Second Edition

HANDBOOK OF Physical-Chemical Properties and Environmental Fate for Organic Chemicals

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Volume I
Introduction and Hydrocarbons

Volume II
Halogenated Hydrocarbons

Volume III
Oxygen Containing Compounds

Volume IV
Nitrogen and Sulfur Containing Compounds
and Pesticides

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Nitrogen and Sulfur Containing Compounds and Pesticides

Donald Mackay
Wan Ying Shiu
Kuo-Ching Ma
Sum Chi Lee

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Preface

This handbook is a compilation of environmentally relevant physical-chemical data for similarly structured groups of chemical substances. These data control the fate of chemicals as they are transported and transformed in the multimedia environment of air, water, soils, sediments, and their resident biota. These fate processes determine the exposure experienced by humans and other organisms and ultimately the risk of adverse effects. The task of assessing chemical fate locally, regionally, and globally is complicated by the large (and increasing) number of chemicals of potential concern; by uncertainties in their physical-chemical properties; and by lack of knowledge of prevailing environmental conditions such as temperature, pH, and deposition rates of solid matter from the atmosphere to water, or from water to bottom sediments. Further, reported values of properties such as solubility are often in conflict. Some are measured accurately, some approximately, and some are estimated by various correlation schemes from molecular structures. In some cases, units or chemical identity are wrongly reported. The user of such data thus has the difficult task of selecting the "best" or "right" values. There is justifiable concern that the resulting deductions of environmental fate may be in substantial error. For example, the potential for evaporation may be greatly underestimated if an erroneously low vapor pressure is selected.

To assist the environmental scientist and engineer in such assessments, this handbook contains compilations of physical-chemical property data for over 1000 chemicals. It has long been recognized that within homologous series, properties vary systematically with molecular size, thus providing guidance about the properties of one substance from those of its homologs. Where practical, plots of these systematic property variations can be used to check the reported data and provide an opportunity for interpolation and even modest extrapolation to estimate unmeasured properties of other substances. Most handbooks treat chemicals only on an individual basis and do not contain this feature of chemical-to-chemical comparison, which can be valuable for identifying errors and estimating properties. This most recent edition includes about 1250 compounds and contains about 30 percent additional physical-chemical property data. There is a more complete coverage of PCBs, PCDDs, PCDFs, and other halogenated hydrocarbons, especially brominated and fluorinated substances that are of more recent environmental concern. Values of the physical-chemical properties are generally reported in the literature at a standard temperature of 20 or 25°C. However, environmental temperatures vary considerably, and thus reliable data are required on the temperature dependence of these properties for fate calculations. A valuable enhancement to this edition is the inclusion of extensive measured temperature-dependent data for the first time. The data focus on water solubility, vapor pressure, and Henry's law constant but include octanol/water and octanol/air partition coefficients where available. They are provided in the form of data tables and correlation equations as well as graphs.

We also demonstrate in Chapter 1 how the data may be taken a stage further and used to estimate likely environmental partitioning tendencies, i.e., how the chemical is likely to become distributed between the various media that comprise our biosphere. The results are presented numerically and pictorially to provide a visual impression of likely environmental behavior. This will be of interest to those assessing environmental fate by confirming the general fate characteristics or behavior profile. It is, of course, only possible here to assess fate in a "typical" or "generic" or "evaluative" environment. No claim is made that a chemical will behave in this manner in all situations, but this assessment should reveal the broad characteristics of behavior. These evaluative fate assessments are generated using simple fugacity models that flow naturally from the compilations of data on physical-chemical properties of relevant chemicals. Illustrations of estimated environmental fate are given in Chapter 1 using Levels I, II, and III mass balance models. These and other models are available for downloading gratis from the website of the Canadian Environmental Modelling Centre at Trent University (www.trent.ca/cemc).

It is hoped that this new edition of the handbook will be of value to environmental scientists and engineers and to students and teachers of environmental science. Its aim is to contribute to better assessments of chemical fate in our multimedia environment by serving as a reference source for environmentally relevant physical-chemical property data of classes of chemicals and by illustrating the likely behavior of these chemicals as they migrate throughout our biosphere.

Acknowledgments

We would never have completed the volumes for the first and second editions of the handbook and the CD-ROMs without the enormous amount of help and support that we received from our colleagues, publishers, editors, friends, and family. We are long overdue in expressing our appreciation.

We would like first to extend deepest thanks to these individuals: Dr. Warren Stiver, Rebecca Lun, Deborah Tam, Dr. Alice Bobra, Dr. Frank Wania, Ying D. Lei, Dr. Hayley Hung, Dr. Antonio Di Guardo, Qiang Kang, Kitty Ma, Edmund Wong, Jenny Ma, and Dr. Tom Harner. During their past and present affiliations with the Department of Chemical Engineering and Applied Chemistry and/or the Institute of Environment Studies at the University of Toronto, they have provided us with many insightful ideas, constructive reviews, relevant property data, computer know-how, and encouragement, which have resulted in substantial improvements to each consecutive volume and edition through the last fifteen years.

Much credit goes to the team of professionals at CRC Press/Taylor & Francis Group who worked on this second edition. Especially important were Dr. Fiona Macdonald, Publisher, Chemistry; Dr. Janice Shackleton, Input Supervisor; Patrica Roberson, Project Coordinator; Elise Oranges and Jay Margolis, Project Editors; and Marcela Peres, Production Assistant.

We are indebted to Brian Lewis, Vivian Collier, Kathy Feinstein, Dr. David Packer, and Randi Cohen for their interest and help in taking our idea of the handbook to fruition.

We also would like to thank Professor Doug Reeve, Chair of the Department of Chemical Engineering and Applied Chemistry at the University of Toronto, as well as the administrative staff for providing the resources and assistance for our efforts.

We are grateful to the University of Toronto and Trent University for providing facilities, to the Natural Sciences and Engineering Research Council of Canada and the consortium of chemical companies that support the Canadian Environmental Modelling Centre for funding of the second edition. It is a pleasure to acknowledge the invaluable contributions of Eva Webster and Ness Mackay.

Biographies

Donald Mackay, born and educated in Scotland, received his degrees in Chemical Engineering from the University of Glasgow. After working in the petrochemical industry he joined the University of Toronto, where he taught for 28 years in the Department of Chemical Engineering and Applied Chemistry and in the Institute for Environmental Studies. In 1995 he moved to Trent University to found the Canadian Environmental Modelling Centre. Professor Mackay's primary research is the study of organic environmental contaminants, their properties, sources, fates, effects, and control, and particularly understanding and modeling their behavior with the aid of the fugacity concept. His work has focused especially on the Great Lakes Basin; on cold northern climates; and on modeling bioaccumulation and chemical fate at local, regional, continental and global scales.

His awards include the SETAC Founders Award, the Honda Prize for Eco-Technology, the Order of Ontario, and the Order of Canada. He has served on the editorial boards of several journals and is a member of SETAC, the American Chemical Society, and the International Association of Great Lakes Research.

Wan-Ying Shiu is a Senior Research Associate in the Department of Chemical Engineering and Applied Chemistry, and the Institute for Environmental Studies, University of Toronto. She received her Ph.D. in Physical Chemistry from the Department of Chemistry, University of Toronto, M.Sc. in Physical Chemistry from St. Francis Xavier University, and B.Sc. in Chemistry from Hong Kong Baptist College. Her research interest is in the area of physical-chemical properties and thermodynamics for organic chemicals of environmental concern.

Kuo-Ching Ma obtained his Ph.D. from Florida State University, M.Sc. from The University of Saskatchewan, and B.Sc. from The National Taiwan University, all in Physical Chemistry. After working many years in the aerospace, battery research, fine chemicals, and metal finishing industries in Canada as a Research Scientist, Technical Supervisor/Director, he is now dedicating his time and interests to environmental research.

Sum Chi Lee received her B.A.Sc. and M.A.Sc. in Chemical Engineering from the University of Toronto. She has conducted environmental research at various government organizations and the University of Toronto. Her research activities have included establishing the physical-chemical properties of organochlorines and understanding the sources, trends, and behavior of persistent organic pollutants in the atmosphere of the Canadian Arctic.

Ms. Lee also possesses experience in technology commercialization. She was involved in the successful commercialization of a proprietary technology that transformed recycled material into environmentally sound products for the building material industry. She went on to pursue her MBA degree, which she earned from York University's Schulich School of Business. She continues her career, combining her engineering and business experiences with her interest in the environmental field.

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16 Nitrogen and Sulfur Compounds

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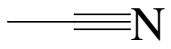
16.1 LIST OF CHEMICALS AND DATA COMPILATIONS

16.1.1 NITRILES (ORGANIC CYANIDES)

16.1.1.1 Acetonitrile



Common Name: Acetonitrile
Synonym: cyanomethane, ethanenitrile, methyl cyanide
Chemical Name: acetonitrile
CAS Registry No: 75-05-8
Molecular Formula: C_2H_3N, CH_3CN
Molecular Weight: 41.052
Melting Point (°C):
  –43.82 (Lide 2003)
Boiling Point (°C):
  81.65 (Lide 2003)
Density (g/cm^3 at 20°C):
  0.7857 (Dreisbach 1961; Weast 1982–83; Dean 1985)
  0.7803 (25°C, Dreisbach 1961)
Molar Volume (cm^3/mol):
  52.7 (calculated-density, Rohrschneider 1973)
  57.4 (exptl. at normal bp, Lee et al. 1972)
  56.3 (calculated-Le Bas method at normal boiling point)
Dissociation Constant, pK:
  29.1 (pK_a, Riddick et al. 1986; Howard 1993)
  32.2 (pK_s, Riddick et al. 1986)
  –10.12 (pK_{BH+}, Riddick et al. 1986)
Enthalpy of Vaporization, ΔH_V (kJ/mol):
  35.01, 31.51 (25°C, bp, Dreisbach 1961)
  32.94, 29.82 (25°C, bp, Riddick et al. 1986)
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
  8.167 (Riddick et al. 1986)
Entropy of Fusion, ΔS_{fus} (J/mol K):
Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F: 1.0

Water Solubility (g/m^3 or mg/L at 25°C):
  $> 3.1 \times 10^6$ (Booth & Everson 1948)
  miscible (Dean 1985; Riddick et al. 1986; Yaws et al. 1990; Howard 1993)

Vapor Pressure (Pa at 25°C or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):
  11870* (interpolated-regression of tabulated data, temp range –47–81.8°C, Stull 1947)
  $\log (P/\text{mmHg}) = 7.12257 - 1315.2/(230 + t/°C)$, (Antoine eq., Dreisbach & Martin 1949)
  11240 (calculated by formula, Dreisbach 1961)
  $\log (P/\text{mmHg}) = 7.07354 - 1279.2/(224.0 + t/°C)$, temp range 5–119°C, (Antoine eq. for liquid state, Dreisbach 1961)
  12156* (25.56°C, measured range 7.3–27.38°C, Putnam et al. 1965)
  $\log (P/\text{mmHg}) = 7.89511 - 1773.06/(T/K)$; temp range 280–300.5 K (Antoine eq., Putnam et al. 1965)
  11510 (Hoy 1970)
  24459* (41.82°C, ebulliometry, measured range 41–82°C, Meyer et al. 1971)
  $\log (P/\text{mmHg}) = 6.23655 - 1397.9228/(239.275 + t/°C)$; temp range 41–82°C (ebulliometry, Meyer et al. 1971)
  $\log (P/\text{mmHg}) = [-0.2185 \times 8173.2/(T/K)] + 7.938662$; temp range: –47.0 to 81.8°C, (Antoine eq., Weast 1972–73)
  11919* (25.3°C, measured range 15.1–89.2°C, Dojcanske & Heinrich 1974)

8306* (saturated-vapor volume, extrapolated from fitted Antoine eq., Mousa 1981)
$\log (P/\text{kPa}) = 6.4914 - 1420.8649/(T/\text{K} - 42.15)$; temp range 438.9–530.1 K (ebulliometry, Mousa 1981)
9864, 15330 (20°C, 30°C, Verschueren 1983)
11790, 11830 (interpolated values-Antoine equations, Boublik et al. 1984)
$\log (P/\text{kPa}) = 6.39532 - 1420.682/(241.852 + t/°\text{C})$, temp range: 15.1–89.2°C (Antoine eq. from reported exptl. data, Boublik et al. 1984)
$\log (P/\text{kPa}) = 7.54606 - 2093.145/(298.369 + t/°\text{C})$, temp range: 7.26–27.4°C (Antoine eq. from reported exptl. data, Boublik et al. 1984)
12310 (calculated-Antoine eq., Dean 1985, 1992)
$\log (P/\text{mmHg}) = 7.11988 - 1314.4/(230 + t/°\text{C})$, temp range: liquid (Antoine eq., Dean 1985, 1992)
11840 (Riddick et al. 1986; Howard et al. 1986; quoted, Banerjee et al. 1990; Howard 1993)
$\log (P/\text{kPa}) = 6.24747 - 1315.2/(230.0 + t/°\text{C})$, temp range not specified (Antoine eq., Riddick et al. 1986)
11800 (extrapolated-Antoine eq., Stephenson & Malanowski 1987)
$\log (P_L/\text{kPa}) = 6.34522 - 1388.446/(-34.856 + T/\text{K})$, temp range: 314–355 K, (Antoine eq., Stephenson & Malanowski 1987)
11840 (selected, Riddick et al. 1986)
$\log (P/\text{kPa}) = 6.24724 - 1315.2/(230 + t/°\text{C})$, temp range not specified (Antoine eq., Riddick et al. 1986)
$\log (P/\text{mmHg}) = 23.1953 - 2.3389 \times 10^3/(T/\text{K}) - 5.4954 \cdot \log (T/\text{K}) + 7.9894 \times 10^{-10} \cdot (T/\text{K}) + 2.3293 \times 10^{-6} \cdot (T/\text{K})^2$; temp range 229–546 K (vapor pressure eq., Yaws 1994)
10604* (22.634°C, comparative ebulliometry, measured range 278–373 K, Ewing & Sanchez Ochoa 2004)
$\ln (P/\text{kPa}) = 14.7340 - 3268.53/(T/\text{K} - 31.615)$, for temp range 290–362 K (comparative ebulliometry, Ewing & Sanchez Ochoa 2004)

Henry's Law Constant (Pa·m^3/mol at 25°C or as indicated and reported temperature dependence equations. Additional data at other temperatures designated* are compiled at the end of this section):
3.50, 2.78 (exptl., calculated-bond contribution, Hine & Mookerjee 1975)
2.07* (headspace-GC, measured range 0–25°C, Snider & Dawson 1985)
2.033 (computed-vapor-liquid equilibrium VLE data, Yaws et al. 1991)
1.474* (20°C, headspace-GC, measured range 6.0–30°C, Benkelberg et al. 1995)
1.474, 1.477, 1.685 (20°C, headspace-GC, deionized water, rain water, artificial seawater, Benkelberg et al. 1995)
$\ln (k_H/\text{atm}) = (13.8 \pm 0.3) - (4106 \pm 101)/T/\text{K})$, temp range: 6–30°C (headspace-GC measurement, Benkelberg et al. 1995)
1.55 (20°C, selected from literature experimentally measured data, Staudinger & Roberts 2001)
$\log K_{AW} = 2.353 - 1627/(T/\text{K})$ (van't Hoff eq. derived from literature data, Staudinger & Roberts 2001)
2.05 (Ostwald concentration coefficient-concn ratio-GC/FID, Bebahani et al. 2002)

Octanol/Water Partition Coefficient, log K_{OW}:
–0.34 (shake flask-GC, Hansch & Anderson 1967; Leo et al. 1969, 1971; Hansch & Leo 1985)
–0.54 (shake flask-GC, Tanii & Hashimoto 1984)
–0.34 (recommended, Sangster 1989, 1993)
–0.34 (recommended, Hansch et al. 1995)

Octanol/Air Partition Coefficient, log K_{OA}:
2.31 (head-space GC, Abraham et al. 2001)

Bioconcentration Factor, log BCF:
–0.523 (estimated-K_{OW} as per regression eq of Bysshe 1982, Howard 1993)

Sorption Partition Coefficient, log K_{OC}:
–0.523 (soil, estimated-K_{OW}, Lyman et al. 1982; quoted, Howard 1993)
–0.714 (calculated-K_{OW}, Kollig 1993)

Environmental Fate Rate Constants, k, or Half-Lives, $t_{½}$:
Volatilization: $t_{½}$ ~ 21 h from a model river of 1-m deep flowing at 1 m/s with a wind velocity of 3 m/s based on Henry's law constant (Lyman et al. 1982; quoted, Howard 1993)

Photolysis:

Oxidation: rate constant k, for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO3} with NO_3 radical and k_{O3} with O_3 or as indicated, *data at other temperatures and/or the Arrhenius expression see reference:

photooxidation $t_{½}$ = 314 – 12559 yr in water, based on measured rate data for reaction with hydroxyl radical in aqueous solution (Dorfman & Adams 1973; Howard et al. 1991)

k_{OH}* = (4.94 ± 0.6) × 10^{-14} cm^3 $molecule^{-1}$ s^{-1} at 297.2 K, measured range 297–424 K (flash photolysis-resonance fluorescence, Harris et al. 1981; quoted, Howard 1993)

k_{OH}* = (1.94 ± 0.37) × 10^{-14} cm^3 $molecule^{-1}$ s^{-1} at 298 K, measured range 250–363 K (flash photolysis-resonance fluorescence, Kurylo & Knable 1984)

k_{OH}* = (2.1 ± 0.3) × 10^{-14} cm^3 $molecule^{-1}$ s^{-1} at 295 K, measured range 295–393 K (discharge flow-EPR, Poulet et al. 1984)

k_{OH}(exptl) = 2.1 × 10^{-14} cm^3 $molecule^{-1}$ s^{-1}, k_{OH}(calc) = 2.0 × 10^{-14} cm^3 $molecule^{-1}$ s^{-1} at 298 K (Atkinson 1985)

k_{OH} = 3 × 10^{-14} cm^3 $molecule^{-1}$ s^{-1} (Atkinson 1985; quoted, Howard et al. 1991; Howard 1993)

k_{OH} = 1.90 × 10^{-14} cm^3 $molecule^{-1}$ s^{-1} and k(soln) = 3.70 × 10^{-14} cm^3 $molecule^{-1}$ s^{-1} for the solution-phase reaction with hydroxyl radical in aqueous solution (Wallington et al. 1988)

k_{OH}* = 2.14 × 10^{-14} cm^3 $molecule^{-1}$ s^{-1} at 298 K (recommended, Atkinson 1989)

Hydrolysis:

k = 5.8 × 10^{-3} M^{-1} h^{-1} at pH 7 and 25°C with $t_{½}$ > 150000 yr (Ellington et al. 1987)

k_{O3}(aq.) ≤ 6 × 10^{-5} M^{-1} s^{-1} for direct reaction with ozone in water at pH 2 and 22°C, with $t_{½}$ ≥ 18 yr at pH 7 (Yao & Haag 1991).

Biodegradation: $t_{½}$(aq. aerobic) = 168 – 672 h, based on aerobic river die-away test data (Ludzack et al. 1958; quoted, Howard et al. 1991); $t_{½}$(aq. anaerobic) = 672 – 2688 h, based on estimated aqueous aerobic biodegradation half-life (Howard et al. 1991).

Biotransformation:

Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants:

Half-Lives in the Environment:

Air: photooxidation $t_{½}$ = 1299 – 12991 h, based on measured rate constant k = 3 × 10^{-14} cm^3 $molecule^{-1}$ s^{-1} for the vapor phase reaction with hydroxyl radical in air (Atkinson 1985; quoted, Howard et al. 1991; Howard 1993);

atmospheric transformation lifetime was estimated to be > 5 d (Kelly et al. 1994).

Surface water: $t_{½}$ = 168 – 672 h, based on aerobic river die-away test data (Howard et al. 1991);

photooxidation $t_{½}$ = 314 – 12559 yr, based on measured rate data for reaction with hydroxyl radical in aqueous solution (Dorfman & Adams 1973; Howard et al. 1991);

$t_{½}$ ≥ 18 yr for direct reaction with ozone in water at pH 7 and 22°C (Yao & Haag 1991).

Groundwater: $t_{½}$ = 336 – 8640 h, based on estimated aqueous aerobic biodegradation half-life (Howard et al. 1991).

Sediment:

Soil: $t_{½}$ = 168 – 672 h, based on estimated aqueous aerobic biodegradation half-life (Howard et al. 1991).

Biota:

TABLE 16.1.1.1.1
Reported vapor pressures of acetonitrile at various temperatures and the coefficients for the vapor pressure equations

$\log P = A - B/(T/K)$	(1)	$\ln P = A - B/(T/K)$	(1a)
$\log P = A - B/(C + t/°C)$	(2)	$\ln P = A - B/(C + t/°C)$	(2a)
$\log P = A - B/(C + T/K)$	(3)		
$\log P = A - B/(T/K) - C \cdot \log(T/K)$	(4)		

(Continued)

TABLE 16.1.1.1.1 (*Continued*)

1.

Stull 1947		Putnam et al. 1965		Meyer et al. 1971		Dojcanske & Heinrich 1974	
summary of literature data		manometer		ebulliometry		in Boublik et al. 1984	
t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa
–47.0	133.3	7.259	4997	41.82	24459	15.1	7359
–26.6	666.6	10.47	5861	46.09	29026	20.1	9413
–16.3	1333	13.791	6914	46.11	29032	25.3	11919
–5.0	2666	18.701	8809	50.36	34288	30.7	15252
7.7	5333	21.905	10244	55.37	41393	35	18292
15.9	7999	23.401	11031	60.64	50155	39.95	22465
27	13332	25.563	12156	65.91	60390	40	22625
43.7	26664	27.38	13187	70.74	71145	44.9	27638
62.5	53329			76.31	85512	50.1	33797
81.8	101325	eq. 1	P/mmHg	81.87	101990	54.9	40517
		A	7.89511	81.89	102010	60	49022
mp/°C	–41.0	B	1773.06			64.4	57182
				bp/°C	81.66	64.95	58102
				eq. 2	P/mmHg	70	68967
				A	6.23655	73.05	76713
				B	1397.923	75.1	81380
				C	239.275	77.2	87952
						81.1	99431
						85.2	112364
						88.2	123189
						89.2	124776

2.

Mousa 1981		Ewing & Sanchez Ochoa 2004			
ebulliometry-pressure gauge		comparative ebulliometry			
T/K	P/kPa	t/°C	P/Pa	t/°C	P/kPa
		set A		set B	
438.9	784.4	4.772	4323#	81.4	100.745
440.9	842.8	5.475	4490#	87.792	122.631
442.6	862.3	8.417	5247#	98.589	168.122
444.5	876.9	12.226	6385#	105.665	204.592
447.9	960.3	14.517	7165#	110.961	235.792
450.5	999.2	17.497	8296	121.144	306.279
455.7	1116.5	19.596	9182	132.086	399.5
460.2	1234.6	22.634	10604	142.063	502.665
505.3	2604.9	27.674	13366	150.533	605.601
508.1	1704.6	30.661	15271	157.974	708.993
512.1	1924.0	36.486	19639	164.152	804.861
519.7	3243.3	42.283	24972	170.346	910.819
521.6	3303.1	47.968	31311	176.446	1025.47
524.8	3482.8	51.872	36387	182.586	1151.97
530.1	3722.1	58.125	45907	188.724	1290.2
		63.263	55169	195.22	1450.28
bp/K	354.8	68.029	65092	200.902	1602.63
		72.425	75440	206.004	1749.88

TABLE 16.1.1.1.1 (*Continued*)

Mousa 1981		Ewing & Sanchez Ochoa 2004			
ebulliometry-pressure gauge		comparative ebulliometry			
T/K	P/kPa	t/°C	P/Pa	t/°C	P/kPa
eq.3	P/kPa	76.178	85311	211.619	2110.77
A	6.4914	79.929	95589	217.22	2303.51
B	1420.8649	81.515	101120	222.602	2523.66
C	–42.15	84.406	110614	228.33	2747.95
		88.462	125129	233.771	2999.22
		95.816	155329	339.66	3254.08
		100.02	175036	244.858	3512.89
				254.64	3760.37
		for temp range 290–373 K		258.929	4001.46
		eq. 2a	P/mmHg	261.882	4174.61
		A	14.734		
		B	3268.53	data fitted to Wagner eq.	
		C	–31.615	for temp range 354.5–535 K	
		# data not used in regression			

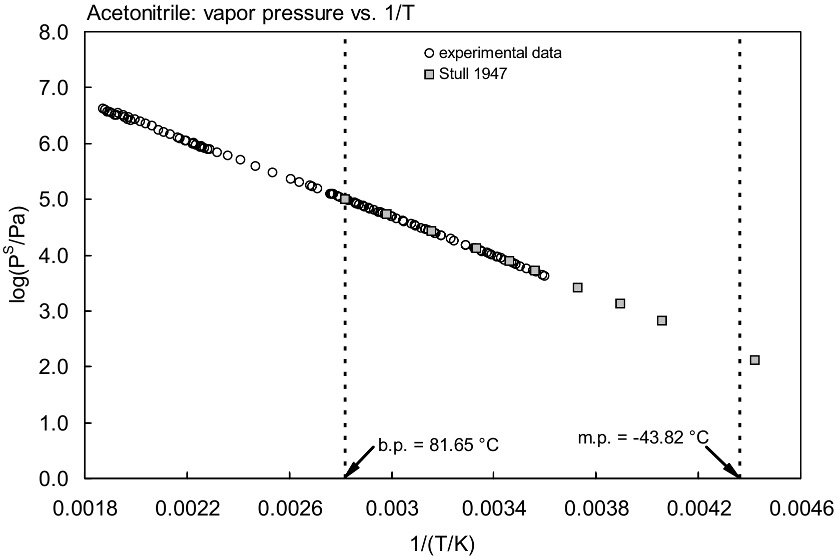


FIGURE 16.1.1.1.1 Logarithm of vapor pressure versus reciprocal temperature for acetonitrile.

TABLE 16.1.1.1.2
Reported Henry's law constants of acetonitrile at various temperatures and temperature dependence equations

$\ln K_{AW} = A - B/(T/K)$ (1) $\log K_{AW} = A - B/(T/K)$ (1a)
$\ln (1/K_{AW}) = A - B/(T/K)$ (2) $\log (1/K_{AW}) = A - B/(T/K)$ (2a)
$\ln (k_H/\text{atm}) = A - B/(T/K)$ (3)
$\ln [H/(\text{Pa m}^3/\text{mol})] = A - B/(T/K)$ (4) $\ln [H/(\text{atm}\cdot\text{m}^3/\text{mol})] = A - B/(T/K)$ (4a)
$K_{AW} = A - B\cdot(T/K) + C\cdot(T/K)^2$ (5)

Snider & Dawson 1985		Benkelberg et al. 1995	
gas stripping-GC		equil. vapor phase concn-GC	
t/°C	H/(Pa m³/mol)	t/°C	H/(Pa m³/mol)
			deionized water
0	0.614	6	0.72
25	2.066	10	1.0706
		20	1.474
enthalpy of transfer:		30	2.356
$\Delta H/(\text{kJ mol}^{-1}) = 30.54$			rain water
		20	1.477
			artificial
		20	1.685
		eq. 3	H/atm
		A	13.8 ± 0.3
		B	4106 ± 101

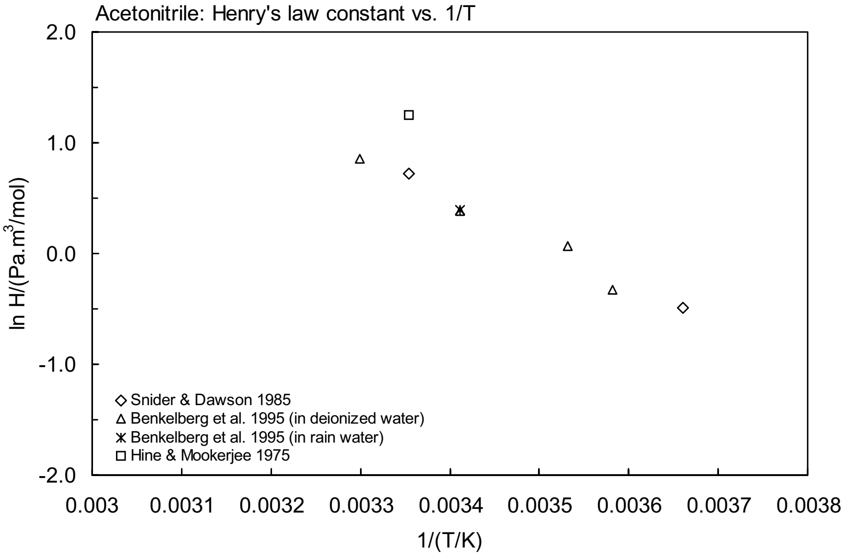
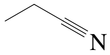


FIGURE 16.1.1.1.2 Logarithm of Henry's law constant versus reciprocal temperature for acetonitrile.

16.1.1.2 Propionitrile



Common Name: Propionitrile
Synonym: propanenitrile, ethyl cyanide, cyanoethane, propyl nitrile
Chemical Name: propionitrile
CAS Registry No: 107-12-0
Molecular Formula: C_3H_5N, CH_3CH_2CN
Molecular Weight: 55.079
Melting Point (°C):
  –92.78 (Lide 2003)
Boiling Point (°C):
  97.14 (Lide 2003)
Density (g/cm^3 at 20°C):
  0.7818 (Weast 1982–83; Dean 1985)
  0.78182, 0.77682 (20°C, 25°C, Riddick et al. 1986)
Molar Volume (cm^3/mol):
  70.4 (calculated-density, Taft et al. 1985; Leahy 1986; Kamlet et al. 1986, 1987)
  78.5 (calculated-Le Bas method at normal boiling point)
Dissociation Constant:
  33.54 (pK_s, Riddick et al. 1986)
Enthalpy of Vaporization, ΔH_{vap}, (kJ/mol):
  37.41, 32.77 (25°C, bp, Dreisbach 1961)
  36.03, 30.96 (25°C, bp, Riddick et al. 1986)
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
  5.045 (Riddick et al. 1986)
Entropy of Fusion, ΔS_{fus} (J/mol K):
Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F: 1.0

Water Solubility (g/m^3 or mg/L at 25°C or as indicated. Additional data at other temperatures designated * are compiled at the end of this section):
  104950 (Seidell 1941)
  105200 (Hansch et al. 1968)
  103000 (Dean 1985; Riddick et al. 1986; Howard 1990)
  55000, 65000 (20°C, 30°C, shake flask-GC, measured range 0–90°C, Stephenson 1994)

Vapor Pressure (Pa at 25°C or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):
  6005* (interpolated-regression of tabulated data, temp range –35–97.1°C, Stull 1947)
  10114* (35.5°C, ebulliometry, measured range 35.5–97.35°C, Dreisbach & Shrader 1949)
  log (P/mmHg) = 7.15217 – 1398.2/(230 + t/°C); temp range 35.5–97.35°C, (Antoine eq., Dreisbach & Martin 1949)
  5333* (22.05°C, measured range –84.66–22.05°C, Milazzo 1956)
  5950 (calculated by formula, Dreisbach 1961)
  log (P/mmHg) = 7.05846 – 1327.9/(221.0 + t/°C), temp range: 17–137°C, (Antoine eq. for liquid state, Dreisbach 1961)
  log (P/mmHg) = [–0.2185 × 8769.0/(T/K)] + 8.079473; temp range: –35 to 97.1°C, (Antoine eq., Weast 1972–73)
  6140 (22.05°C, quoted exptl., Boublik et al. 1973, 1984)
  6163, 6143 (extrapolated values-Antoine eq., Boublik et al. 1984)
  log (P/kPa) = 5.89149 – 1181.562/(206.603 + t/°C), temp range: 35.5–97.39°C (Antoine eq. from reported exptl. data, Boublik et al. 1984)
  log (P/kPa) = 4.43918 – 677.415/(160.551 + t/°C), temp range: –84.7 to 22.05°C (Antoine eq. from reported exptl. data, Boublik et al. 1984)

6140 (extrapolated-Antoine eq., Dean 1985, 1992)
log (P/mmHg) = 5.2782 – 665.52/(159.0 + t/°C), temp range: –84 to 22°C (Antoine eq., Dean 1985, 1992)
5950 (selected, Riddick et al. 1986)
log (P/kPa) = 6.27702 – 1398.2/(230 + t/°C), temp range not specified (Antoine eq., Riddick et al. 1986)
log (P/kPa) = 7.15190 – 1894.10/(T/K); temp range: 9–25°C, (Antoine eq., Riddick et al. 1986)
6306 (calculated-Antoine eq., Stephenson & Malanowski 1987)
log (P_L/kPa) = 7.395 – 3213/(T/K), temp range: 357–413 K, (Antoine eq.-I, Stephenson & Malanowski 1987)
log (P_L/kPa) = 10.31055 – 3994.667/(T/K), temp range: 373–413 K, (Antoine eq.-II, Stephenson & Malanowski 1987)
log (P/mmHg) = 33.7908 – 2.9113 × 10^3/(T/K) – 9.1506·log (T/K) + 1.1173 × 10^{-11}·(T/K) + 3.2756 × 10^{-6}·$(T/K)^2$; temp range 180–564 K (vapor pressure eq., Yaws 1994)

Henry's Law Constant (Pa·m^3/mol at 25°C):
3.800 (partial pressure, Butler & Ramchandani 1935)
3.748 (partial vapor pressure-GC, Buttery et al. 1969)
3.752, 3.752, 4.114 (exptl., calculated-group contribution, calculated-bond contribution, Hine & Mookerjee 1975)
5.947 (Howard 1990)

Octanol/Water Partition Coefficient, log K_{OW}:
0.041 (shake flask, Collander 1951)
0.16 (shake flask-GC, Hansch & Anderson 1967; Hansch et al. 1968)
– 0.10 (shake flask-GC, Tanii & Hashimoto 1984)
0.16 (recommended, Sangster 1989, 1993)
0.16 (recommended, Hansch et al. 1995)

Octanol/Air Partition Coefficient, log K_{OA}:
2.69 (head-space GC, Abraham et al. 2001)

Bioconcentration Factor, log BCF:
– 0.108 (estimated-K_{OW}, Lyman et al. 1982; quoted, Howard 1990)

Sorption Partition Coefficient, log K_{OC}:
0.079 (soil, estimated-K_{OW}, Lyman et al. 1982; quoted, Howard 1990)

Environmental Fate Rate Constants, k, or Half-Lives, $t_{1/2}$:
Volatilization: using Henry's law constant, $t_{1/2}$ = 13.3 h was estimated for a model river 1 m deep flowing 1 m/s with wind speed 3 m/s (Lyman et al. 1982; quoted, Howard 1990).
Photolysis:
Oxidation: rate constant k, for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO3} with NO_3 radical and k_{O3} with O_3 or as indicated, *data at other temperatures and/or the Arrhenius expression see reference:
k_{OH}* = (1.94 ± 0.20) × 10^{-13} cm^3 $molecule^{-1}$ s^{-1} at 298.2 K, measured range 298–423 K (flash photolysis-resonance fluorescence, Harris et al. 1981)
k_{OH} = 1.9 × 10^{-13} cm^3 $molecule^{-1}$ s^{-1} at 298 K (Atkinson 1985)
k_{OH} = 1.94 × 10^{-13} cm^3 $molecule^{-1}$ s^{-1} at 298.2 K, k(soln) = 1.60 × 10^{-13} cm^3 $molecule^{-1}$ s^{-1} for the solution-phase reaction with hydroxyl radical in aqueous solution (Wallington et al. 1988)
photooxidation $t_{1/2}$ = 83 d in air, based on experimental rate constant assuming $t_{1/2}$ = 12 h of sunlight for the vapor-phase reaction with hydroxyl radical in air and $t_{1/2}$ > 100 d for the reaction with ozone in the atmosphere (Howard 1990)
k_{OH} = 0.194 × 10^{-12} cm^3 $molecule^{-1}$ s^{-1} at 298.2 K (review, Atkinson 1989)
Hydrolysis:
Biodegradation:
Biotransformation:
Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants:

Half-Lives in the Environment:

Air: $t_{½}$ = 83 d, based on experimental rate constant assuming 12 h of sunlight for the vapor-phase reaction with hydroxyl radical in air and $t_{½} > 100$ d for the reaction with ozone in the atmosphere (Harris et al. 1981; quoted, Howard 1990).

TABLE 16.1.1.2.1
Reported aqueous solubilities and vapor pressures of propionitrile at various temperatures

$\log P = A - B/(T/K)$	(1)	$\ln P = A - B/(T/K)$	(1a)
$\log P = A - B/(C + t/°C)$	(2)	$\ln P = A - B/(C + t/°C)$	(2a)
$\log P = A - B/(C + T/K)$	(3)		
$\log P = A - B/(T/K) - C\cdot\log(T/K)$	(4)		

Aqueous solubility		Vapor pressure					
Stephenson 1994		Stull 1947		Dreisbach & Shrader 1949		Milazzo 1956	
shake flask-GC		summary of literature data		ebulliometry			
t/°C	S/g·m⁻³	t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa
0	62000	–35.0	133.3	35.5	10114	–84.66	1
20	55000	–13.8	666.6	43.76	16500	–77.01	2
30	65000	–3.0	1333	70.45	42066	–67.42	6
40	79000	8.8	2666	84.44	67661	–65.49	7
50	94000	22	5333	97.35	101325	–59.72	13
60	98000	30.1	7999			–52.96	17
70	134000	41.4	13332			–46.19	49
80	156000	58.2	26664			–34.95	133
90	195000	77.7	53329			–22.85	356
		97.1	101325			–13.08	707
						–2.95	1347
		mp/°C	–91.9			6.36	2400
						16.42	4146
						22.05	5333

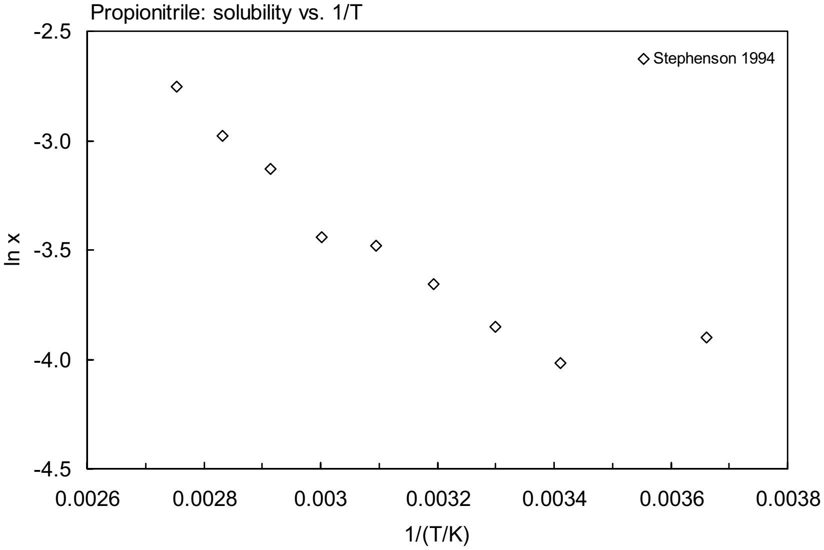


FIGURE 16.1.1.2.1 Logarithm of mole fraction solubility (ln *x*) versus reciprocal temperature for propionitrile.

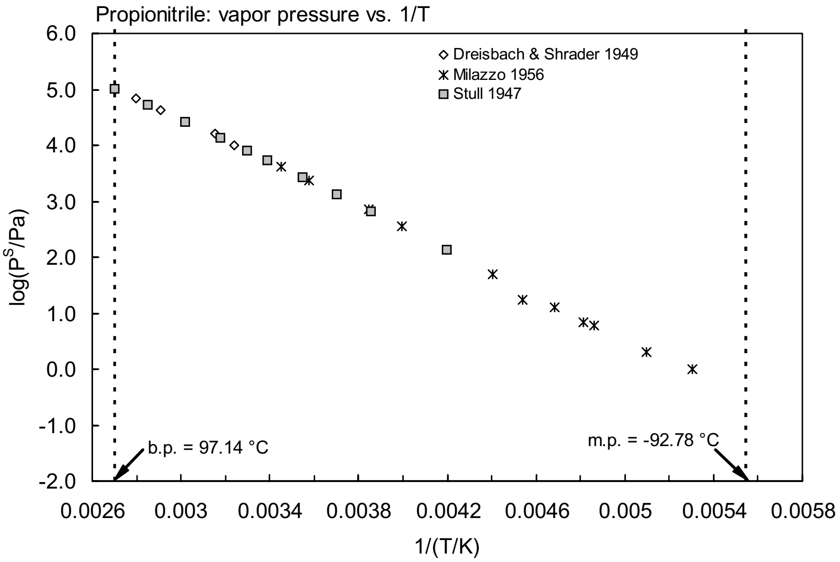
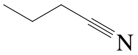


FIGURE 16.1.1.2.2 Logarithm of vapor pressure versus reciprocal temperature for propionitrile.

16.1.1.3 Butyronitrile



Common Name: *n*-Butyronitrile
Synonym: butanenitrile
Chemical Name: butyronitrile
CAS Registry No: 109-74-0
Molecular Formula: C_4H_7N, $CH_3CH_2CH_2CN$
Molecular Weight: 69.106
Melting Point (°C):
  –111.9 (Lide 2003)
Boiling Point (°C):
  117.6 (Lide 2003)
Density (g/cm^3):
  0.7911, 0.7865 (20°C, 25°C, Riddick et al. 1986)
Dissociation Constant, pK_a:
Molar Volume (cm^3/mol):
  88.4 (30°C, Stephenson & Malanowski 1987)
  100.7 (calculated-Le Bas method at normal boiling point)
Enthalpy of Vaporization, ΔH_V (kJ/mol):
  39.33, 34.43 (25°C, bp, Riddick et al. 1986)
Enthalpy of Sublimation, ΔH_{subl} (kJ/mol):
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
  5.021 (Riddick et al. 1986)
Entropy of Fusion, ΔS_{fus} (J/mol K):
Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F: 1.0

Water Solubility (g/m^3 or mg/L at 25°C or as indicated. Other data at other temperatures designated * are compiled at the end of this section):
  33000 (selected, Riddick et al. 1986)
  33500* (20°C, shake flask-GC/TC, measured range 0–90°C, Stephenson 1994)

Vapor Pressure (Pa at 25°C or as indicated and the reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):
  1333* (25.7°C, summary of literature data, temp range –20 to 117.5°C, Stull 1947)
  3592* (30.64°C, ebulliometry, measured range 30.64–120.223°C, Meyer et al. 1971)
  $\log (P/mmHg) = 6.771124 - 1444.5851/(t/°C + 223.275)$; temp range 30.64–120.223°C (Antoine eq., ebulliometric measurements, Meyer et al. 1971)
  13831* (59.807°C, ebulliometry, measured range 59.807–127.707°C, Meyer & Hotz 1976)
  2546 (selected, Riddick et al. 1986)
  $\log (P/kPa) = 6.25390 - 1452.076/(t/°C + 224.1855)$; temp range not specified (Riddick et al. 1986)
  $\log (P_L/kPa) = 6.25397 - 1452.076/(-46.9645 + T/K)$; temp range 332–401 K (Antoine eq., Stephenson & Malanowski 1987)
  $\log (P/mmHg) = 4.8780 - 2.5505 \times 10^3/(T/K) + 3.6306\cdot\log (T/K) - 1.663 \times 10^{-2}\cdot(T/K) + 1.0604 \times 10^{-5}\cdot(T/K)^2$; temp range 161–582 K (vapor pressure eq., Yaws 1994)

Henry's Law Constant (Pa m^3/mol at 25°C):

Octanol/Water Partition Coefficient, log K_{OW}:
  0.53 (shake flask-GC, Tanii & Hashimoto 1984)
  0.53 (recommended, Sangster 1993; Hansch et al. 1995)

Bioconcentration Factor, log BCF or log K_B:

Sorption Partition Coefficient, log K_{OC}:

TABLE 16.1.1.3.1
Reported aqueous solubilities and vapor pressures of butyronitrile at various temperatures

$\log P = A - B/(T/K)$ (1) $\quad \ln P = A - B/(T/K)$ (1a)
$\log P = A - B/(C + t/°C)$ (2) $\quad \ln P = A - B/(C + t/°C)$ (2a)
$\log P = A - B/(C + T/K)$ (3)
$\log P = A - B/(T/K) - C\cdot\log(T/K)$ (4)

Aqueous solubility		Vapor pressure					
Stephenson 1994		Stull 1947		Meyer et al. 1971		Meyer & Hotz 1976	
shake flask-GC		summary of literature data		ebulliometry		ebulliometry	
t/°C	S/g·m^{-3}	t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa
0	37500	–20.0	133.3	30.64	3592	59.807	13831
20	33500	2.10	666.6	39.03	5459	65.615	17513
30	33100	13.4	1333	49.913	9041	71.638	22151
40	32500	25.7	2666	59.226	13527	77.023	27111
50	32300	38.4	5333	67.536	18888	83.599	34366
60	32100	47.3	7999	77.313	27448	89.462	42109
70	31900	59.0	13332	86.71	39316	96.022	52382
80	34000	76.7	26664	93.675	48525	102.279	63984
90	36100	96.8	53329	100.638	60811	109.175	79081
		117.5	101325	100.701	60928	115.651	95737
				107.041	74214	121.838	114148
		mp/°C		112.04	88451	127.707	134135
				117.254	100344		
				120.223	109170		
				bp/°C	117.583		
				$\log P = A - B/(C + t/°C)$			
					P/mmHg		
				A	6.771124		
				B	1444.5851		
				C	223.275		

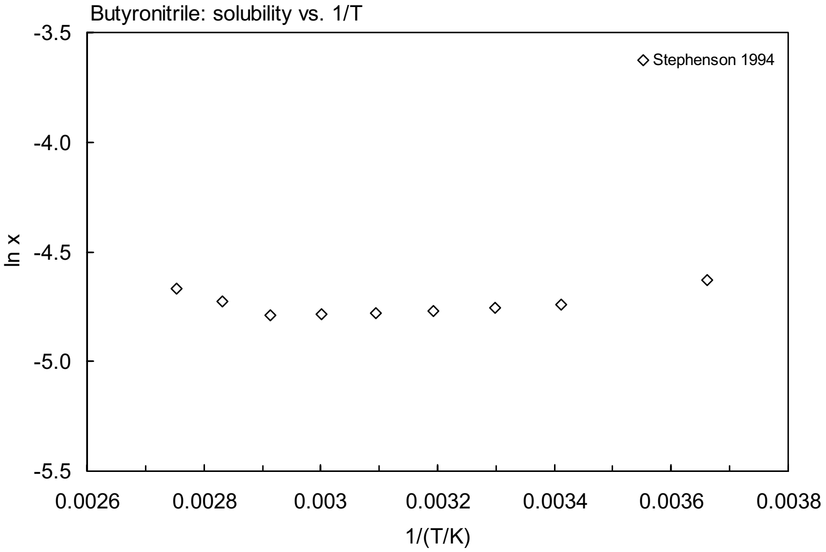


FIGURE 16.1.1.3.1 Logarithm of mole fraction solubility (ln *x*) versus reciprocal temperature for butyronitrile.

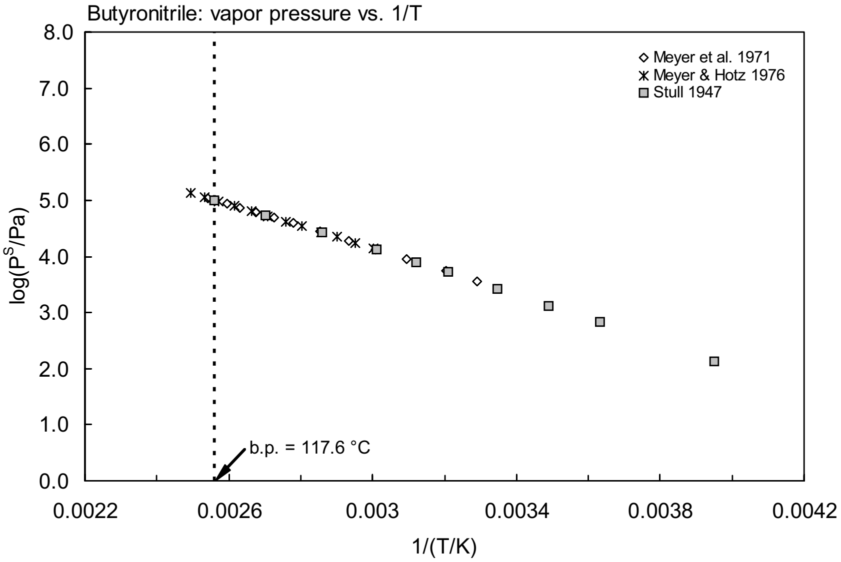
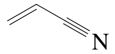


FIGURE 16.1.1.3.2 Logarithm of vapor pressure versus reciprocal temperature for butyronitrile.

16.1.1.4 Acrylonitrile (2-Propenenitrile)



Common Name: Acrylonitrile
Synonym: cyanoethylene, propenenitrile, 2-propenenitrile, vinyl cyanide
Chemical Name: acrylonitrile, cyanoethylene
CAS Registry No: 107-13-1
Molecular Formula: C_3H_3N, CH_2=CHCN
Molecular Weight: 53.063
Melting Point (°C):
 –83.48 (Lide 2003)
Boiling Point (°C):
 77.30 (Riddick et al. 1986; Howard 1989; Lide 2003)
Density (g/cm^3 at 20°C):
 0.8060, 0.8004 (20°C, 25°C, Riddick et al. 1986)
Molar Volume (cm^3/mol):
 65.8 (20°C, calculated-density)
 71.1 (calculated-Le Bas method at normal boiling point)
Dissociation Constant, pK$_a$:
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
 6.230 (Riddick et al. 1986)
Entropy of Fusion, ΔS_{fus} (J/mol K):
Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F: 1.0

Water Solubility (g/m^3 or mg/L at 25°C or as indicated. Additional data at other temperatures designated * are compiled at the end of this section):
 79000 (Klein et al. 1957)
 75000 (Günther et al. 1968)
 73500 (20°C, Windholz 1976)
 73240 (shake flask-LSC, Veith et al. 1980)
 7.35 wt%* (20°C, Kirk-Othmer Encyclopedia 3rd ed., measured range 0–60°C, quoted, Basu et al. 1983)
 73500 (20°C, Riddick et al. 1986)
 69000*, 66400 (20°C, 30°C, shake flask-GC, measured range 0–70°C, Stephenson 1994)

Vapor Pressure (Pa at 25°C or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):
 14340* (interpolated-regression of tabulated data, temp range –51 to 78.5°C, Stull 1947)
 11732* (20°C, temp range 20–77°C, Gudkov et al. 1964; quoted, Boublik et al. 1984)
 14100 (Hoy 1970)
 log (P/mmHg) = [–0.2185 × 7941.4/(T/K)] + 7.851016; temp range: –51 to 78.5°C, (Antoine eq., Weast 1972–73)
 14720 (extrapolated-Antoine eq., Boublik et al. 1984)
 log (P/kPa) = 4.77668 – 649.583/(155.006 + t/°C), temp range 20–70°C (Antoine eq. from reported exptl. data, Boublik et al. 1984)
 14370 (Daubert & Danner 1985)
 15240 (calculated-Antoine eq., Dean 1985, 1992)
 log (P/mmHg) = 7.03855 – 1232.53/(222.47 + t/°C), temp range –20 to 140°C (Antoine eq., Dean 1985, 1992)
 11000 (20°C, Riddick et al. 1986)
 log (P/kPa) = 6.643 – 11644.7/(T/K), temp range not specified (Antoine eq., Riddick et al. 1986)
 14560 (interpolated-Antoine eq.-II, Stephenson & Malanowski 1987)
 log (P_L/kPa) = 6.12021 – 1288.9/(–38.74 + T/K); temp range 257–352 K (Antoine eq.-I, Stephenson & Malanowski 1987)
 log (P_L/kPa) = 6.4811 – 1518.381/(–12.003 + T/K); temp range 283–343 K (Antoine eq.-II, Stephenson & Malanowski 1987)

15600 (calculated-solvatochromic parameters, Banerjee et al. 1990)

log (P/mmHg) = 35.921 – 2.7763 × 10^3/(T/K) – 10.101·log (T/K) – 3.1547 × 10^{-10}·(T/K) + 4.7299 × 10^{-6}·$(T/K)^2$; temp range 190–535 K (vapor pressure eq., Yaws 1994)

Henry's Law Constant (Pa·m^3/mol at 25°C):

11.14	(Bocek 1976; quoted, Basu et al. 1983; Howard 1989)
8.918	(calculated-P/C, Mabey et al. 1982)
9.420	(quoted, WERL Treatability Database, Ryan et al. 1988)

Octanol/Water Partition Coefficient, log K_{OW}:

0.25	(shake flask-HPLC, Pratesi et al. 1979)
0.00	(shake flask, Fujisawa & Masuhara 1980, 1981)
0.09	(shake flask-GC, Tanii & Hashimoto 1984)
0.25	(Hansch & Leo 1985)
0.25	(recommended, Sangster 1989)
0.25	(recommended, Hansch et al. 1995)

Octanol/Air Partition Coefficient, log K_{OA}:

Bioconcentration Factor, log BCF:

1.68	(bluegill sunfish, Barrows et al. 1978)
0.00	(estimated-S, Kenaga 1980)
1.68, 0.32	(bluegill sunfish, calculated-K_{OW}, Veith et al. 1980)
0.017	(microorganisms-water, calculated-K_{OW}, Mabey et al. 1982)

Sorption Partition Coefficient, log K_{OC}:

0.954 (soil, calculated-S, Kenaga 1980)

–0.071 (sediment-water, calculated-K_{OW}, Mabey et al. 1982)

1.101, 1.006; 1.09 (Captina silt loam, McLaurin sandy loam; weighted mean, batch equilibrium-sorption isotherm, Walton et al. 1992)

–0.0899 (calculated-K_{OW}, Walton et al. 1992)

–0.0890 (calculated-K_{OW}, Kollig 1993)

Environmental Fate Rate Constants, k, or Half-Lives, $t_{½}$:

Volatilization: $t_{½}$ = 6, 1.2, 4.8 d in a typical pond, river and lake are 6, 1.2, and 4.8 d, respectively, with the reaeration for oxygen in typical bodies of water (Lyman et al. 1982; quoted, Howard 1989)

evaporation $t_{½}$ = 795 min from water with an assumed 1-m depth (Basu et. al. 1983).

Photolysis:

Oxidation: rate constant k, for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO3} with NO_3 radical and k_{O3} with O_3 or as indicated, *data at other temperatures see reference:

k < 1 × 10^8 M^{-1} h^{-1} for singlet oxygen, and 36 M^{-1} h^{-1} for peroxy radical at 25°C (Mabey et al. 1982)

$t_{½}$ = 4.0 h for photooxidation in the troposphere (Callahan et al. 1979)

k_{OH} = (40.6 ± 4.1) × 10^{-13} cm^3 $molecule^{-1}$ s^{-1} at 299 K (flash photolysis-resonance fluorescence technique, Harris et al. 1981)

k_{O3} < 1 × 10^{-19} cm^3 $molecule^{-1}$ s^{-1} at 296 ± 2 K, and tropospheric lifetimes, τ > 115 d and τ = 3 d due to reactions with O_3 and OH radical, respectively (Atkinson et al. 1982)

k_{O3} < 1 × 10^{-19} cm^3 $molecule^{-1}$ s^{-1} at 296 ± 2 K (Atkinson et al. 1983; quoted, Atkinson & Carter 1984)

$t_{½}$ = 3.5 d for the reaction with photochemically produced hydroxyl radical by the sunlight (Edney et al. 1983; quoted, Howard 1989)

k_{OH} = 4.8 × 10^{-12} cm^3 $molecule^{-1}$ s^{-1} at 298.7 K, and k_{OH} = 3.4 × 10^{-12} cm^3 $molecule^{-1}$ s^{-1} at 296 K (review, flash photolysis-resonance fluorescence technique Atkinson 1985)

photooxidation $t_{½}$ = 3.4–189 h, based on measured rate constant for the reaction with hydroxyl radical in air (Howard et al. 1991)

k_{OH} = (3.4 – 4.80) × 10^{-12} cm^3 $molecule^{-1}$ s^{-1} at 296–298.2 K (review, Atkinson 1989)

Hydrolysis: k(acid) = 4.2×10^{-2} M^{-1} h^{-1} at pH 5.0 with $t_{1/2}$ = 188 yr and k(base) = 6.1×10^{-2} M^{-1} h^{-1} at pH 9.0 with $t_{1/2}$ = 13 yr (Ellington et al. 1987; quoted, Howard et al. 1991, Kollig 1993);

$t_{1/2}$ = 1210 yr at pH 7.0, based on measured acid and base catalyzed hydrolysis constants (Ellington et al. 1987; quoted, Howard et al. 1991)

$t_{1/2}$ = 69 d at pH 2, $t_{1/2}$ = 440000 d at pH 7 and $t_{1/2}$ = 4.7 d at pH 12 in natural waters (Capel & Larson 1995).

Biodegradation: $t_{1/2}$(aq. aerobic) = 30–552 h, based on river die-away test data (Going et al. 1979; Ludzack et al. 1958; quoted, Howard et al. 1991); $t_{1/2}$(aq. anaerobic) = 120–2208 h, based on estimated aqueous aerobic biodegradation half-life (Howard et al. 1991)

^{14}C labeled acrylonitrile at concentrations up to 100 ppm was completely degraded within 2.0 d in a London soil under aerobic conditions (Donberg et al. 1992)

$t_{1/2}$(aerobic) = 1.3 d, $t_{1/2}$(anaerobic) = 5 d in natural waters (Capel & Larson 1995)

Biotransformation: k = of 3×10^{-9} mL $cell^{-1}$ h^{-1} for bacterial transformation in water (Mabey et al. 1982).

Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants:

Half-Lives in the Environment:

Air: $t_{1/2}$ = 4.0 h for photooxidation in the troposphere (Callahan et al. 1979);

$t_{1/2}$ = 3.5 d for the reaction with photochemically produced hydroxyl radical by the sunlight (Edney et al. 1983; quoted, Howard 1989);

photooxidation $t_{1/2}$ = 13.4–189 h, based on measured rate constant for the reaction with hydroxyl radicals in air (Atkinson 1985; quoted, Howard et al. 1991);

atmospheric transformation lifetime was estimated to be 1 – 5 to > 5 d (Kelly et al. 1994).

Surface water: $t_{1/2}$ = 30–552 h, based on estimated aqueous aerobic biodegradation half-life (Howard et al. 1991)

Biodegradation $t_{1/2}$(aerobic) = 100 d, $t_{1/2}$(anaerobic) = 400 d; hydrolysis $t_{1/2}$ = 69 d at pH 2, $t_{1/2}$ = 440000 d at pH 7 and $t_{1/2}$ = 4.7 d at pH 12 in natural waters (Capel & Larson 1995).

Groundwater: $t_{1/2}$ = 60–1104 h based on estimated aqueous aerobic biodegradation half-life (Howard et al. 1991).

Sediment:

Soil: $t_{1/2}$ < 10 d in soil (USEPA 1979; quoted, Ryan et al. 1988);

$t_{1/2}$ = 30–552 h based on estimated aqueous aerobic biodegradation half-life (Howard et al. 1991).

Biota:

TABLE 16.1.1.4.1
Reported aqueous solubilities and vapor pressures of acrylonitrile at various temperatures

Aqueous solubility				Vapor pressure			
Othmer Encyclopedia		Stephenson 1994		Stull 1947		Gudkov et al. 1964	
Basu et al. 1983		shake flask-GC		summary of literature data		in Boublik et al. 1984	
t/°C	S/g·m^{-3}	t/°C	S/g·m^{-3}	t/°C	P/Pa	t/°C	P/Pa
0	72000	0	65800	–51.0	133.3	20	11732
20	73500	10	66800	–30.7	666.6	30	18932
40	79000	20	69000	–20.3	1333	40	27998
60	91000	30	66400	–9.0	2666	50	38530
		40	68800	3.8	5333	60	57328
		50	73600	11.8	7999	70	78660
		60	73900	22.8	13332		
		70	85600	38.7	26664		
				58.3	53329		
				78.5	101325		
				mp/°C	–82.0		

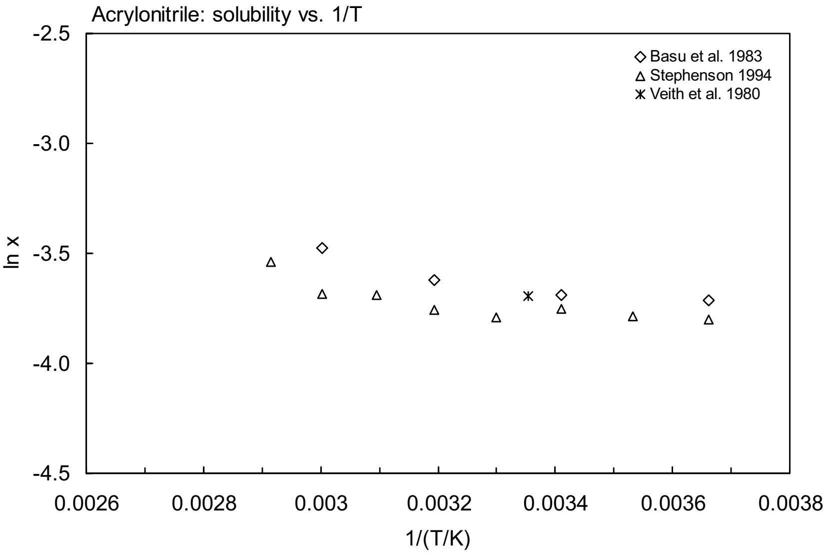


FIGURE 16.1.1.4.1 Logarithm of mole fraction solubility (ln *x*) versus reciprocal temperature for acrylonitrile.

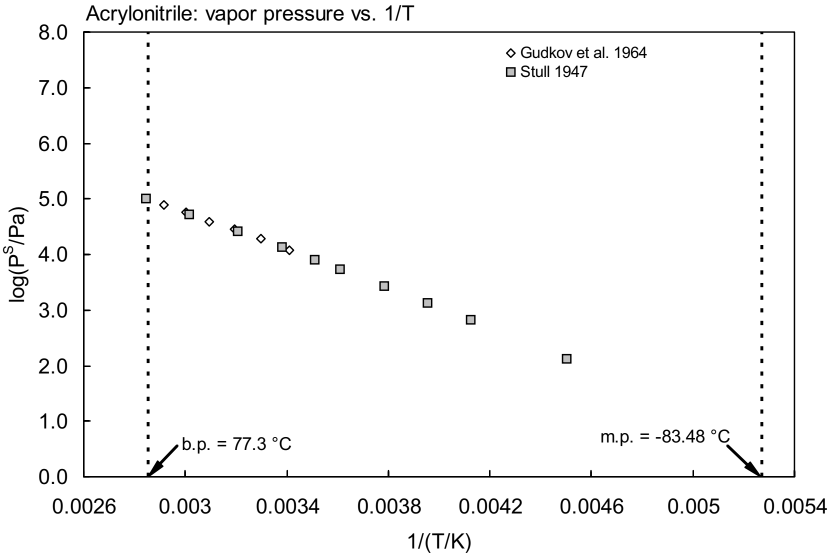
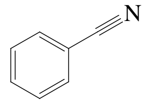


FIGURE 16.1.1.4.2 Logarithm of vapor pressure versus reciprocal temperature for acrylonitrile.

16.1.1.5 Benzonitrile



Common Name: Benzonitrile
Synonym: benzenecarbonitrile, cyanobenzene, phenyl cyanide
Chemical Name: benzonitrile, benzoic acid nitrile
CAS Registry No: 100-47-0
Molecular Formula: C_6H_5CN
Molecular Weight: 103.122
Melting Point (°C):
  –13.99 (Lide 2003)
Boiling Point (°C):
  191.1 (Lide 2003)
Density (g/cm^3 at 20°C):
  1.0006 (25°C, Dean 1985; Riddick et al. 1986)
Molar Volume (cm^3/mol):
  103.1 (25°C, calculated-density)
  107.9 (calculated-Le Bas method at normal boiling point)
Dissociation Constant, pK_a:
Enthalpy of Vaporization, ΔH_V (kJ/mol):
  55.48, 45.94 (25°C, bp, Riddick et al. 1986)
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
  10.88 (Riddick et al. 1986)
Entropy of Fusion, ΔS_{fus} (J/mol K):
Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F: 1.0

Water Solubility (g/m^3 or mg/L at 25°C or as indicated. Additional data at other temperatures designated * are compiled at the end of this section):
  4330 (shake flask-UV, McGowan et al. 1966)
  2000 (Dean 1985; Riddick et al. 1986)
  10000 (selected, Yaws et al. 1990)
  4000* (shake flask-GC/TC, measured range 0–90°C, Stephenson 1994)

Vapor Pressure (Pa at 25°C and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):
  133.3* (38.4°C, static method, measured range 38.4–190.6°C, Kahlbaum 1898)
  133.3* (28.2°C, summary of literature data, temp range 28.2–190.6°C, Stull 1947)
  $\log (P/\text{mmHg}) = [-0.2185 \times 11341.0/(T/\text{K})] + 8.239760$; temp range: 28.2–190.6°C (Antoine eq., Weast 1972–73)
  78.86 (calculated-Antoine eq., Dean 1985, 1992)
  $\log (P/\text{mmHg}) = 6.74631 - 1436.72/(181 + t/°\text{C})$, temp range: liquid (Antoine eq., Dean 1985, 1992)
  100.0 (Riddick et al. 1986)
  $\log (P/\text{kPa}) = 5.87121 - 1436.72/(181.0 + t/°\text{C})$, temp range not specified (Antoine eq., Riddick et al. 1986)
  106.0 (extrapolated-Antoine eq., Stephenson & Malanowski 1987)
  $\log (P_L/\text{kPa}) = 6.79506 - 2066.71/(-32.19 + T/\text{K})$, temp range 301–464 K (Antoine eq.-I, Stephenson & Malanowski 1987)

Henry's Law Constant (Pa·m^3/mol at 25°C):
  55.32 (computed-vapor-liquid equilibrium VLE data, Yaws et al. 1991)

Octanol/Water Partition Coefficient, log K_{OW}:
  1.56 (shake flask-UV spectrophotometry, Fujita et al. 1964; quoted, Leo et al. 1969; Hansch & Leo 1979)
  1.56 (shake flask-UV, Holmes & Lough 1976)

1.67 (calculated-fragment const., Rekker 1977)
1.56 (shake flask at pH 7, Unger et al. 1978)
1.66 (RP-HPLC-k′ correlation, Miyake & Terada 1982)
1.65 ± 0.01 (HPLC-RV correlation-ALPM, Garst & Wilson 1984)
1.50 (HPLC-k′ correlation, Haky & Young 1984)
1.56 (shake flask-GC, Tanii & Hashimoto 1984)
1.56 (RP-HPLC-capacity ratio, Minick et al. 1988)
1.45 (RP-HPLC-RT correlation, ODS column with masking agent, Bechalany et al. 1989)
1.56 (recommended, Sangster 1989, 1993)
1.56 (shake flask-GC, Alcorn et al. 1993)
1.56 (recommended, Hansch et al. 1995)

Octanol/Air Partition Coefficient, log K_{OA}:
4.46 (head-space GC, Abraham et al. 2001)

Bioconcentration Factor, log BCF:

Sorption Partition Coefficient, log K_{OC}:

Environmental Fate Rate Constants, k, or Half-Lives, $t_{½}$:
Volatilization:
Photolysis:
Oxidation: rate constant k; for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO3} with NO_3 radical and k_{O3} with O_3 or as indicated, *data at other temperatures see reference:
$k_{OH} = 3.3 \times 10^{-13}$ cm^3 molecule^{-1} s^{-1} at room temp. (Zetzsch 1982; Atkinson 1989)
k_{OH}(calc) = 4.2×10^{-13} cm^3 molecule^{-1} s^{-1} at room temp. (Atkinson 1985)
k_{OH}(calc) = 3.9×10^{-13} cm^3 molecule^{-1} s^{-1} at room temp. (Atkinson et al. 1985)
k_{OH}(calc) = 3.6×10^{-13} cm^3 molecule^{-1} s^{-1}, k_{OH}(obs) = 3.3×10^{-13} cm^3 molecule^{-1} s^{-1} at room temp. (SAR structure-activity relationship, Atkinson 1987)
k_{OH}(calc) = 4.1×10^{-13} cm^3 molecule^{-1} s^{-1} (molecular orbital calculations, Klamt 1993)
Hydrolysis:
Biodegradation:
Biotransformation:
Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants:

Half-Lives in the Environment:
Surface water: an estimated $t_{½}$ = 1.3 d in Rhine River in case of first order reduction process (Zoeteman et al. 1980)

TABLE 16.1.1.5.1
Reported aqueous solubilities and vapor pressures of butyronitrile at various temperatures

Aqueous solubility		Vapor pressure					
Stephenson 1994		Kahlbaum 1898*				Stull 1947	
shake flask-GC		static-manometer				summary of literature data	
t/°C	S/g·m^{-3}	t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa
0	3500	38.4	133.3	141.4	26664	28.2	133.3
10	3300	45.3	266.6	155.8	39997	55.3	666.6
20	4000	50.0	400.0	165.8	53329	69.2	1333
40	4500	53.8	533.3	174.4	66661	83.4	2666
50	3800	56.9	666.6	181.6	79993	99.6	5333
60	4200	69.1	1333.2	187.7	93326	109.8	7999

(*Continued*)

TABLE 16.1.1.5.1 (*Continued*)

Aqueous solubility		Vapor pressure					
Stephenson 1994		Stull 1947		Meyer et al. 1971		Meyer & Hotz 1976	
shake flask-GC		summary of literature data		ebulliometry		ebulliometry	
t/°C	S/g·m^{-3}	t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa
70	6000	83.0	2666.4	190.6	101325	123.5	13332
80	9500	92.1	3999.7			144.1	26664
90	9100	98.5	5332.9	*complete list see ref.		156.7	53329
		103.9	6666.1			190.6	101325
ΔH_{sol}/(kJ mol^{-1})		113.7	9999.2				
25 °C		121.3	13332			mp/°C	−12.9

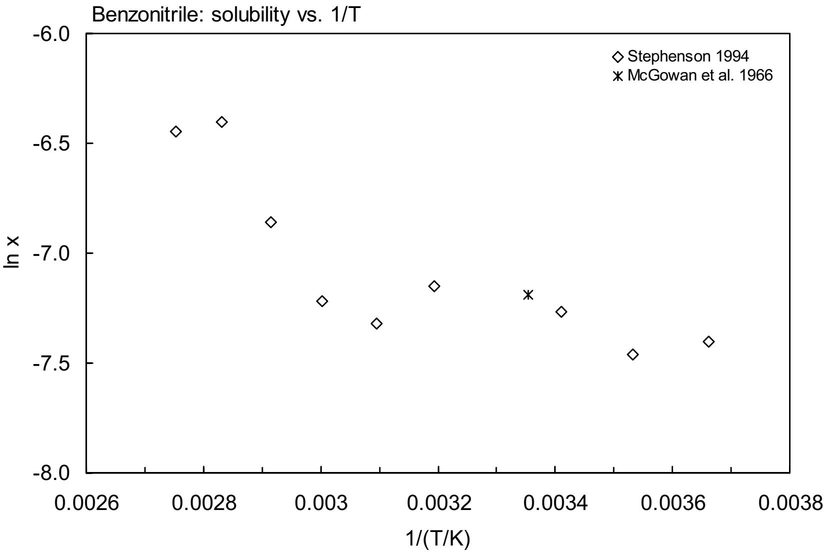


FIGURE 16.1.1.5.1 Logarithm of mole fraction solubility (ln *x*) versus reciprocal temperature for benzonitrile.

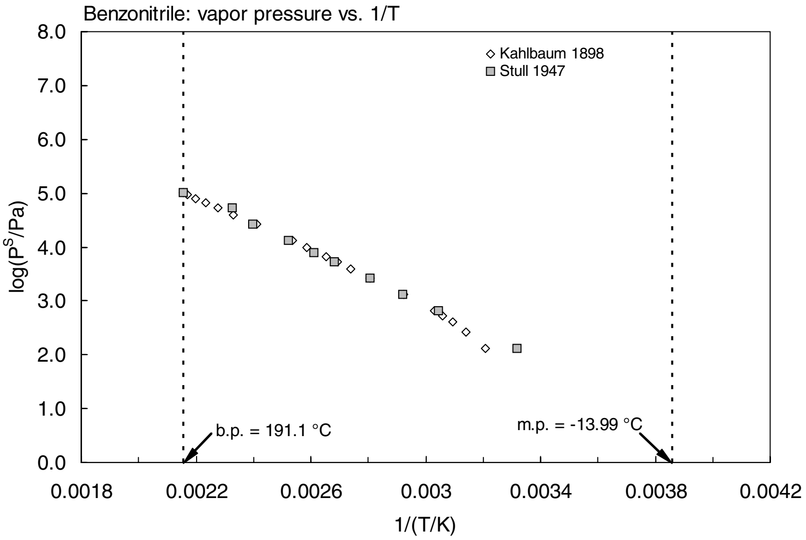
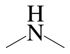


FIGURE 16.1.1.5.2 Logarithm of vapor pressure versus reciprocal temperature for benzonitrile.

16.1.2 ALIPHATIC AMINES

16.1.2.1 Dimethylamine



Common Name: Dimethylamine
Synonym: aminomethylmethane, N-methylmethanamine
Chemical Name: aminomethylmethane, dimethylamine
CAS Registry No: 124-40-3
Molecular Formula: C_2H_7N, CH_3NHCH_3
Molecular Weight: 45.084
Melting Point (°C):
–92.18 (Lide 2003)
Boiling Point (°C):
6.88 (Lide 2003)
Density (g/cm^3 at 20°C):
0.6804 (0°C, Weast 1982–83)
0.6556, 0.6496 (20°C, 25°C, Riddick et al. 1986)
Molar Volume (cm^3/mol):
68.8 (20°C, calculated-density)
67.5 (calculated-Le Bas method at normal boiling point)
Dissociation Constant, pK_a:
10.732 (Perrin 1965; Weast 1982–83; Howard 1990)
10.77 (protonated cation + 1, Dean 1985)
10.77 (Sangster 1989)
Enthalpy of Vaporization, ΔH_V (kJ/mol):
23.84, 24.61 (25°C, bp, Dreisbach 1961)
23.65, 24.61 (25°C, bp, Riddick et al. 1986)
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
5.941 (Riddick et al. 1986)
Entropy of Fusion, ΔS_{fus} (J/mol K):
Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F: 1.0

Water Solubility (g/m^3 or mg/L at 25°C):
very soluble (Dean 1985)
620000 (selected, Yaws et al. 1990)
miscible (Stephenson 1993b)

Vapor Pressure (Pa at 25°C and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):
101141* (280.018 K, static method, measured range 201.387–280.018 K, Ashton et al. 1939)
236420* (extrapolated-regression of tabulated data, temp range –87.2 to + 7.4°C, Stull 1947)
196800 (calculated by formula, Dreisbach 1961)
log (P/mmHg) = 7.06396 – 1024.4/(238.0 + t/°C), temp range –55 to 37°C, (Antoine eq. for liquid state, Dreisbach 1961)
log (P/mmHg) = [–0.2185 × 6660.0/(T/K)] + 7.995166; temp range –87.7 to 162.6°C, (Antoine eq., Weast 1972–73)
172220 (20°C, Verschueren 1983)
206180 (extrapolated-Antoine eq., Boublik et al. 1984)
log (P/kPa) = 6.21132 – 962.001/(221.852 + t/°C), temp range –71.77 to 6.858°C (Antoine eq. from reported exptl. data, Boublik et al. 1984)
202620 (Daubert & Danner 1985)
206000 (extrapolated-Antoine eq., Dean 1985, 1992)
log (P/mmHg) = 7.08212 – 960.242/(221.67 + t/°C), temp range –72 to 6°C (Antoine eq., Dean 1985, 1992)

196800 (quoted lit., Riddick et al. 1986)
log (P/kPa) = 6.18886 – 1-024.40/(238.0 + t/°C), temp range not specified (Antoine eq., Riddick et al. 1986)
205300 (interpolated-Antoine eq-II., Stephenson & Malanowski 1987)
log (P_L/kPa) = 6.29031 – 993.586/(–48.12 + T/K), temp range 201–280 K (Antoine eq.-I, Stephenson & Malanowski 1987)
log (P_L/kPa) = 6.20646 – 965.728/(–50.151 + T/K), temp range 277–360 K (Antoine eq.-II, Stephenson & Malanowski 1987)
log (P_L/kPa) = 7.81489 – 2369.425/(141.433 + T/K), temp range 358–438 K (Antoine eq.-III, Stephenson & Malanowski 1987)
log (P/mmHg) = 36.9182 – 2.4965 × 10^3/(T/K) – 10.417·log (T/K) – 1.6287 × 10^{-9}·(T/K) + 4.6496 × 10^{-6}·$(T/K)^2$; temp range 181–438 K (vapor pressure eq., Yaws 1994)

Henry's Law Constant (Pa·m^3/mol at 25°C):
1.796 (exptl., Hine & Mookerjee 1975; quoted, Howard 1990)
1.796, 1.03 (calculated-group contribution, calculated-bond contribution, Hine & Mookerjee 1975)
2.718 (calculated-molecular structure, Russell et al. 1992)

Octanol/Water Partition Coefficient, log K_{OW}:
–0.38 (shake flask-RC at pH 13, Wolfenden 1978)
–0.38 (Hansch & Leo 1985)
–0.38 (recommended, Sangster 1989; 1993)
–0.38 (recommended, Hansch et al. 1995)

Octanol/Air Partition Coefficient, log K_{OA}:
2.00 (calculated-S_{oct} and vapor pressure P, Abraham et al. 2001)

Bioconcentration Factor, log BCF:
–0.523 (calculated-K_{OW}, Lyman et al. 1982; quoted, Howard 1990)

Sorption Partition Coefficient, log K_{OC}:
2.638 (adsorption isotherm average for five soils, Rao & Davidson 1982; quoted, Howard 1990)
0.602; 2.212; 2.706 (Podzol soil; Alfisol soil; sediment, von Oepen et al. 1991)
2.63 (soil, calculated-MCI, Sabljic et al. 1995)

Environmental Fate Rate Constants, k, or Half-Lives, $t_{½}$:
Volatilization: using Henry's law constant, $t_{½}$ = 35.1 h was estimated for a model river of 1 m deep flowing at 1 m/s with a wind velocity of 3 m/s (Lyman et al. 1982; selected, Howard 1990).
Photolysis:
Oxidation: rate constant k, for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO3} with NO_3 radical and k_{O3} with O_3 or as indicated:
k_{OH} = 6.54 × 10^{-11} cm^3 $molecule^{-1}$ s^{-1} at 299 K (Atkinson et al. 1977; quoted, Carlier et al. 1986; Atkinson 1989)
photooxidation $t_{½}$ = 5.9 h in air was estimated for the vapor phase reaction with hydroxyl radical of 5 × 10^5 radicals/cm^3 in air (Atkinson et al. 1978; Atkinson 1985; quoted, Howard 1990);
k_{O3} = (2.61 ± 0.30) × 10^{-18} cm^3 $molecule^{-1}$ s^{-1} at 296 ± 2 K (Atkinson & Carter 1984; quoted, Atkinson 1985)
k_{OH} = 6.5 × 10^{-11} cm^3 ± $molecule^{-1}$ s^{-1} for the gas-phase reaction with 5 × 10^5 OH radicals/cm^3 at room temp. having a loss rate of 2.8 d^{-1} (Atkinson 1985)
k_{OH}(calc) = 63 × 10^{-12} cm^3 $molecule^{-1}$ s^{-1} at room temp. (Atkinson 1987).
Hydrolysis:
Biodegradation: aqueous aerobic $t_{½}$ = 2–79 h, based on river die-away test data (Digeronimo et al. 1979; Dojlido 1979; selected, Howard et al. 1991); aqueous anaerobic $t_{½}$ = 8–316 h, based on estimated unacclimated aqueous aerobic biodegradation half-life (Howard et al. 1991).
Biotransformation:
Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants:

Half-Lives in the Environment:

Air: $t_{½}$ = 5.9 h was estimated for the vapor phase reaction with hydroxyl radical of 5 × 10^5 radicals/cm^3 in air (Atkinson et al. 1978; Atkinson 1985; quoted, Howard 1990);

photooxidation $t_{½}$ = 0.892–9.20 h, based on measured rate constant for the gas-phase reaction with OH radical (Atkinson 1985; quoted, Howard et al. 1991) and ozone (Tuazon et al. 1978; selected, Howard et al. 1991).

Surface water: $t_{½}$ = 2–79 h, based on estimated unacclimated aqueous aerobic biodegradation half-life (Howard et al. 1991).

Groundwater: $t_{½}$ = 4–158 h, based on estimated unacclimated aqueous aerobic biodegradation half-life (Howard et al. 1991).

Sediment:

Soil: $t_{½}$ = 86–336 h, based on soil die-away test data (Tate & Alexander 1976; Greene et al. 1981; selected, Howard et al. 1991).

Biota:

TABLE 16.1.2.1.1
Reported vapor pressures of dimethylamine at various temperatures and the coefficients for the vapor pressure equations

$\log P = A - B/(T/K)$ (1) $\ln P = A - B/(T/K)$ (1a)
$\log P = A - B/(C + t/°C)$ (2) $\ln P = A - B/(C + t/°C)$ (2a)
$\log P = A - B/(C + T/K)$ (3)
$\log P = A - B/(T/K) - C \cdot \log (T/K)$ (4)
$\log P = A - B/(T/K) - C \log (T/K) + D \cdot (T/K) - E \cdot (T/K)^2 + F \cdot (T/K)^3$ (5)

Ashton et al. 1939				Stull 1947	
static method				summary of literature data	
T/K	P/Pa			t/°C	P/Pa
201.387	648	bp/K	280.04	–87.7	133.3
213.802	1959	mp/K	180.97	–72.2	666.6
222.078	3780	$\Delta H_V/(kJ\ mol^{-1})$ = 26.48 (bp)		–64.6	1333
232.137	7775	$\Delta H_{fus}/(kJ\ mol^{-1})$ = 5.94 (mp)		–56.0	2666
242.078	14743			–46.7	5333
249.640	22949	eq. 5	P/mmHg	–40.7	7999
256.449	33269	A	32.26370	–32.6	13332
262.977	46404	B	2460.10	–20.4	26664
270.182	65491	C	8.6390	–7.1	53329
275.934	84860	D	7.6055×10^{-3}	7.4	101325
279.980	100974	E	3.51389×10^{-5}		
277.680	91519	F	5.3241×10^{-8}	mp/°C	–96.0
280.018	101141				

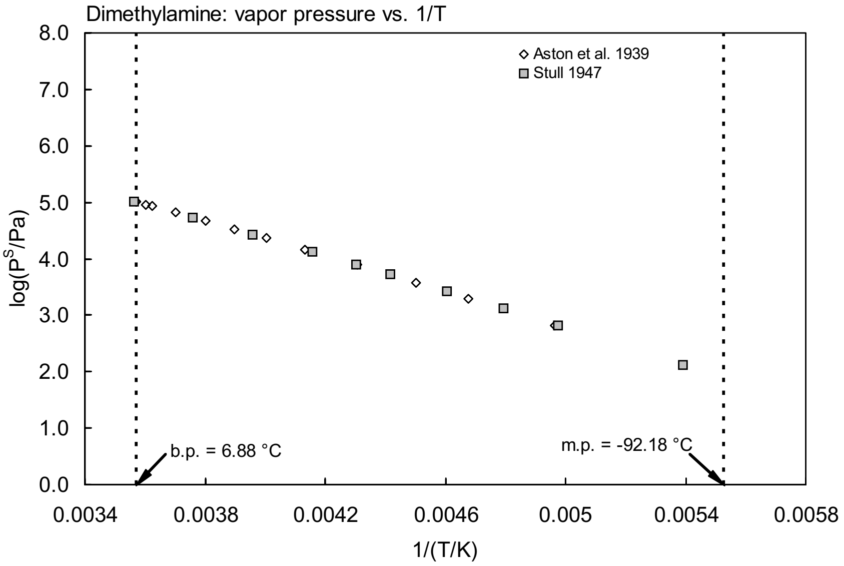
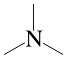


FIGURE 16.1.2.1.1 Logarithm of vapor pressure versus reciprocal temperature for dimethylamine.

16.1.2.2 Trimethylamine



Common Name: Trimethylamine
Synonym: dimethylamino methane, TMA
Chemical Name: trimethylamine
CAS Registry No: 75-50-3
Molecular Formula: C_3H_9N, $CH_3N(CH_3)_2$
Molecular Weight: 59.110
Melting Point (°C):
 –117.1 (Lide 2003)
Boiling Point (C):
 2.87 (Lide 2003)
Density (g/cm^3 at 20°C):
 0.6356 (Weast 1982–83)
Molar Volume (cm^3/mol):
 93 (20°C, calculated-density)
 93.3 (calculated-Le Bas method at normal boiling point)
Dissociation Constant, pK_a:
 9.801, 9.987 (Perrin 1972; quoted, Howard 1990)
 9.80 (pK_a, protonated cation + 1, Dean 1985)
 9.79 (pK_a, Sangster 1989)
Enthalpy of Vaporization, ΔH_V (kJ/mol):
 22.85, 24.13 (25°C, bp, Dreisbach 1961)
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
Entropy of Fusion, ΔS_{fus} (J/mol K):
Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F: 1.0

Water Solubility (g/m^3 or mg/L at 25°C) or as indicated:
 410000 (Dean 1985)
 890000 (30°C, Howard 1990)
 291000 (selected, Yaws et al. 1990)
 miscible (Stephenson 1993b)

Vapor Pressure (Pa at 25°C or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this chapter):
 221715* (isoteniscope, measured range 0–40°C, Swift & Hochanadel 1945)
 log (P/mmHg) = 24.91300 – 2018.37/(T/K) – 6.0303 · log (T/K); temp range 0–40°C (isoteniscope method, Swift & Hochanadel 1945)
 265200* (extrapolated-regression of tabulated data, temp range –97.1 to + 2.9°C, Stull 1947)
 226540 (calculated by formula, Dreisbach 1961)
 log (P/mmHg) = 6.97038 – 968.7/(234.0 + t/°C), temp range –58 to 32°C (Antoine eq. for liquid state, Dreisbach 1961)
 log (P/mmHg) = [–0.2185 × 6361.7/(T/K)] + 7.952370; temp range –97.1 to 2.9°C (Antoine eq., Weast 1972–73)
 192500 (20°C, 30°C, Verschueren 1983)
 219300, 221800 (extrapolated-Antoine eq., interpolated-Antoine eq., Boublik et al. 1984)
 log (P/kPa) = 5.98554 – 1957.276/(237.664 + t/°C), temp range –80.3 to 3.45°C (Antoine eq. from reported exptl. data, Boublik et al. 1984)
 log (P/kPa) = 5.87712 – 894.366/(228.276 + t/°C), temp range 0–40°C (Antoine eq. from reported exptl. data, Boublik et al. 1984)
 214200 (Daubert & Danner 1985)
 219000 (extrapolated-Antoine eq., Dean 1985, 1992)
 log (P/mmHg) = 6.85755 – 955.94/(237.52 + t/°C), temp range –80 to 3°C (Antoine eq., Dean 1985, 1992)
 219900 (extrapolated-Antoine eq., Stephenson & Malanowski 1987)

log (P_L/kPa) = 6.01402 – 968.978/(–34.253 + T/K), temp range 192–277 K (Antoine eq., Stephenson & Malanowski 1987)

log (P/mmHg) = 58.6807 – 2.686 × 10^3/(T/K) – 20.36·log (T/K) + 1.3131 × 10^{-2}·(T/K) – 6.563 × 10^{-13}·$(T/K)^2$; temp range 156–433 K (vapor pressure eq., Yaws 1994)

Henry's Law Constant (Pa·m^3/mol at 25°C):

6.672 (exptl., Hine & Mookerjee 1975)
12.71, 2.16 (calculated-group contribution, calculated-bond contribution, Hine & Mookerjee 1975)
15.64 (calculated-molecular structure, Russell et al. 1992)

Octanol/Water Partition Coefficient, log K_{OW}:

0.27 (shake flask-TN, Sandell 1962; quoted, Leo et al. 1971)
0.27; 0.20 (calculated-f const., calculated-π const., Rekker 1977)
0.16 (shake flask, Hansch & Leo 1985)
0.16 (recommended, Sangster 1989)
0.16 (recommended, Hansch et al. 1995)

Octanol/Air Partition Coefficient, log K_{OA}:

Bioconcentration Factor, log BCF:

< 0.0 (estimated-K_{OW}, Lyman et al. 1982; quoted, Howard 1990)

Sorption Partition Coefficient, log K_{OC}:

1.462 (soil, estimated-K_{OW}, Lyman et al. 1982; quoted, Howard 1990)
0.602 (soil, estimated-solubility, Lyman et al. 1982; quoted, Howard 1990)
0.778; 2.365; 2.831 (Podzol soil; Alfisol soil;, sediments von Oepen et al. 1991)

Environmental Fate Rate Constants, k, or Half-Lives, $t_{½}$:

Volatilization: using Henry's law constant, $t_{½}$ = 11 h was estimated for a model river 1 m deep flowing at 1 m/s with a wind velocity of 3 m/s (Lyman et al. 1982; quoted, Howard 1990).

Photolysis:

Hydrolysis:

Oxidation: rate constant k, for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO3} with NO_3 radical and k_{O3} with O_3 or as indicated, *data at other temperatures see reference:

k_{OH} = 6.09 × 10^{-11} cm^3 molecule^{-1} s^{-1} at 299 K (Atkinson et al. 1977; Atkinson 1989)

photooxidation $t_{½}$ = 62 d in water, based on rate constant k = 1.3 × 10^{10} L mol^{-1} s^{-1} for the reaction with photochemically produced hydroxyl radicals of 1 × 10^{-17} mol · L^{-1} in water (Mill et al. 1980; Güesten et al. 1981; quoted, Howard 1990)

k_{OH} = 6.10 × 10^{-11} cm^3 molecule^{-1} s^{-1} for the gas-phase reaction with 1 × 10^6 OH radicals/cm^3 with a loss rate of 5.0 d^{-1} and rate constant k_{O3} = 9.70 × 10^{-18} cm^3 molecule^{-1} s^{-1} for the gas-phase reaction with 7 × 10^{11} O_3 molecules/cm^3 with a loss rate of 0.6 d^{-1} both at room temp. (Atkinson & Carter 1984)

calculated k_{OH} = 64 × 10^{-12} cm^3 molecule^{-1} s^{-1} at room temp. (SAR, Atkinson 1987).

Biodegradation:

Biotransformation:

Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants:

Half-Lives in the Environment:

Air: photooxidation $t_{½}$ = 4.0 h, based on rate constant k = 6.09 × 10^{-11} cm^3 molecule^{-1} s^{-1} for the vapor-phase reaction with photochemically produced hydroxyl radical of 8 × 10^5 radicals/cm^3 in air at 25.5°C and $t_{½}$ = 1.4 d, based on rate constant k = 9.73 × 10^{-18} cm^3 molecule^{-1} s^{-1} for the vapor-phase reaction with ozone of 6 × 10^{11} molecules/cm^3 in air at 24.4°C (Atkinson 1985; GEMS 1986; quoted, Howard 1990).

Surface water: $t_{½}$ = 62 d, based on rate constant k = 1.3 × 10^{10} L mol^{-1} s^{-1} for the reaction with photochemically produced hydroxyl radicals of 1 × 10^{-17} mol L^{-1} in water (Mill et al. 1980; Güesten et al. 1981; quoted, Howard 1990).

TABLE 16.1.2.2.1
Reported vapor pressures of trimethylamine at various temperatures and the coefficients for the vapor pressure equations

$\log P = A - B/(T/K)$ (1) $\ln P = A - B/(T/K)$ (1a)
$\log P = A - B/(C + t/°C)$ (2) $\ln P = A - B/(C + t/°C)$ (2a)
$\log P = A - B/(C + T/K)$ (3)
$\log P = A - B/(T/K) - C \cdot \log (T/K)$ (4)

Aston et al. 1944		Swift & Hochanadel 1945		Stull 1947	
static method		isoteniscope		summary of literature data	
t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa
–80.315	805	0	91059	–97.1	133.3
–74.081	1367	15	158520	–81.7	666.6
–62.339	3354	20	188651	–73.8	1333
–51.938	6777	25	221715	–65.0	2666
–46.842	9305	30	259444	–55.2	5333
–41.774	12548	35	302107	–48.8	7999
–35.617	17684	40	349437	–40.3	13332
–28.507	25624			–27.0	26664
–24.155	31772	bp/K	276.03	–12.5	53329
–23.067	33494			2.90	101325
–20.164	38401	eq. 4	P/mmHg		
–15.974	46505	A	24.91300	mp/°C	–117.1
–11.422	56802	B	2018.37		
–8.985	63039	C	6.0303		
–7.399	67346				
–3.113	80208	$\Delta H_V/(\text{kJ mol}^{-1})$ = 23.93			
0.780	93495		at bp		
2.928	101526				
3.454	103611				

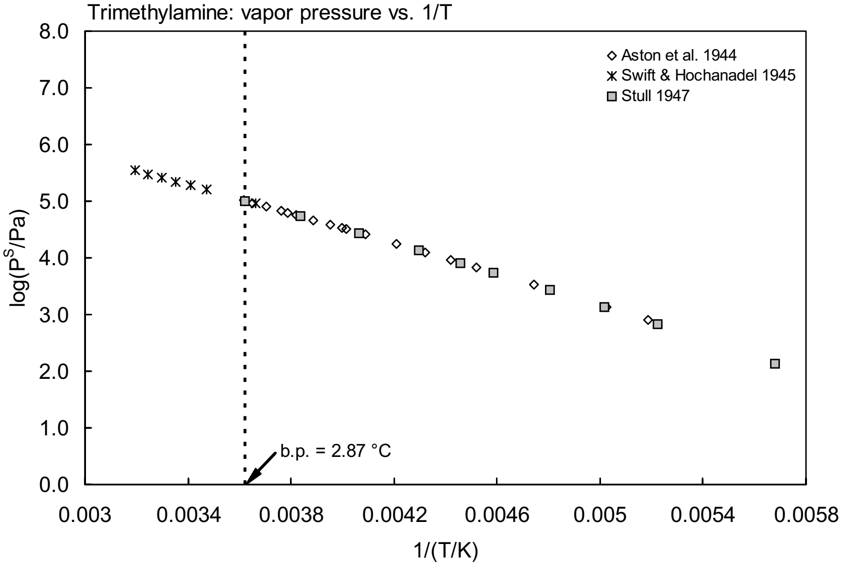


FIGURE 16.1.2.2.1 Logarithm of vapor pressure versus reciprocal temperature for trimethylamine.

16.1.2.3 Ethylamine

Common Name: Ethylamine
Synonym: aminoethane, ethanamine, monoethylamine
Chemical Name: aminoethane, ethylamine
CAS Registry No: 75-04-7
Molecular Formula: C_2H_7N, $CH_3CH_2NH_2$
Molecular Weight: 45.084
Melting Point (°C):
–80.5 (Lide 2003)
Boiling Point (°C):
16.5 (Lide 2003)
Density (g/cm^3 at 20°C):
0.6829 (Dreisbach 1961; Weast 1982–83)
0.6769 (25°C, Dreisbach 1961)
Molar Volume (cm^3/mol):
65.4 (5°C, Stephenson & Malanowski 1987)
66.0 (calculated-Le Bas method at normal boiling point)
Dissociation Constant, pK_a:
10.79 (Perrin 1972)
10.81 (20°C, Weast 1982–83)
10.63 (protonated cation + 1, Dean 1985)
10.70 (Sangster 1989)
Enthalpy of Vaporization, ΔH_V (kJ/mol):
27.08, 27.57 (25°C, bp, Dreisbach 1961)
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
Entropy of Fusion, ΔS_{fus} (J/mol K):
Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F: 1.0

Water Solubility (g/m^3 or mg/L at 25°C):
miscible (Dean 1985; Howard 1990; Stephenson 1993b)

Vapor Pressure (Pa at 25°C or as indicated and reported temperature dependence equations. Additional data at other temperatures designated* are compiled at the end of this section):
156200* (extrapolated-regression of tabulated data, temp range –82.3 to 16.6°C, Stull 1947)
141620 (calculated by formula, Dreisbach 1961)
$\log (P/\text{mmHg}) = 7.3862 - 1137.30/(235.85 + t/°C)$; temp range –43 to 47°C (Antoine eq. for liquid state, Dreisbach 1961)
93325* (20°C, temp range 1.95 to 20°C, Bittrich et al. 1962)
$\log (P/\text{mmHg}) = [-0.2185 \times 6845.1/(T/K)] + 7.973674$; temp range –82.3 to 176°C, (Antoine eq., Weast 1972–73)
121570, 172220 (20°C, 30°C, Verschueren 1983)
139100 (extrapolated-Antoine eq., Boublik et al. 1984)
$\log (P/\text{kPa}) = 5.12561 - 559.427/(162.579 + t/°C)$; temp range 1.95–14.65°C (Antoine eq. from reported exptl. data, Boublik et al. 1984)
139700 (Daubert & Danner 1985)
141000 (calculated-Antoine eq., Dean 1985, 1992)
$\log (P/\text{mmHg}) = 7.05413 - 987.31/(220.0 + t/°C)$; temp range –20 to 90°C (Antoine eq., Dean l985, 1992)
137500, 141200 (calculated-Antoine eq.-II, III, Stephenson & Malanowski 1987)
$\log (P_L/\text{kPa}) = 6.57462 - 1167.57/(-34.18 + T/K)$; temp range 213–297 K (Antoine eq.-I, Stephenson & Malanowski 1987)
$\log (P_L/\text{kPa}) = 6.43082 - 1140.62/(-32.433 + T/K)$; temp range 290–449 K (Antoine eq.-II, Stephenson & Malanowski 1987)

log (P_L/kPa) = 6.21526 – 1009.66/(–49.804 + T/K); temp range 291–367 K (Antoine eq.-III, Stephenson & Malanowski 1987)
log (P_L/kPa) = 6.48782 – 1176.995/(–26.674 + T/K); temp range 377–456 K (Antoine eq.-IV, Stephenson & Malanowski 1987)
140900 (calculated-Cox eq., Chao et al. 1990)
log (P/mmHg) = 33.2962 – 2.4307 × 10^3/(T/K) – 9.0779·log (T/K) – 1.3848 × 10^{-9}·(T/K) + 3.8183 × 10^{-6}·$(T/K)^2$; temp range 192–456 K (vapor pressure eq., Yaws 1994)

Henry's Law Constant (Pa·m^3/mol at 25°C):

1.012	(partial pressure, Butler & Ramchandani 1935)
0.683	(exptl., Hine & Mookerjee 1975)
0.859, 0.730	(calculated-group contribution, calculated-bond contribution, Hine & Mookerjee 1975)
0.421	(calculated-molecular structure, Russell et al. 1992)

Octanol/Water Partition Coefficient, log K_{OW}:

–0.30	(shake flask-titration with ion correction, Korenman et al. 1973)
–0.16, –0.14; –0.19	(calculated-fragment const.; calculated-π const., Rekker 1977)
–0.13	(Hansch & Leo 1985)
–0.13	(recommended, Sangster 1989)
–0.14	(calculated-CLOGP, Jäckel & Klein 1991)
–0.13	(recommended, Hansch et al. 1995)

Octanol/Air Partition Coefficient, log K_{OA}:

Bioconcentration Factor, log BCF:

< 0.0	(estimated-K_{OW}, Lyman et al. 1982; quoted, Howard 1990)

Sorption Partition Coefficient, log K_{OC}:

Environmental Fate Rate Constants, k, or Half-Lives, $t_{½}$:

Volatilization: using Henry's law constant, $t_{½}$ = 2.0 d was estimated for a model river of 1 m deep flowing at 1 m/s with a wind velocity of 3 m/s (Howard 1990).

Photolysis:

Oxidation: rate constant k, for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO3} with NO_3 radical and k_{O3} with O_3 or as indicated, *data at other temperatures see reference:

photooxidation $t_{½}$ > 9.9 d for the gas-phase reaction with OH radical in air, based on the rate of disappearance of hydrocarbon due to reaction with hydroxyl radical (Darnall et al. 1976)

k_{OH} = 2.77 × 10^{-11} cm^3·$molecules^{-1}$·s^{-1} at 299 K (Atkinson et al. 1977; quoted, Carlier et al. 1986)

photooxidation $t_{½}$ = 321 d in water, based on a rate constant k = 2.5 × 10^9 L·mol^{-1}·s^{-1} for the aqueous-phase reaction with photochemically produced OH radical of 1 × 10^{-17} mol·L^{-1} (Mill et al. 1980; Güesten et al. 1981; quoted, Howard 1990)

k_{O3} = (2.76 ± 0.34) × 10^{-20} cm^3·$molecules^{-1}$·s^{-1} at 296 ± 2 K under atmospheric conditions (Atkinson & Carter 1984)

k_{OH} = 27.7 × 10^{-12} cm^3 $molecule^{-1}$ s^{-1} at 299.6 K (Atkinson 1989)

Hydrolysis:

Biodegradation:

Biotransformation:

Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants:

Half-Lives in the Environment:

Air: $t_{½}$ > 9.9 d for the gas-phase reaction with hydroxyl radical in air, based on the rate of disappearance of hydrocarbon due to reaction with hydroxyl radical (Darnall et al. 1976);

photooxidation $t_{½}$ = 8.6 h, based on rate constant k = 6.54 × 10^{-11} cm^3·$molecules^{-1}$·s^{-1} for the vapor-phase reaction with an average hydroxyl radical of 5 × 10^5 radicals/cm^3 at 25.5°C (Atkinson 1985; quoted, Howard 1990).

Surface water: $t_{½}$ = 321 d, based on a rate constant $k = 2.5 \times 10^9$ $L \cdot mol^{-1} \cdot s^{-1}$ for the aqueous-phase reaction with photochemically produced hydroxyl radical of 1×10^{-17} $mol \cdot L^{-1}$ (Mill et al. 1980; Güesten et al. 1981; quoted, Howard 1990).

TABLE 16.1.2.3.1
Reported vapor pressures of ethylamine at various temperatures

Stull 1947		Bittrich et al. 1962	
summary of literature data			
t/°C	P/Pa	t/°C	P/Pa
–82.3	133.3	1.95	53329
–66.4	666.6	4.55	59995
–58.3	1333	6.85	66661
–48.6	2666	9.15	73327
–39.8	5333	11.05	79993
–33.4	7999	12.85	86659
–25.1	13332	14.65	93325
–12.3	26664		
2.0	53329		
16.6	101325		
mp/°C	–80.6		

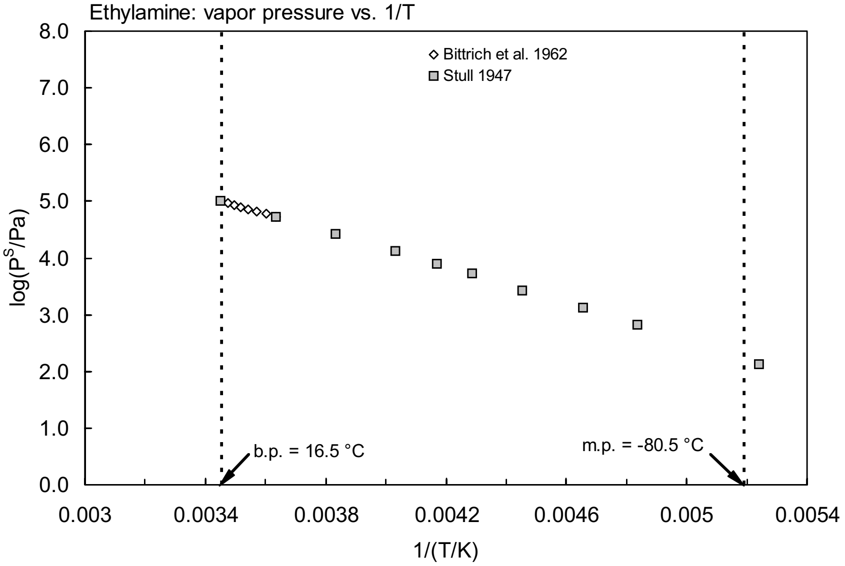
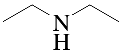


FIGURE 16.1.2.3.1 Logarithm of vapor pressure versus reciprocal temperature for ethylamine.

16.1.2.4 Diethylamine



Common Name: Diethylamine
Synonym: aminoethylethane, *N*-ethylethanamine
Chemical Name: aminoethylethane, diethylamine
CAS Registry No: 109-89-7
Molecular Formula: $C_4H_{11}N$, $CH_3CH_2NHCH_2CH_3$
Molecular Weight: 73.137
Melting Point (°C):
    –49.8 (Lide 2003)
Boiling Point (°C):
    55.5 (Lide 2003)
Density (g/cm^3 at 20°C):
    0.6993, 0.6926 (20°C, 25°C, Dreisbach. 1961)
    0.7056 (Weast 1982–83)
    0.7070, 0.7016 (20°C, 25°C, Riddick et al. 1986)
Molar Volume (cm^3/mol):
    103.4 (20°C, calculated-density)
    109.0 (exptl. at normal bp, Lee et al. 1972)
    111.9 (calculated-Le Bas method at normal boiling point,)
Dissociation Constant, pK_a:
    10.98 (Perrin 1965; quoted, Howard 1990)
    10.80 (35°C, Perrin 1972)
    10.80 (protonated cation + 1, Dean 1985)
    11.07 (Sangster 1989)
Enthalpy of Vaporization, ΔH_V (kJ/mol):
    31.38, 29.50 (25°C, bp, Dreisbach 1961)
    31.32, 29.07 (25°C, bp, Riddick et al. 1986)
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
Entropy of Fusion, ΔS_{fus} (J/mol K):
Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F: 1.0

Water Solubility (g/m^3 or mg/L at 25°C or as indicated):
    815000 (14°C, quoted, Verschueren 1983)
    miscible (Dean 1985; Riddick et al. 1986; Yaws et al. 1990)
    miscible (Stephenson 1993b)

Vapor Pressure (Pa at 25°C and or as indicated reported temperature dependence equations. Additional data at other temperatures designated* are compiled at the end of this section):
    26664* (21°C, summary of literature data, temp range –33.0 to 55.5°C, Stull 1947)
    31130 (calculated by formula, Dreisbach 1961)
    log (P/mmHg) = 7.14099 – 1209.9/(229.0 + t/°C); temp range –15 to 90°C (Antoine eq. for liquid state, Dreisbach 1961)
    39997* (31.45°C, temp range 31.45–60.58°C, Bittrich & Kauer 1962)
    31471* (25.17°C, temp range 19.73–40.22°C, Kilian & Bittrich 1965)
    log (P/mmHg) = [–0.2185 × 7307.5/(T/K)] + 7.701718; temp range –33.0 to 210°C (Antoine eq., Weast 1972–73)
    26660, 38660 (20°C, 30°C, Verschueren 1983)
    30110, 31310 (extrapolated-Antoine eq., interpolated-Antoine eq., Boublik et al. 1984)
    log (P/kPa) = 4.97981 – 580.448/(143.68 + t/°C); temp range 31.45–60.58°C (Antoine eq. from reported exptl. data, Boublik et al. 1984)
    log (P/kPa) = 5.84728 – 994.478/(203.53 + t/°C); temp range 19.758–40.22°C (Antoine eq. from reported exptl. data, Boublik et al. 1984)

31130 (selected, Riddick et al. 1986)
log (P/kPa) = 4.92649 – 583.297/(144.145 + t/°C); temp range not specified (Antoine eq., Riddick et al. 1986)
31490 (extrapolated-Antoine eq., Stephenson & Malanowski 1987)
log (P_L/kPa) = 5.96802 – 1058.538/(–61.331 + T/K); temp range 302–328 K (Antoine eq.-I, Stephenson & Malanowski 1987)
log (P_L/kPa) = 5.92678 – 1028.405/(–66.2061 + T/K); temp range 325–437 K (Antoine eq.-II, Stephenson & Malanowski 1987)
log (P/mmHg) = 5.8016 – 583.3/(144.1 + t/°C); temp range 31–61°C (Antoine eq., Dean 1992)
log (P/mmHg) = $32.626 - 2.4918 \times 10^3/(T/K) - 9.3285 \cdot \log (T/K) + 3.990 \times 10^{-3} \cdot (T/K) + 1.1732 \times 10^{-12} \cdot (T/K)^2$; temp range 223–497 K (vapor pressure eq., Yaws 1994)

Henry's Law Constant (Pa·m³/mol at 25°C):

2.596	(exptl., Hine & Mookerjee 1975)
2.537, 2.37	(calculated-group contribution, calculated-bond contribution, Hine & Mookerjee 1975)
6.67	(calculated-vapor liquid equilibrium VLE data, Yaws et al. 1991)

Octanol/Water Partition Coefficient, log K_{OW}:

0.43	(shake flask, Collander 1951)
0.57	(shake flask-titration, Sandell 1962)
0.60, 0.61; 0.70	(calculated-fragment const.; calculated-π const., Rekker 1977)
0.58	(Hansch & Leo 1985)
0.58	(20°C, shake flask-GC, Takayama et al. 1985)
0.81	(HPLC-k′ correlation, Eadsforth 1986)
0.58	(recommended, Sangster 1989)
0.58	(recommended, Hansch et al. 1995)

Octanol/Air Partition Coefficient, log K_{OA}:

Bioconcentration Factor, log BCF:

0.210	(calculated-K_{OW}, Lyman et al. 1982; quoted, Howard 1990)

Sorption Partition Coefficient, log K_{OC}:

1.699	(soil, calculated-K_{OW}, Lyman et al. 1982; quoted, Howard 1990)

Environmental Fate Rate Constants, k, or Half-Lives, $t_{1/2}$:

Volatilization: using Henry's law constant, $t_{1/2}$ ~ 31.6 h for a model river 1 m deep flowing at 1 m/s with a wind velocity of 3 m/s (estimated, Lyman et al. 1982; quoted, Howard 1990).
Photolysis:
Oxidation: photooxidation $t_{1/2}$ > 9.9 d for the gas-phase reaction with hydroxyl radical in air, based on the rate of disappearance of hydrocarbon due to reaction with OH radical (Darnall et al. 1976);
photooxidation $t_{1/2}$ = 0.21 d in air, based on an estimated second-order rate constant k = 77.1×10^{-12} cm³ molecule⁻¹ s⁻¹ for the vapor-phase reaction with photochemically produced hydroxyl radicals of 5×10^5 radicals/cm³ in air (Atkinson 1987; quoted, Howard 1990).
Hydrolysis:
Biodegradation:
Biotransformation:
Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants:

Half-Lives in the Environment:

Air: $t_{1/2}$ > 9.9 d for the gas-phase reaction with hydroxyl radicals in air, based on the rate of disappearance of hydrocarbon due to reaction with hydroxyl radical (Darnall et al. 1976);
$t_{1/2}$ = 0.21 d, based on an estimated rate constant k ~ 77.1×10^{-12} cm³ molecule⁻¹ s⁻¹ for the vapor-phase reaction with photochemically produced hydroxyl radicals of 5×10^5 radicals/cm³ in air (Atkinson 1987; quoted, Howard 1990).

TABLE 16.1.2.4.1
Reported vapor pressures of diethylamine at various temperatures

Stull 1947		Bittrich & Kauer 1962		Kilian & Bittrich 1965	
summary of literature data					
t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa
–33.0	1333	31.45	39997	19.73	24718
–22.6	2666	34.75	46663	25.17	31471
–11.3	5333	38.05	53329	30.31	39343
–4.0	7999	41.1	59995	34.99	47596
6.0	13332	43.85	66661	40.22	58582
21.0	26664	46.5	73327		
38.0	53329	48.85	79993		
55.5	101325	51.10	86659		
		53.20	93325		
mp/°C	–38.9	55.53	101325		
		57.05	106658		
		59.00	113324		
		60.58	119990		

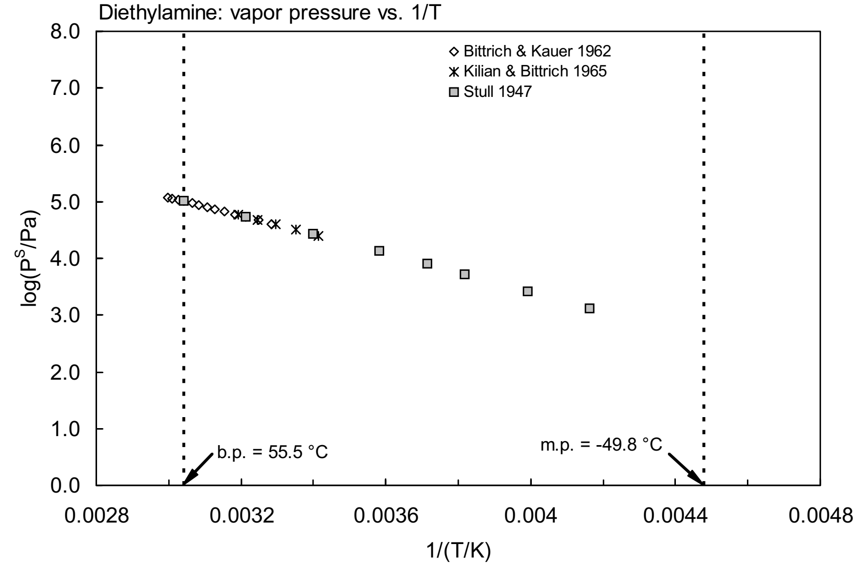
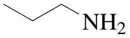


FIGURE 16.1.2.4.1 Logarithm of vapor pressure versus reciprocal temperature for diethylamine.

16.1.2.5 *n*-Propylamine



Common Name: Propylamine
Synonym: 1-aminopropane, 1-propanamine, *n*-propylamine
Chemical Name: aminopropane, *n*-propylamine
CAS Registry No: 107-10-8
Molecular Formula: C_3H_9N, $CH_3CH_2CH_2NH_2$
Molecular Weight: 59.110
Melting Point (°C):
  –84.75 (Lide 2003)
Boiling Point (°C):
  47.22 (Lide 2003)
Density (g/cm^3 at 20°C):
  0.7173 (Dreisbach 1961; Weast 1982–83; Dean 1985; Riddick et al. 1986)
  0.7123 (25°C, Dreisbach 1961)
Molar Volume (cm^3/mol):
  82.4 (liquid molar volume, Kamlet et al. 1986, 1987)
  88.2 (calculated-Le Bas method at normal boiling point)
Dissociation Constant, pK:
  10.74, 10.789 (20°C, Perrin 1972)
  10.71 (pK$_a$, 20°C, Weast 1982–83)
  10.57 (pK$_{BH^+}$, Dean 1985; Riddick et al. 1986)
  10.68 (pK$_a$, Sangster 1989)
Enthalpy of Vaporization, ΔH_V (kJ/mol):
  31.13, 29.73 (25°C, bp, Dreisbach 1961)
  31.26, 29.54 (25°C, bp, Riddick et al. 1986)
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
  10.974 (Riddick et al. 1986)
Entropy of Fusion, ΔS_{fus} (J/mol K):
Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F: 1.0

Water Solubility (g/m^3 or mg/L at 25°C):
  miscible (Dean 1985; Stephenson 1993b)
  miscible (Riddick et al. 1986; Howard 1990; Yaws et al. 1990)

Vapor Pressure (Pa at 25°C and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):
  41800* (interpolated-regression of tabulated data, temp range –64.4 to 48.5°C, Stull 1947)
  41050 (calculated by formula, Dreisbach 1961)
  log (P/mmHg) = 7.2672 – 1218.1/(229.9 + t/°C); temp range –20 to 81°C (Antoine eq. for liquid state, Dreisbach 1961)
  42100* (ebulliometry, calculated-Antoine eq., Osborn & Douslin 1968)
  log (P/mmHg) = 6.92646 – 1044.028/(t/°C + 210.833); temp range 23–77.6°C (ebulliometric method, Antoine eq., Osborn & Douslin 1968)
  log [(P/atm) = [1 – 320.379 ± (T/K)] × 10^{0.922208 – 10.51259 × 10^{-4}·(T/K) + 11.25530 × 10^{-7}·(T/K)^2}, temp range: 34–77.6°C (ebulliometric method, Cox eq., Osborn & Douslin 1968)
  log (P/mmHg) = [–0.2185 × 7408.0/(T/K)] + 7.867998; temp range –64.4 to 214.5°C (Antoine eq., Weast 1972–73)
  32660 (20°C, 31°C, Verschueren 1983)
  38550; 42110 (22.97°C, quoted exptl., calculated-Antoine eq., Boublik et al. 1984)
  log (P/kPa) = 6.05146 – 1044.082/(210.84 + t/°C); temp range 22.97–77.6°C (Antoine eq. from reported exptl. data of Osborn & Douslin 1968, Boublik et al. 1984)
  42120 (calculated-Antoine eq., Dean 1985, 1992)

log (P/mmHg) = 6.92651 – 1044.05/(210.84 + t/°C); temp range: 23–77°C (Antoine eq., Dean l985, 1992)
41050 (Riddick et al. 1986)
log (P/kPa) = 6.05136 – 1044.028/(210.833 + t/°C); temp range not specified (Antoine eq., Riddick et al. 1986)
42120 (interpolated-Antoine eq., Stephenson & Malanowski 1987)
log (P_L/kPa) = 6.04693 – 1041.725/(–62.596 + T/K); temp range 295–351 K (Antoine eq., Stephenson & Malanowski 1987)
42125 (calculated-Cox eq., Chao et al. 1990)
log (P/mmHg) = 24.6420 – 2.3152 × 10^3/(T/K) – 5.8711·log (T/K) – 4.6258 × 10^{-11}·(T/K) + 1.582 × 10^{-6}·$(T/K)^2$; temp range 190–497 (vapor pressure eq., Yaws 1994)

Henry's Law Constant (Pa m^3/mol at 25°C):
1.274 (partial pressure, Butler & Ramchandani 1935)
0.784; 0.732 (exptl.; calculated-group contribution, Hine & Mookerjee 1975)
1.330 (calculated-bond contribution, Hine & Mookerjee 1975)
0.637 (calculated-molecular structure, Russell et al. 1992)
2.01 (gas stripping-GC, Altschuh et al. 1999)

Octanol/Water Partition Coefficient, log K_{OW}:
0.28 (shake flask-GC, Korenman et al. 1973)
0.37, 0.39; 0.31‘ (calculated-f const.; calculated-π const., Rekker 1977)
0.48 (shake flask-GC, pH 13, Yakayama et al. 1985)
0.48 (recommended, Sangster 1989)
0.48 (recommended, Hansch et al. 1995)

Octanol/Air Partition Coefficient, log K_{OA}:

Bioconcentration Factor, log BCF:
–0.886 (estimated-K_{OW}, Lyman et al. 1982; quoted, Howard 1990)

Sorption Partition Coefficient, log K_{OC}:
< 1.699 (soil, estimated-K_{OW}, Lyman et al. 1982; quoted, Howard 1990)

Environmental Fate Rate Constants, k, or Half-Lives, $t_{1/2}$:
Volatilization: using Henry's law constant, $t_{1/2}$ ~ 2.44 d was estimated for a model river 1 m deep flowing at 1 m/s with a wind speed of 3 m/s (estimated, Lyman et al. 1982; quoted, Howard 1990).
Photolysis:
Oxidation: photooxidation $t_{1/2}$ = 12 h in air, based on estimated rate constant k = 3.21 × 10^{-12} cm^3·$molecule^{-1}$·s^{-1} for the vapor-phase reaction with hydroxyl radical of 5 × 10^5/cm^3 at 25°C in the atmosphere (Atkinson 1987; quoted, Howard 1990).
Hydrolysis:
Biodegradation:
Biotransformation:
Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants:

Half-Lives in the Environment:
Air: $t_{1/2}$ = 12 h, based on estimated second-order rate constant of 3.21 × 10^{-12} cm^3·$molecule^{-1}$·s^{-1} for the vapor-phase reaction with hydroxyl radical of 5 × 10^5/cm^3 at 25°C in the atmosphere (Atkinson 1987; quoted, Howard 1990).

TABLE 16.1.2.5.1
Reported vapor pressures of *n*-propylamine at various temperatures

Stull 1947		Osborn & Douslin 1968	
summary of literature data		ebulliometric method	
t/°C	P/Pa	t/°C	P/Pa
–64.4	133.3	22.973	38547
–46.3	666.6	27.750	47359
–37.2	1333	32.564	57803
–27.1	2666	37.414	70109
–16.0	5333	42.304	84525
–9.0	7999	47.229	101325
0.50	13332	52.193	120798
15.0	26664	57.195	143268
31.5	53329	62.235	169052
48.5	101325	67.314	198530
		72.430	232087
mp/°C	–83.0	77.587	270110

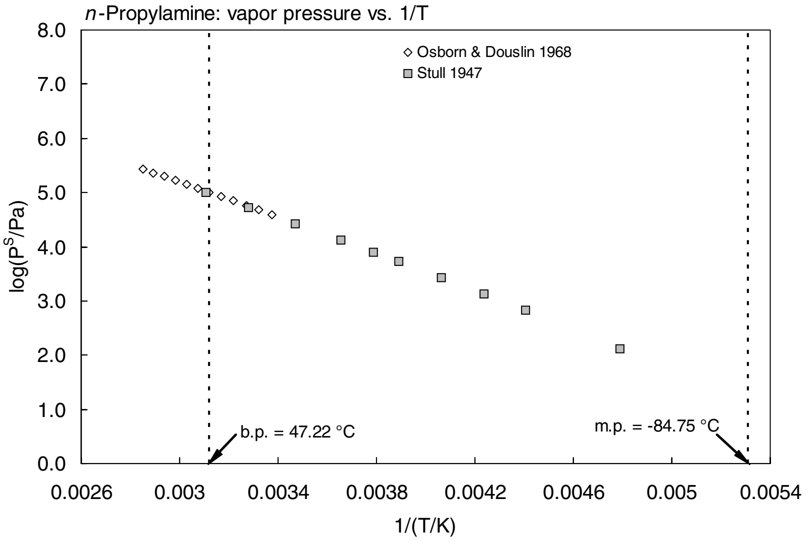
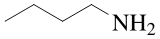


FIGURE 16.1.2.5.1 Logarithm of vapor pressure versus reciprocal temperature for *n*-propylamine.

16.1.2.6 *n*-Butylamine



Common Name: Butylamine
Synonym: 1-aminobutane, *n*-butylamine. 1-butanamine
Chemical Name: 1-aminobutane, *n*-butylamine
CAS Registry No: 109-73-9
Molecular Formula: $C_4H_{11}N$, $CH_3CH_2CH_2CH_2NH_2$
Molecular Weight: 73.137
Melting Point (°C):
  –49.1 (Dreisbach 1961; Riddick et al. 1986; Stephenson & Malanowski 1987; Lide 2003)
Boiling Point (°C):
  77.0 (Lide 2003)
Density (g/cm^3 at 20°C):
  0.7414 (Dreisbach 1961; Weast 1982–83)
  0.7392 (Riddick et al. 1986)
Molar Volume (cm^3/mol):
  98.8 (20°C, calculated-density)
  110.4 (calculated-Le Bas method at normal boiling point)
Dissociation Constant, pK:
  10.77 (Perrin 1965; pK$_a$, 20°C, Weast 1982–83; Howard 1990)
  10.65 (Perrin 1972)
  10.64 (pK$_a$, protonated + 1, Dean 1985; Sangster 1989)
  10.77 (pK$_{BH+}$, Riddick et al. 1986)
Enthalpy of Vaporization, ΔH_V (kJ/mol):
  35.54, 32.11 (25°C, bp, Dreisbach 1961)
  35.74, 31.80 (25°C, bp, Riddick et al. 1986)
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
Entropy of Fusion, ΔS_{fus} (J/mol K):
Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F: 1.0

Water Solubility (g/m^3 or mg/L at 25°C):
  miscible (Dean 1985; Howard 1990; Yaws et al. 1990)
  miscible (Riddick et al. 1986)
  miscible (Stephenson 1993b)

Vapor Pressure (Pa at 25°C and reported temperature dependence equations):
  13850 (Hoy 1970; Abraham 1984)
  12230 (calculated by formula, Dreisbach 1961)
  $\log (P/\text{mmHg}) = 7.213 - 1308.4/(224.2 + t/°C)$; temp range 4–114°C (Antoine eq. for liquid state, Dreisbach 1955)
  9600 (20°C, Verschueren 1983)
  12230 (quoted lit., Riddick et al. 1986; quoted, Howard 1990)
  $\log (P/\text{kPa}) = 6.07009 - 1157.810/(207.80 + t/°C)$; temp range not specified (Antoine eq., Riddick et al. 1986)
  12520 (extrapolated-Antoine eq., Stephenson & Malanowski 1987)
  $\log (P_L/\text{kPa}) = 6.2635 - 1258.745/(-54.49 + T/K)$; temp range 313–350 K (Antoine eq., Stephenson & Malanowski 1987)
  $\log (P/\text{mmHg}) = 25.0711 - 2.5701 \times 10^3/(T/K) - 5.8985 \cdot \log (T/K) + 7.9399 \times 10^{-10} \cdot (T/K) + 1.192 \times 10^{-6} \cdot (T/K)^2$; temp range 124–532 K (vapor pressure eq., Yaws 1994)

Henry's Law Constant (Pa m^3/mol at 25°C):
  1.526 (partial pressure, Butler & Ramchandani 1935)
  1.528 (exptl., Hine & Mookerjee 1975)

1.676, 1.68 (calculated-group contribution, calculated-bond contribution, Hine & Mookerjee 1975)
0.880 (calculated-molecular structure, Russell et al. 1992)
1.785 (gas stripping-GC, Altschuh et al. 1999)

Octanol/Water Partition Coefficient, log K_{OW}:
0.68 (shake flask, Collander 1951)
0.88 (shake flask-titration, Sandell 1962)
0.81 (shake flask, unpublished result, Leo et al. 1971; Hansch & Leo 1987)
0.74 (shake flask-titration, Korenman et al. 1973)
0.90, 0.92; 0.81 (calculated-f const.; calculated-π const., Rekker 1977)
0.80 (inter-lab. shake flask average, Eadsforth & Moser 1983)
0.97 (shake flask-GC, Takayama et al. 1985)
0.86 (recommended, Sangster 1989)
0.97 (recommended, Hansch et al. 1995)

Octanol/Air Partition Coefficient, log K_{OA}:
3.61 (calculated-S_{oct} and vapor pressure P, Abraham et al. 2001)

Bioconcentration Factor, log BCF:
0.505 (calculated-K_{OW}, Lyman et al. 1982; quoted, Howard 1990)

Sorption Partition Coefficient, log K_{OC}:
1.903 (soil, calculated-K_{OW}, Lyman et al. 1982; quoted, Howard 1990)
1.176, 2.021, 2.029 (Podzol soil, Alfisol soil, sediment, von Oepen et al. 1991)
1.880 (soil, quoted exptl., Meylan et al. 1992)
1.780 (soil, calculated-MCI χ and fragment contribution, Meylan et al. 1992)

Environmental Fate Rate Constants, k, or Half-Lives, $t_{1/2}$:

Volatilization: using Henry's law constant, $t_{1/2}$ =1.95 d was predicted for evaporation from a model river 1 m deep, flowing at 1 m/s with a wind velocity of 3 m/s (Lyman et al. 1982; quoted, Howard 1990).

Photolysis:

Oxidation: estimated vapor phase photooxidation $t_{1/2}$ = 0.479 d in air, based on a result of reaction with photochemically produced hydroxyl radical at a concentration of 5×10^5 radicals/cm^3 (USEPA 1986; quoted, Howard 1990).

Hydrolysis:

Biodegradation:

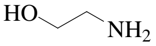
Biotransformation:

Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants:

Half-Lives in the Environment:

Air: estimated vapor phase $t_{1/2}$ = 0.479 d, based on a result of reaction with photochemically produced hydroxyl radical at a concentration of 5×10^5 radicals/cm^3 (USEPA 1986; quoted, Howard 1990).

16.1.2.7 Ethanolamine



Common Name: Ethanolamine
Synonym: β-aminoethyl alcohol, ethylolamine, 2-hydroxyethylamine, β-hydroxyethylamine, monoethanolamine, MEA
Chemical Name: ethanolamine, 2-aminoethanol
CAS Registry No: 141-43-5
Molecular Formula: C_2H_7NO, $HOCH_2CH_2NH_2$
Molecular Weight: 61.098
Melting Point (°C):
10.5 (Lide 2003)
Boiling Point (°C):
171 (Lide 2003)
Density (g/cm^3 at 20°C):
1.0180 (Weast 1982–83)
1.0147 (Riddick et al. 1986)
Molar Volume (cm^3/mol):
60.4 (Stephenson & Malanowski 1987)
73.4 (calculated-Le Bas method at normal boiling point)
Dissociation Constant, pK:
9.48, 9.4994 (Perrin 1972; quoted, Howard 1990)
9.50 (pK_{BH^+}, Riddick et al. 1986)
Enthalpy of Vaporization, ΔH_V (kJ/mol):
92.09, 49.831 (25°C, bp, Riddick et al. 1986)
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
20.50 (Riddick et al. 1986)
Entropy of Fusion, ΔS_{fus} J/mol K:
Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F: 1.0

Water Solubility (g/m^3 or mg/L at 25°C):
miscible (Dean 1985)
miscible (Riddick et al. 1986; quoted, Howard 1990)

Vapor Pressure (Pa at 25°C and reported temperature dependence equations. Additional data at other temperatures deisgnated * are compiled at the end of this section):
893* (65.4°C, Ramsay-Young method, measured range 65.4–170.9°C, Matthews et al. 1950)
log (P/mmHg) = 44.008 – 4089/(T/K) – 11.446 ± log (T/K); temp range 65.4–170.9°C (Kirchhoff eq., ebulliometry, Matthews et al. 1950)
8707* (106.1°C, ebulliometry, measured range 106.1–170.37°C, McDonald et al. 1959)
log (P/mmHg) = 7.7380 –1772.11/(186.25 + t/°C); temp range 106–170°C, or pressure range 65.31–760 mmHg (ebulliometry, McDonald et al. 1959)
53.32 (20°C, Verschueren 1983)
41.64, 46.67 (extrapolated values-Antoine eq., Boublik et al. 1984)
log (P/kPa) = 6.54175 – 1554.149/(171.175 + t/°C); temp range 65.5–170.9°C (Antoine eq. from reported exptl. data, Boublik et al. 1984)
log (P/kPa) = 6.86239 – 1725.168/(185.556 + t/°C); temp range 106.1–170.37°C (Antoine eq. from reported exptl. data, Boublik et al. 1984)
42.51 (extrapolated-Antoine eq., Dean 1985, 1992)
log (P/mmHg) = 7.4568 – 1577.67/(172.37 + t/°C); temp range 65–171°C (Antoine eq., Dean 1985, 1992)
48.0 (Riddick et al. 1986)
log (P/kPa) = 6.86290 – 1732.11/(186.215 + t/°C); temp range not specified (Antoine eq., Riddick et al. 1986)
47.34 (extrapolated-Antoine eq., Stephenson & Malanowski 1987)
log (P_L/kPa) = 6.8629 – 1732.11/(–86.6 + T/K); temp range 310–444 K (liquid, Antoine eq., Stephenson & Malanowski 1987)

34.66 (from Dow Chemical's Handbook, Howard 1990)

$\log (P/\text{mmHg}) = 72.9125 - 5.8595 \times 10^3/(T/K) - 21.914\cdot\log (T/K) - 7.1511 \times 10^{-10}\cdot(T/K) + 5.9841 \times 10^{-6}\cdot(T/K)^2$; temp range 284–638 K (vapor pressure eq., Yaws 1994)

Henry's Law Constant ($Pa\cdot m^3/mol$ at 25°C):

0.0041 (calculated-bond method, Hine & Mookerjee 1975)

Octanol/Water Partition Coefficient, log K_{OW}:

–1.31	(shake flask, Collander 1951)
–1.29; –1.35	(calculated-f const., calculated-π const., Rekker 1977)
–1.31	(recommended, Sangster 1993)
–1.31	(recommended, Hansch et al. 1995)

Octanol/Air Partition Coefficient, log K_{OA}:

Bioconcentration Factor, log BCF:

< 0.0 (estimated-K_{OW}, Lyman et al. 1982; quoted, Howard 1990)

Sorption Partition Coefficient, log K_{OC}:

0.699 (soil, estimated-K_{OW}, Lyman et al. 1982; quoted, Howard 1990)

Environmental Fate Rate Constants, k, or Half-Lives, $t_{1/2}$:

Volatilization:

Photolysis:

Hydrolysis:

Oxidation: photooxidation $t_{1/2}$ = 11 h in air, based on an estimated rate constant k ~ 3.5×10^{-11} cm^3 ± $molecule^{-1}$ s^{-1} for the vapor phase reaction with photochemically produced hydroxyl radical of 5×10^5 radicals/cm^3 in air (Atkinson 1987; quoted, Howard 1990).

Biodegradation:

Biotransformation:

Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants:

Half-Lives in the Environment:

Air: half-life of 11 h, based on an estimated rate constant of 3.5×10^{-11} cm^3 $molecule^{-1}$ s^{-1} for the vapor phase reaction with photochemically produced hydroxyl radical of 5×10^5 radicals/cm^3 in air (Atkinson 1987; quoted, Howard 1990).

TABLE 16.1.2.7.1
Reported vapor pressures of ethanolamine at various temperatures and the coefficients for the vapor pressure equations

$\log P = A - B/(T/K)$ (1) $\ln P = A - B/(T/K)$ (1a)
$\log P = A - B/(C + t/°C)$ (2) $\ln P = A - B/(C + t/°C)$ (2a)
$\log P = A - B/(C + T/K)$ (3)
$\log P = A - B/(T/K) - C\cdot\log(T/K)$ (4)

Matthews et al. 1950				McDonald et al. 1959	
Ramsay-Young method				ebulliometric method	
t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa
65.4	893	137.9	32264	106.1	8707
65.5	947	144.6	42236	108.43	10058
69.5	1160	150.0	54195	112.29	11427
70.0	1253	161.4	73860	114.55	12702
75.4	1760	170.9	100125	116.79	14049
81.1	2320			125.73	20454
86.4	3280	bp/K	444.1	159.79	71862
90.0	3813			169.20	97584
96.4	5440	$\Delta H_V/(kJ\ mol^{-1}) = 46.07$ at bp		170.37	101325
101.7	7146	Kirchhoff, Rankine, Dupre			
105.5	8559	eq. 4	P/mmHg	mp/°C	10.31
112.1	11306	A	44.008	eq. 2	P/mmHg
117.3	14012	B	4809	A	7.7380
125.0	19452	C	11.446	B	173211
132.0	25771			C	186.215

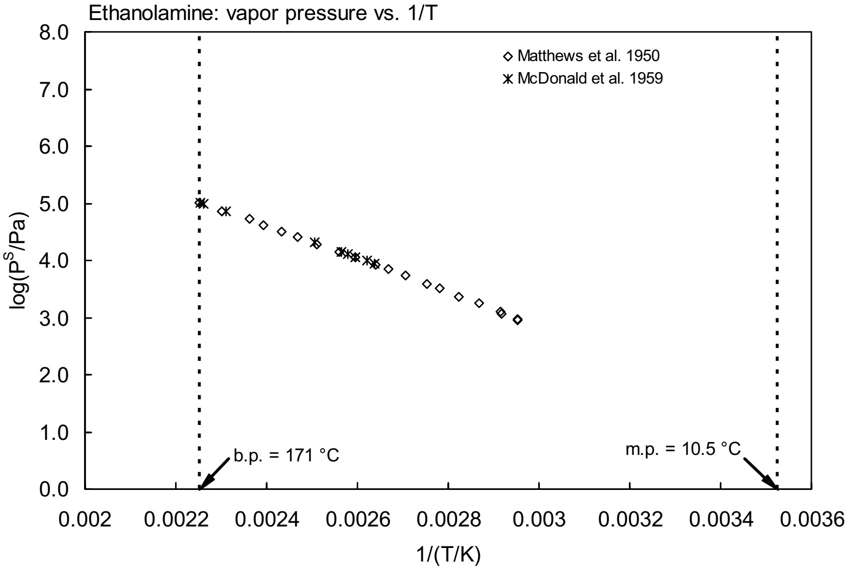
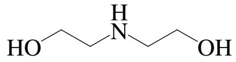


FIGURE 16.1.2.7.1 Logarithm of vapor pressure versus reciprocal temperature for ethanolamine.

16.1.2.8 Diethanolamine



Common Name: Diethanolamine
Synonym: 2,2′-amino-diethanol, 3-aza-1,5-pentanediol, diethylolamine, bis(hydroxyethyl)amine, 2,2′-dihydroxydiethylamine, β,β′-dihydroxydiethylamine, 2,2′-iminobisethanol, 2,2′-iminodiethanol
Chemical Name: diethanolamine
CAS Registry No: 111-42-2
Molecular Formula: $C_4H_{11}NO_2$, $HOCH_2CH_2NHCH_2CH_2OH$
Molecular Weight: 105.136
Melting Point (°C):
28.0 (Weast 1982–83; Dean 1985; Riddick et al. 1986; Stephenson & Malanowski 1987; Lide 2003)
Boiling Point (°C):
268.8 (Lide 2003)
Density (g/cm^3 at 20°C):
1.0966 (Weast 1982–83)
1.0936 (25°C, Riddick et al. 1986)
Molar Volume (cm^3/mol):
96.5 (30°C, Stephenson & Malanowski 1987)
126.7 (calculated-Le Bas method at normal boiling point)
Dissociation Constant, pK:
8.88, 8.97 (Perrin 1972)
8.88 (pK_{BH^+}, Dean 1985; Riddick et al. 1986)
Enthalpy of Vaporization, ΔH_V (kJ/mol):
70.3, 65.229 (25°C, bp, Riddick et al. 1986)
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
25.104 (Riddick et al. 1986)
Entropy of Fusion, ΔS_{fus} (J/mol K):
Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F: 0.934 (mp at 28°C)

Water Solubility (g/m^3 or mg/L at 25°C):
954000 (Verschueren 1983)
964000 (Dean 1985)
954000 (20°C, Riddick et al. 1986)
miscible (from Dow Chemical's Handbook, Howard 1990)

Vapor Pressure (Pa at 25°C and reported temperature dependence equations):
< 1.333 (20°C, Verschueren 1983)
0.040 (extrapolated-Antoine eq., Dean 1985, 1992)
$\log (P/\text{mmHg}) = 8.1388 - 2327.9/(174.4 + t/°C)$; temp range 194–241°C (Antoine eq., Dean 1985, 1992)
0.030 (quoted lit., Riddick et al. 1986)
$\log (P/\text{kPa}) = 7.26458 - 2328.56/(174.399 + t/°C)$; temp range not specified (Antoine eq., Riddick et al. 1986)
$\log (P_L/\text{kPa}) = 7.26044 - 2326.23/(-98.907 + T/K)$; temp range: 423–542 K (liquid, Antoine eq., Stephenson & Malanowski 1987)
0.0373 (quoted from Dow Chemical's Handbook, Howard 1990)
$\log (P/\text{mmHg}) = 122.0877 - 8.8422 \times 10^3/(T/K) - 40.422 \cdot \log (T/K) + 1.4062 \times 10^{-2} \cdot (T/K) + 1.1986 \times 10^{-12} \cdot (T/K)^2$; temp range 301–542 K (vapor pressure eq., Yaws 1994)

Henry's Law Constant (Pa·m^3/mol at 25°C):
5.42×10^{-9} (Hine & Mookerjee 1975)

Octanol/Water Partition Coefficient, log K_{OW}:

–1.43 (shake flask, Collander 1951)
–1.51 (calculated-fragment const., Rekker & De Kort 1979)
–1.43 (recommended, Sangster 1993)
–1.43 (recommended, Hansch et al 1995)

Octanol/Air Partition Coefficient, log K_{OA}:

Bioconcentration Factor, log BCF:

< 0.0 (estimated-K_{OW}, Howard 1990)

Sorption Partition Coefficient, log K_{OC}:

0.602 (soil, estimated-K_{OW}, Howard 1990)

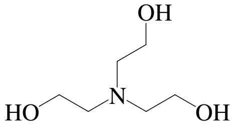
Environmental Fate Rate Constants, k, or Half-Lives, $t_{1/2}$:

Volatilization:
Photolysis:
Hydrolysis:
Oxidation: photooxidation $t_{1/2}$ = 0.72–7.2 h in air, based on estimated rate constant for the reaction with hydroxyl radical in air (Atkinson 1987; quoted, Howard 1990; Howard et al. 1991).
Biodegradation: aqueous aerobic $t_{1/2}$ = 14.4–168 h, based on measured half-life in surface water grab sample experiment (Boethling & Alexander 1979; quoted, Howard et al. 1991) and aqueous aerobic screening test data (Gerike & Fischer 1979; Bridie et al. 1979; quoted, Howard et al. 1991); aqueous anaerobic $t_{1/2}$ = 57.6–672 h, based on estimated unacclimated aqueous aerobic biodegradation half-life (Howard et al. 1991).
Biotransformation:
Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants:

Half-Lives in the Environment:

Air: photooxidation $t_{1/2}$ = 0.72–7.2 h, based on estimated rate constant for the reaction with hydroxyl radical in air (Atkinson 1987; quoted, Howard 1990; Howard et al. 1991);
atmospheric transformation lifetime by reaction with water was estimated to be < 1 d (Kelly et al. 1994).
Surface water: $t_{1/2}$ = 14.4–168 h, based on estimated unacclimated aqueous aerobic biodegradation half-life (Howard et al. 1991).
Groundwater: $t_{1/2}$ = 28.8–336 h, based on estimated unacclimated aqueous aerobic biodegradation half-life (Howard et al. 1991).
Sediment:
Soil: $t_{1/2}$ = 14.4–168 h, based on estimated unacclimated aqueous aerobic biodegradation half-life (Howard et al. 1991).
Biota:

16.1.2.9 Triethanolamine



Common Name: Triethanolamine
Synonym: 2,2′,2″-nitrilotriethanol, 2,2′,2″-nitrilotrisethanol, triethylolamine, trihydroxytriethylamine, trolamine, tris(hydroxyethyl)–amine, TEA
Chemical Name: triethanolamine
CAS Registry No: 102-71-6
Molecular Formula: $C_6H_{15}NO_3$, $(HOCH_2CH_2)_3N$
Molecular Weight: 149.188
Melting Point (°C):
  20.5 (Lide 2003)
Boiling Point (°C):
  335.4 (Dean 1985; Riddick et al. 1986; Stephenson & Malanowski 1987; Lide 2003)
Density (g/cm^3 at 20°C):
  1.1242 (Weast 1982–83; Dean 1985)
  1.1196 (25°C, Riddick et al. 1986)
Molar Volume (cm^3/mol):
  133.3 (Stephenson & Malanowski 1987)
  182.1 (calculated-Le Bas method at normal boiling point)
Dissociation Constant, pK:
  7.92 (Perrin 1972; quoted, Howard 1990)
  7.76 (pK_{BH^+}, Dean 1985; Riddick et al. 1986)
Enthalpy of Vaporization, ΔH_V (kJ/mol):
  67.475 (bp, Riddick et al. 1986)
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
  27.20 (Riddick et al. 1986)
Entropy of Fusion, ΔS_{fus} (J/mol K):
Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F: 1.0

Water Solubility (g/m^3 or mg/L at 25°C):
  miscible (Dean 1985; Howard 1990)
  miscible (Riddick et al. 1986)

Vapor Pressure (Pa at 25°C and reported temperature dependence equations):
  < 1.33 (20°C, Verschueren 1983)
  0.0131 (extrapolated-Antoine eq., Boublik et al. 1984)
  log (P/kPa) = 9.19319 – 4543.817/(297.839 + t/°C), temp range: 252.7–305.6°C (Antoine eq. from reported exptl. data, Boublik et al. 1984)
  0.0100 (extrapolated-Antoine eq., Dean 1985, 1992)
  log (P/mmHg) = 10.0675 – 4542.78/(297.76 + t/°C), temp range: 252–305°C (Antoine eq., Dean l985, 1992)
  < 1.30 (20°C, Riddick et al. 1986)
  log (P/kPa) = 7.67989 – 2962.73/(186.75 + t/°C), temp range not specified (Antoine eq., Riddick et al. 1986)
  log (P_L/kPa) = 9.53861 – 4951.87/(49.99 + T/K), temp range: 523–579 K, (Antoine eq., Stephenson & Malanowski 1987)
  4.79×10^{-4} (quoted from Dow Chemical's Handbook, Howard 1990)
  log (P/mmHg) = 135.3206 –1.0312×10^4/(T/K) –44.637·log (T/K) + 1.4368×10^{-2}·(T/K) – 1.7552×10^{-13}·(T/K)^2; temp range 294–787 K (vapor pressure eq., Yaws 1994)

Henry's Law Constant (Pa·m^3/mol at 25°C):
  3.42×10^{-14} (Hine & Mookerjee 1975)

Octanol/Water Partition Coefficient, log K_{OW}:

–1.32, –1.75	(calculated, Verschueren 1983)
–1.59	(Howard 1990)
–1.00	(recommended, Hansch et al. 1995)

Octanol/Air Partition Coefficient, log K_{OA}:

Bioconcentration Factor, log BCF:

< 0.0	(estimated-K_{OW}, Howard 1990)

Sorption Partition Coefficient, log K_{OC}:

0.477	(soil, estimated-K_{OW}, Howard 1990)

Environmental Fate Rate Constants, k, or Half-Lives, $t_{½}$:

Volatilization:

Photolysis:

Hydrolysis:

Oxidation: photooxidation $t_{½}$ = 4.0 h in air, based on an estimated rate constant k ~ 10.4×10^{-11} $cm^3 \cdot molecule^{-1}$ s^{-1} for the vapor phase reaction with photochemically produced hydroxyl radical of 5×10^5 radicals/cm^3 in air at 25°C (Atkinson 1987; quoted, Howard 1990).

Biodegradation:

Biotransformation:

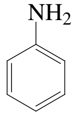
Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants:

Half-Lives in the Environment:

Air: $t_{½}$ = 4.0 h, based on an estimated rate constant k ~ 10.4×10^{-11} cm^3 $molecule^{-1}$ s^{-1} for the vapor phase reaction with photochemically produced hydroxyl radical of 5×10^5 radicals/cm^3 in air at 25°C (Atkinson 1987; quoted, Howard 1990).

16.1.3 AROMATIC AMINES

16.1.3.1 Aniline



Common Name: Aniline
Synonym: phenylamine, aminobenzene, benzeneamine, benzenamine
Chemical Name: aniline
CAS Registry No: 62-53-3
Molecular Formula: $C_6H_5NH_2$
Molecular Weight: 93.127
Melting Point (°C):
–6.02 (Lide 2003)
Boiling Point (°C):
184.1 (Lide 2003)
Density (g/cm^3 at 20°C):
1.02173, 1.01750 (20°C, 25°C, Dreisbach 1955)
1.02173 (20°C, Weast 1982–83)
Molar Volume (cm^3/mol):
91.2 (20°C, calculated-density)
110.2 (calculated-Le Bas method at normal boiling point)
Dissociation Constant, pK$_a$:
4.596 (Perrin 1972; Howard 1989)
4.600 (McLeese et al. 1979; Riddick et al. 1986; Sangster 1989)
4.630 (Weast 1982–83)
4.58, 3.96 (quoted, HPLC, Miyake et al. 1987)
Enthalpy of Vaporization, ΔH_V (kJ/mol):
54.28, 43.17 (25°C, bp, Dreisbach 1955)
55.843, 44.53 (25°C, bp, Riddick et al. 1986)
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
Entropy of Fusion, ΔS_{fus} (J/mol K):
Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F: 1.0

Water Solubility (g/m^3 or mg/L at 25°C):
36650 (Hill & Macy 1924)
36070 (Seidell 1941)
38670 (shake flask-residue volume method, Booth & Everson 1948)
36220 (shake flask-interferometry, Donahue & Bartell 1952)
34100 (Stephen & Stephen 1963)
36600 (Kenaga 1980)
34000 (Verschueren 1983)
56900 (calculated-activity coeff. γ by UNIFAC, Fu & Luthy 1985, 1986)
33800 (selected, Riddick et al. 1986)
34200 (selected, Yaws et al. 1990)

Vapor Pressure (Pa at 25°C and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):
133.3 (43.7°C, static method, measured range 43.7–183.9°C, Kahlbaum 1898)
85.71* (extrapolated-regression of tabulated data, temp range 34.8–184.4°C Stull 1947)
log (P/mmHg) = 7.57170 – 1941.7/(230 + t/°C) (Antoine eq., Dreisbach & Martin 1949)
10351* (112.92°C, ebulliometry, measured range 112.92–183.93°C, Dreisbach & Shrader 1949)
89.52 (calculated by formula, Dreisbach 1955; quoted, Riddick et al. 1986)

log (P/mmHg) = 7.24179 – 1674.3/(200.0 + t/°C); temp range 90–250°C (Antoine eq. for liquid state, Dreisbach 1955)

6806* (102.59°C, ebulliometry, measured range 102.59–185.15°C, McDonald et al. 1959)

log (P/mmHg) = 7.25375 – 1684.35/(201.175 + t/°C, temp range 103–185°C (Antoine eq., ebulliometry, McDonald et al. 1959)

133.3* (31.55°C, calculated-thermodynamic properties, temp range 31.55–184.40°C, Hatton et al. 1962)

log (P/mmHg) = [–0.2185 × 11307.6/(T/K)] + 8.221995; temp range 34.8–422.4°C (Antoine eq., Weast 1972–73)

88.30 (extrapolated-Antoine eq., Boublik et al. 1973)

log (P/mmHg) = 7.3201 – 1731.515/(205.049 + t/°C); temp range 102.6–185.2°C (Antoine eq. from reported exptl. data of McDonald et al.1959, Boublik et al. 1973)

log (P/mmHg) = [–0.2185 × 11307.6/(T/K)] + 8.221995; temp range 34.8–422.4°C (Antoine eq., Weast 1972–73)

82.71 (calculated-Cox eq., Chao et al. 1983)

log (P/atm) = [1– 457.025/(T/K)] × 10^{0.911551 – 6.64936 × 10^{-4}·(T/K) + 5.25455 × 10^{-7}·(T/K)^2}; temp range: 267.3–695.0 K (Cox eq., Chao et al. 1983)

80 ± 6 (gas saturation-HPLC/UV, Sonnefeld et al. 1983)

40.0 (20°C, Verschueren 1983)

88.0, 48.24 (extrapolated-Antoine eq., Boublik et al. 1984)

log (P/kPa) = 6.43196 – 1722.154/(205.002 + t/°C); temp range 102.6–185.2°C (Antoine eq. from reported exptl. data, Boublik et al. 1984)

log (P/kPa) = 5.68977 – 1234.569/(151.207 + t/°C); temp range 112.9–183.9°C (Antoine eq. from reported exptl. data, Boublik et al. 1984)

65.18 (Daubert & Danner 1985)

89.30 (extrapolated-Antoine eq., Dean 1985, 1992)

log (P/mmHg) = 7.32010 – 1731.515/(206.049 + t/°C); temp range 102–185°C (Antoine eq., Dean l985, 1992)

log (P/kPa) = 5.69066 – 1941.7/(230.0 + t/°C), temp range not specified (Antoine eq., Riddick et al. 1986)

89.60 (calculated-Antoine eq., Stephenson & Malanowski 1987)

log (P_L/kPa) = 6.40627 – 1702.817/(–70.155 + T/K); temp range 304–458 K (Antoine eq.-I, Stephenson & Malanowski 1987)

log (P_L/kPa) = 8.1019 – 2728/(T/K); temp range 273–338 K (Antoine eq.-II, Stephenson & Malanowski 1987)

log (P_L/kPa) = 6.41147 – 1708.239/(–69.454 + T/K); temp range 373–458 K (Antoine eq.-III, Stephenson & Malanowski 1987)

log (P_L/kPa) = 6.44338 – 1682.348/(–78.065 + T/K); temp range: 455–523 K (Antoine eq.-IV, Stephenson & Malanowski 1987)

86.70 (calculated-Cox eq., Chao et al. 1990)

log (P/mmHg) =124.3764 –7.1676 × 10^3/(T/K) –42.763·log (T/K) + 1.7336 × 10^{-2}·(T/K) + 5.7138 × 10^{-15}·(T/K)^2; temp range 267–699 K (vapor pressure eq., Yaws 1994)

Henry's Law Constant (Pa·m^3/mol at 25°C):

13778 (Hakuta et al. 1977)

12.16 (measured, Yoshida et al. 1983)

0.193 (gas stripping-GC, Altschuh et al. 1999)

Octanol/Water Partition Coefficient, log K_{OW}:

0.90 (shake flask-UV, Fujita et al. 1964)

0.90 (shake flask, Iwasa et al. 1965)

0.90 (shake flask-UV, Hansch et al. 1968)

0.90 (Leo et al. 1971; Hansch & Leo 1979; Hansch & Leo 1983, Hansch & Leo 1985)

0.89 (shake flask-UV at pH 5.6, Umeyama et al. 1971)

0.90 (HPLC-k′ correlation, Carlson et al. 1975)

0.85 (shake flask, Lu & Metcalf 1975)

0.90 (HPLC-RT correlation, Mirrlees et al. 1976)

0.93 ± 0.05 (shake flask at pH 7, Unger et al. 1978)

0.90, 0.98, 0.85 (shake flask, Hansch & Leo 1979)

0.91 (HPLC-k′ correlation, Könemann et al. 1979)

0.90 (shake flask-UV, Briggs 1981)

1.03 (RP-HPLC-k′ correlation, D'Amboise & Hanai 1982)
0.90 (HPLC-k′ correlation, Hammers et al. 1982)
0.90 (inter-laboratory studies. shake flask average, Eadsforth & Moser 1983)
1.09 (inter-laboratory studies, HPLC-RT correlation, average, Eadsforth & Moser 1983; Brooke et al. 1990)
1.34, 1.27, 1.08 (HPLC-RT correlation, Harnish et al. 1983)
1.08 (shake flask average, OECD/EEC lab. comparison tests, Harnish et al. 1983)
0.79, 0.96 (HPLC-RV correlation-ALPM, Garst & Wilson 1984)
0.89 (shake flask-UV at pH 7.4, El Tayar et al. 1984)
0.99 (calculated-activity coeff. γ from UNIFAC, Campbell & Luthy 1985)
0.81, 1.08 (HPLC-k′ correlation, Eadsforth 1986)
0.91 (RP-HPLC-RT correlation, Eadsforth 1986)
0.98 (shake flask-UV at pH 7.5, Martin-Villodre et al. 1986)
0.93 (HPLC method average, Ge et al. 1987)
0.78 (HPLC-k′ correlation, Miyake et al. 1987)
1.18 (calculated-activity coeff. γ from UNIFAC, Banerjee & Howard 1988)
0.940 ± 0.006 (shake flask/slow-stirring-GC, De Bruijn et al. 1989)
0.90 (recommended, Sangster 1989, 1993)
0.942 ± 0.010; 0.940 ± 0.006 (shake flask/stir-flask method by BRE; RITOX, inter-laboratory studies, Brooke et al. 1990)
0.90 (shake flask-GC, Alcorn et al. 1993)
1.21, 0.89, 0.87, 1.09 (HPLC-k′ correlation, different combinations of stationary and mobile phases under isocratic conditions, Makovskaya et al. 1995)
0.92 (shake flask-dialysis tubing-HPLC/UV, both phases, Andersson & Schrăder 1999)
0.88 (microemulsion electrokinetic chromatography-retention factor correlation, Jia et al. 2003)

Octanol/Air Partition Coefficient, log K_{OA}:

Bioconcentration Factor, log BCF:
0.78 (fish, Lu & Metcalf 1975)
0.30 (calculated-S, Kenaga 1980)
< 1.0 (fish, Freitag et al. 1982)
< 1.0, 0.602, 3.01 (golden orfe, algae, activated sludge, Freitag et al. 1982)
0.602 (alga *Chlorella fusca*, wet wt. basis, Geyer et al. 1984)
0.845 (alga *Chlorella fusca*, calculated-K_{OW}, Geyer et al. 1984)
< 1.0, < 1.0, 2.70 (golden ide, algae, activated sludge, Freitag et al. 1985)
2.77 (*Daphnia magna*, based on elimination phase, Dauble et al. 1986)
1.87 (*Daphnia magna*, based on ^{14}C and exposure water, Dauble et al. 1986)
0.70 (fish, correlated-K_{OW}, Isnard & Lambert 1988)
0.78 (quoted, Isnard & Lambert 1988, 1989)
0.41 (zebrafish, Kalsch et al. 1991)
0.41 (zebrafish, Zok et al. 1991)
0.41; 1.04, –0.87, 0.03 (quoted exptl.; calculated values-K_{OW}, Bintein et al. 1993)

Sorption Partition Coefficient, log K_{OC}:
3.11; 2.11 (H-montmorillonite at pH 8.35; pH 6.80, Bailey et al. 1968)
1.86 (soil average, Moreale & Van Bladel 1976)
1.41 (average of seven agricultural soils, Briggs 1981)
3.59 (colloidal organic carbon/ground water, Means et al.1982)
2.11; 2.61 (soil; more acidic soil, Pillai et al. 1982)
2.49; 2.11 (nonsterile Hagerstown soil; sterile Hagerstown soil, Pillai et al. 1982)
2.96; 2.61 (nonsterile Palouse soil; sterile Palouse soil, Pillai et al. 1982)
1.17 (soil, quoted as log K_{OM}, Sabljic 1987)
2.12, 2.05, 2.06 (calculated values: Podzol soil, Alfisol soil, sediment, von Oepen et al. 1991)
0.596 (calculated-K_{OW}, Kollig 1993)

1.08, 1.25, 0.98 (RP-HPLC-k′ correlation on 3 different stationary phases, Szabo et al. 1995)
1.41 (soil, calculated-MCI $^1\chi$, Sabljic et al. 1995)
2.07; 1.65 (HPLC-screening method; calculated-PCKOC fragment method, Müller & Kördel 1996)
2.70, 1.64, 2.08, 2.04, 2.29 (first generation Eurosoils ES-1, ES-2, ES-3, ES-4, ES-5, shake flask-batch equilibrium-HPLC/UV, Gawlik et al. 1998)
2.384, 1.503, 1.279, 1.437, 2.136 (second generation Eurosoils ES-1, ES-2, ES-3, ES-4, ES-5, shake flask-batch equilibrium-HPLC/UV and HPLC-k′ correlation, Gawlik et al. 2000)
1.0–1.54 (5 soils, pH 2.8–7.2, batch equilibrium-sorption isotherm, Li et al. 2000)

Environmental Fate Rate Constants, k, or Half-Lives, $t_{½}$:

Volatilization: estimated $t_{½}$ = 12 d from a measured Henry's law constant of 1.2×10^{-4} atm m^3 mol^{-1} (Yoshida et al. 1983; quoted, Howard 1989) for a model river of 1-m deep with a 1 m/s current and a 3 m/s wind (Lyman et al. 1982; quoted, Howard 1989);
volatilization $t_{½}$(calc) = 55 d (Toräng et al. 2002).

Photolysis: first-order rate constants for photosensitized reactions in water with various humic substances as sensitizers: k = 0.17 h^{-1} with aquatic humus from Aucilla River, k = 0.12 h^{-1} with Aldrich humic acid, k = 0.091 h^{-1} with Fluka humic acid and k = 0.11 h^{-1} with Contech fulvic acid in sunlight, corresponding to half-lives of 4 to 8 h (Zepp et al. 1981); photolysis $t_{½}$ = > 50 yr at 15°C and a pH 5–9 (Toräng et al. 2002).

Oxidation: rate constant k; for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO3} with NO_3 radical and k_{O3} with O_3 or as indicated, *data at other temperatures and/or the Arrhenius expression see reference:
k = 1×10^4 M^{-1} s^{-1} for oxidation by RO_2 radical at 30°C in aquatic systems with $t_{½}$ = 0.8 d (Howard 1972; Hendry et al. 1974; quoted, Mill 1982)
k < 2×10^2 M^{-1} s^{-1} for oxidation by singlet oxygen at 25°C in aquatic systems with $t_{½}$ > 100 yr (Foote 1976; Mill 1979; quoted, Mill 1982)
k_{OH} = 1.20×10^{-10} cm^3 molecule^{-1} s^{-1}, k_{OH}(av.) = 1.17×10^{-10} cm^3 molecule^{-1} s^{-1} at 296 K (flash photolysis -RF, Rinke & Zetzsch 1984; Witte et al. 1986)
k_{OH}* = 1.10×10^{-10} cm^3 molecule^{-1} s^{-1} at 298 K, measured range: 239–362 K (flash photolysis-resonance fluorescence, Witte et al. 1986)
k_{OH}(calc) = 1.54×10^{-10} cm^3·molecule^{-1} s^{-1} at room temp. (Atkinson et al. 1985)
k_{OH}(obs) ≈ 6.0×10^{-11} cm^3 molecule^{-1} s^{-1}; k_{OH}(calc.) = 1.16×10^{-10} cm^3 molecule^{-1} s^{-1} at room temp. (Atkinson 1985)
k_{OH}(calc) = 1.36×10^{-10} cm^3 molecule^{-1} s^{-1}, k_{OH}(obs.) = 1.17×10^{-10} cm^3 molecule^{-1} s$^{-1,}$ (SAR structure-activity relationship, Atkinson 1987)
k_{OH}*(exptl) = 1.18×10^{-10} cm^3 molecule^{-1} s^{-1} at 296 ± 2 K, measured range: 265–455 K; and k_{O3} = 1.12×10^{-18} cm^3 molecule^{-1} s^{-1} at 296 ± 2 K (relative rate method, Atkinson et al. 1987)
k_{OH}* = 1.11×10^{-10} cm^3 molecule^{-1} s^{-1} at 298 K (recommended, Atkinson 1989)
k_{OH}(calc) = 1.385×10^{-10} cm^3 molecule^{-1} s^{-1} (molecular orbital calculations, Klamt 1993)

Hydrolysis:

Biodegradation: completely degraded by a soil inoculum in 4 d (Alexander & Lustigman 1966; quoted, Verschueren 1983; Howard 1989);
completely degraded in 20 d by bacteria in river mud (Calamari et al. 1980; quoted, Howard 1989);
k = 0.23 d^{-1} and corresponding to a $t_{½}$ = 3 d in samples of White Lake water at 29°C (Subba-Rao et al. 1982);
average rate of biodegradation k = 19.0 mg COD g^{-1} h^{-1} for 94.5% removal (Scow 1982);
biodegradation $t_{½}$ = 4.5 d in unpolluted and $t_{½}$ < 0.5 d in polluted pond water as model environments (Lyons et al. 1984);
0.46 mM aniline solution degraded by strain Ani1 within 14 d in water (Schnell et al. 1989);
average exptl. k = 0.044 h^{-1} compared to the group-contribution method predicted rate constants of 0.050 h^{-1} (nonlinear) and 0.018 h^{-1} (Tabak & Govind 1993);
first-order k = 1.0 d^{-1} for batch expt. with Elbe water at 20°C (Börnick et al. 2001);
field first-order degradation k ~ 1.8 d^{-1} for 2 different dates with water temperatures of 21.9 and 14.7°C, respectively, in Rhine river and rate constant obtained in laboratory shake flask batch tests with Rhine water averaged 1.5 d^{-1} at 15°C and 2.0 d^{-1} at 20°C (Toräng et al. 2002).

Biotransformation: mean bacteria transformation rate constant for all three sites of $(1.1 \pm 0.8) \times 10^{-11}$ L·organism^{-1}·h^{-1} (Paris & Wolfe 1987; quoted, Steen 1991).

Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants:

$k_1 = 0.052 \pm 0.0067$ h^{-1}; $k_2 = 7.200 \pm 1.3000$ h^{-1} (Kalsch et al. 1991)

$k_1 = 11.10 \pm 3.2000$ h^{-1} (zebrafish, Zok et al. 1991)

Half-Lives in the Environment:

Air: atmospheric lifetimes of 2.3 h in clean troposphere and 1.2 h in moderately polluted atmosphere, based on gas-phase reaction with hydroxyl radical at room temp.; atmospheric lifetimes of 15.0 d in clean troposphere and 5.0 d in moderately polluted atmosphere, based on gas-phase reaction with O_3 at room temp. (Atkinson et al. 1987)

$t_{1/2}$ ~ 3.3 h, based on reaction with photochemically produced hydroxyl radical (Howard 1989); atmospheric transformation lifetime was estimated to be < 1 d (Kelly et al. 1994).

Surface water: estimated $t_{1/2}$ = 2.3 d in Rhine river in case of a first order reduction process (Zoeteman et al. 1980; quoted, Howard 1989);

estimated $t_{1/2}$ = 0.3–3.0 d in river waters (Zoeteman et al. 1980);

$t_{1/2}$ = 4 to 8 h in May sunlight with both commercial humic acids and aquatic humus as photosensitizers near-surface water and $t_{1/2}$ ~ 1 wk in distilled water (Zepp et al. 1981);

$t_{1/2}$ = 6 d in eutropic pond and $t_{1/2}$ = 21 d in an oligotrophic lake (Subba-Rao et al. 1982; quoted, Howard 1989);

biodegradation $t_{1/2}$ = 4.5 d in unpolluted and $t_{1/2}$ < 0.5 d in polluted pond water as model environments (Lyons et al. 1984);

$t_{1/2}$ = 4–33 d at 15°C (Ingerslev & Nyholm 2000);

$t_{1/2}$ ~ 9 h in the Rhine river at 15 and 22°C (Toräng et al. 2002).

Ground water: estimated $t_{1/2}$ ~ 30–300 d (Zoeteman et al. 1980).

Sediment:

Soil:

Biota:

TABLE 16.1.3.1.1
Reported vapor pressures of aniline at various temperatures and the coefficients for the vapor pressure equations

$\log P = A - B/(T/K)$ (1) $\ln P = A - B/(T/K)$ (1a)
$\log P = A - B/(C + t/°C)$ (2) $\ln P = A - B/(C + t/°C)$ (2a)
$\log P = A - B/(C + T/K)$ (3)
$\log P = A - B/(T/K) - C \cdot \log (T/K)$ (4)

Stull 1947		**Dreisbach & Shrader 1949**		**McDonald et al. 1959**		**Hatton et al. 1962**	
summary of literature data		**ebulliometry**		**ebulliometry**		**calc-thermodynamic properties**	
t/°C	**P/Pa**	**t/°C**	**P/Pa**	**t/°C**	**P/Pa**	**t/°C**	**P/Pa**
34.8	133.3	112.92	10351	102.59	6806	31.55	133.3
57.9	666.6	125.16	17039	117.22	12295	41.82	666.6
69.4	1333	153.2	42103	137.5	25439	52.59	1333
82.0	2666	168.21	67701	160.08	51913	68.62	2666
96.7	5333	183.93	101325	182.4	97103	82.11	5333
106.0	7999			184.24	101912	97.02	7999
119.9	13332	bp/°C	183.93	185.15	104589	119.41	13332
140.1	26664					138.90	26664
161.9	53329			mp/°C	–6.02	161.05	53329
184.4	101325					184.40	101325
				eq. 2	P/mmHg		
mp/°C	–6.2			A	7.25375		
				B	1684.35		
				C	201.175		

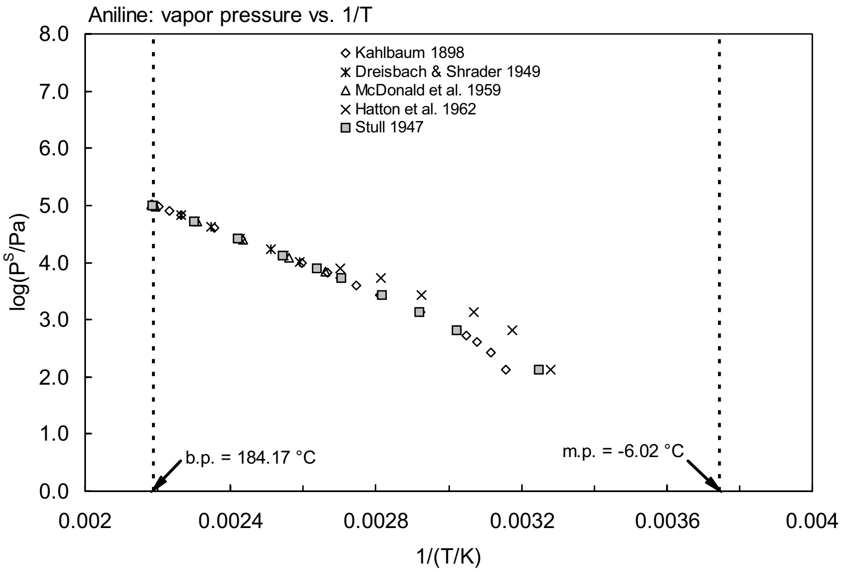
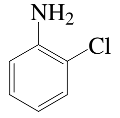


FIGURE 16.1.3.1.1 Logarithm of vapor pressure versus reciprocal temperature for aniline.

16.1.3.2 2-Chloroaniline



Common Name: 2-Chloroaniline
Synonym: 1-amino-2-chlorobenzene, *o*-aminochlorobenzene, *o*-chloroaniline, 2-chlorophenylamine
Chemical Name: 1-amino-2-chlorobenzene, *o*-chloroaniline, 2-chloroaniline
CAS Registry No: 95-51-2
Molecular Formula: $C_6H_4NH_2Cl$
Molecular Weight: 127.572
Melting Point (°C):
−1.94 (β-2-chloroaniline, Dreisbach 1955; Weast 1872–83, Riddick et al. 1986)
−14.0 (α-2-chloroaninline, Weast 1982–83; Verschueren 1983; Howard 1989)
−1.9 (Lide 2003)
Boiling Point (°C):
208.8 (Kahlbaum 1898; Stull 1947; Dreisbach 1955; Weast 1982–83; Lide 2003)
Density (g/cm^3 at 20°C):
1.21266, 1.20787 (20°C, 25°C, Dreisbach 1955)
1.21251, 1.20775 (20°C, 25°C, Riddick et al. 1986)
Molar Volume (cm^3/mol):
105.2 (20°C, Stephenson & Malanowski 1987)
131.1 (calculated-Le Bas method at normal boiling point)
Dissociation Constant, pK_a:
2.661 (Perrin 1972; quoted, Howard 1989)
2.650 (Weast 1982–83)
2.640 (protonated cation + 1, Dean 1985)
2.640 (Riddick et al. 1986)
Enthalpy of Vaporization, ΔH_V (kJ/mol):
57.5 ± 5 (25°C, Piacente et al. 1985)
56.756, 44.35 (25°C, bp, Riddick et al. 1986)
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
11.88 (Riddick et al. 1986)
Entropy of Fusion, ΔS_{fus} (J/mol K):
Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F: 1.0

Water Solubility (g/m^3 or mg/L at 25°C or as indicated):
8760 (Dreisbach 1955)
3765 (20°C, shake flask-GC, Chiou 1981; Chiou & Schmedding 1981; Chiou et al. 1982)
3763 (calculated-K_{OW}, Müller & Klein 1992)
4740 (calculated-group contribution method, Kühne et al. 1995)

Vapor Pressure (Pa at 25°C or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):
40.31* (extrapolated-regression of tabulated data, measured range 64.4–208.8°C, Kahlbaum 1898)
37.77* (extrapolated-regression of tabulated data, temp range 46.3–208.8°C, Stull 1947)
log (P/mmHg) = 7.63311 – 2085.5/(230 + t/°C) (Antoine eq., Dreisbach & Martin 1949)
7605* (124.48°C, ebulliometry, measured range 124.48–208.84°C, Dreisbach & Shrader 1949)
33.77 (calculated by formula, Dreisbach 1955; selected, Riddick et al. 1986)
log (P/mmHg) = 7.19240 – 1762.74/(200.0 + t/°C); temp range 110–330°C (Antoine eq. for liquid state, Dreisbach 1955)
log (P/mmHg) = [–0.2185 × 12441.0/(T/K)] + 8.56946; temp range 46.3–208.8°C (Antoine eq., Weast 1972–73)
33.88 (calculated-Antoine eq., Dean 1985, 1992)

log (P/mmHg) = 7.56265 – 1998.6/(220.0 + t/°C), temp range 20–108°C (Antoine eq., Dean 1985, 1992)
log (P/mmHg) = 7.19240 – 1762.74/(200.0 + t/°C), temp range: 108–300°C (Antoine eq., Dean 1985, 1992)
35.30* (torsion-weighing effusion, Piacente et al. 1985)
log (P/kPa) = (8.63 ± 0.16) – (3006 ± 56)/(T/K); temp range: 287–336 K (Antoine eq., combined torsion-weighing effusion, Piacente et al. 1985)
log (P/kPa) = 6.75801 – 2085.50/(230.0 + t/°C); temp range not specified (Antoine eq., Riddick et al. 1986)
18.97 (extrapolated-Antoine eq., Stephenson & Malanowski 1987)
log (P_L/kPa) = 5.84227 – 1432.2/(–108.81 + T/K); temp range 397–482 K (Antoine eq., Stephenson & Malanowski 1987)
log (P/mmHg) = 90.6491 – 6.041 × 10^3/(T/K) – 31.118·log (T/K) + 1.1564 × 10^{-2}·(T/K) + 4.8388 × 10^{-13}·$(T/K)^2$; temp range 271–722 K (vapor pressure eq., Yaws 1994)

Henry's Law Constant (Pa·m^3/mol at 25°C):
0.760 (calculated-P/C, Howard 1989)
0.425 (calculated-P/C, Meylan & Howard 1991)
0.143 (estimated-bond contribution, Meylan & Howard 1991)

Octanol/Water Partition Coefficient, log K_{OW}:
1.81 (shake flask, Fujita et al. 1964)
1.90 (Leo et al. 1971; Hansch & Leo 1979; Hansch & Leo 1985)
1.92 (exptl., Leo et al. 1971; McCall 1975; Rekker 1977)
1.92 (HPLC-k′ correlation, Carlson et al. 1975)
1.63 (calculated-π const., Norrington et al. 1975)
1.61, 1.73 (calculated-π const., calculated-f const., Rekker 1977)
1.90, 1.92 (shake flask, Hansch & Leo 1979)
1.74 (HPLC-k′ correlation, Könemann et al. 1979)
1.74 (calculated-f const., Rekker & De Kort 1979)
1.91 ± 0.01 (HPLC-k′, Hammers et al. 1982)
1.99 (HPLC-k′ correlated, Hammers et al. 1982)
1.926 ± 0.021 (slow-stirring-GC, De Bruijn et al. 1989)
1.88 (recommended, Sangster 1993)
1.93 ± 0.14, 1.55 ± 0.51 (solvent generated liquid-liquid chromatography SGLLC-correlation, RP-HPLC-k′ correlation, Cichna et al. 1995)
1.90 (recommended, Hansch et al. 1995)

Octanol/Air Partition Coefficient, log K_{OA}:

Bioconcentration Factor, log BCF:
< 2.0 (Kawasaki 1980)
1.30 (estimated, Canton et al. 1985)
1.18 (zebrafish, Zok et al. 1991)
0.301–0.57 (carp, Tsuda et al. 1993)
1.18; 1.56, 0.73, 0.94 (quoted; calculated values-K_{OW}, Bintein et al. 1993)

Sorption Partition Coefficient, log K_{OC}:

Environmental Fate Rate Constants, k, or Half-Lives, $t_{1/2}$:
Volatilization: using Henry's law constant, $t_{1/2}$ ~ 5.6 d was estimated for a model river of 1-m deep (Lyman et al. 1982; quoted, Howard 1989);
estimated $t_{1/2}$ = 64 d from a representative environmental pond (stagnant) (USEPA 1987; quoted, Howard 1989).
Photolysis:
Oxidation: rate constant of 5.1 × 10^{-12} cm^3/molecule·s for the reaction with hydroxyl radical in a typical ambient atmosphere at 25°C with $t_{1/2}$ ~ 2 d (GEMS 1987; quoted, Howard 1989).
Hydrolysis:
Biodegradation: average biodegradation rate of 25 mg COD g^{-1} h^{-1} for 95.6% removal (Scow 1982).

Biotransformation:

Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants:

$k_1 = 7.10\ h^{-1}$ (zebrafish, Zok et al. 1991)

$k_2 = 0.19\ h^{-1}$ (carp, Tsuda et al. 1993)

Half-Lives in the Environment:

Air: estimated atmospheric $t_{1/2} = 2$ d, based on the reaction with sunlight-produced hydroxyl radical (GEMS 1987; quoted, Howard 1989).

Surface water:

Groundwater:

Sediment:

Soil:

Biota: $t_{1/2} = 3.6$ h in carp with excretion rate constant $k = 0.19\ h^{-1}$ (Tsuda et al. 1993).

TABLE 16.1.3.2.1
Reported vapor pressures of 2-chloroaniline at various temperatures and the coefficients for the vapor pressure equations

$\log P = A - B/(T/K)$ (1) $\ln P = A - B/(T/K)$ (1a)

$\log P = A - B/(C + t/°C)$ (2) $\ln P = A - B/(C + t/°C)$ (2a)

$\log P = A - B/(C + T/K)$ (3)

$\log P = A - B/(T/K) - C \cdot \log (T/K)$ (4)

Kahlbaum 1898		**Stull 1947**		**Piacente et al. 1985**		**Piacente et al. 1985**	
static method		**summary of literature data**		**torsion-weighing effusion**		**torsion-weighing effusion**	
t/°C	**P/Pa**	**t/°C**	**P/Pa**	**t/°C**	**P/Pa**	**t/°C**	**P/Pa**
				run 62	average		average
64.4	400	46.3	133.3	14	18	23	36
72.3	666.6	72.3	666.6	20	32	24	41
84.8	1333	84.8	1333	27	45	28	50
92.9	2000	99.2	2666	32	72	30	66
99.2	2666	115.6	5333	34	96	31	62
104.2	3333	125.7	7999	34.5	86	32	83
108.4	4000	139.5	13332	38	117	34	87
112.0	4666	160.0	26664	43	200	35	90
115.2	6333	183.7	53329	34	203	38	112
118.1	6000	208.8	101325	48.5	251	41	167
120.7	6666			52.5	347	43	190
131.4	9999	mp/°C	-	54	362	45	200
139.5	13332			63	505	47	218
160.0	26664					49	269
173.6	39997	**Dreisbach & Shrader 1949**				51	275
183.7	53329	**ebulliometry**				51	309
192.0	66661	**t/°C**	**P/Pa**			55	343
199.4	79993					56	354
208.8	101325	124.48	7605			57	398
		131.54	10114				
		145.3	16500			overall vapor pressure eq.	
		154.55	42066			eq. 1	P/kPa
		192.71	67661			A	8.63 ± 0.16
		208.84	101325			B	3006 ± 56
						$\Delta H_V/(kJ\ mol^{-1}) = 57.5 \pm 5$ at 25°C	

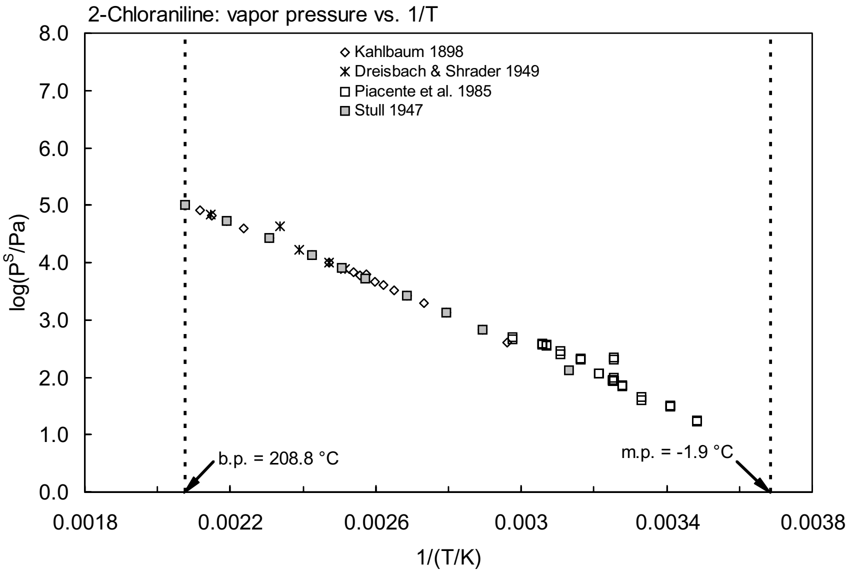
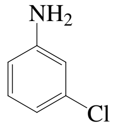


FIGURE 16.1.3.2.1 Logarithm of vapor pressure versus reciprocal temperature for 2-chloroaniline.

16.1.3.3 3-Chloroaniline



Common Name: 3-Chloroaniline
Synonym: 1-amino-3-chlorobenzene, *m*-chloroaniline, 3-chlorophenylamine
Chemical Name: 1-amino-3-chlorobenzene, *m*-chloroaniline, 3-chloroaniline
CAS Registry No: 108-42-9
Molecular Formula: $C_6H_4NH_2Cl$
Molecular Weight: 127.572
Melting Point (°C):
–10.28 (Lide 2003)
Boiling Point (°C):
230.5 (Lide 2003)
Density (g/cm^3 at 20°C):
1.21606 (20°C, Weast 1982–83)
1.2150 (22°C, Dean 1985; Budavari 1989)
Molar Volume (cm^3/mol):
105.0 (22°C, calculated-density, Stephenson & Malanowski 1987)
131.1 (calculated-Le Bas method at normal boiling point)
Dissociation Constant, pK_a:
3.52 (Perrin 1972)
3.50 (McLeese et al. 1979)
3.46 (Weast 1982–83)
3.52 (protonated cation + 1, Dean 1985)
Enthalpy of Vaporization, ΔH_V (kJ/mol):
61.04, 46.016 (25°C, bp, Dreisbach 1955)
60.9 ± 5 (25°C, Piacente et al. 1985)
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
10.25 (Dreisbach 1955)
Entropy of Fusion, ΔS_{fus} (J/mol K):
Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F: 1.0

Water Solubility (g/m^3 or mg/L at 25°C):
5442 (20°C, shake flask-GC, Chiou 1981; Chiou & Schmedding 1981; Chiou et al. 1982)
5447 (calculated-K_{OW}, Müller & Klein 1992)
4740 (calculated-group contribution method, Kühne et al. 1995)

Vapor Pressure (Pa at 25°C and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):
13.14* (extrapolated-regression of tabulated data, measured range 81.7–228.5°C, Kahlbaum 1898)
11.94* (extrapolated-regression of tabulated data, temp range 63.5–228.5°C, Stull 1947)
11.17 (calculated by formula, Dreisbach 1955)
log (P/mmHg) = 7.23603 – 1857.75/(196.64 + t/°C); temp range 125–350°C (Antoine eq. for liquid state, Dreisbach 1955)
log (P/mmHg) = [–0.2185 × 133854.6/(T/K)] + 8.761546; temp range 63.5–228.5°C (Antoine eq., Weast 1972–73)
11.06 (calculated-Antoine eq., Dean 1985, 1992)
log (P/mmHg) = 7.59939 – 2073.75/(215.0 + t/°C), temp range 15–125°C (Antoine eq., Dean 1985, 1992)
log (P/mmHg) = 7.23603 – 1857.75/(196.64 + t/°C), temp range 125–310°C (Antoine eq., Dean 1985, 1992)
15.60* (torsion-weighing effusion, Piacente et al. 1985)

log (P/kPa) = (8.86 ± 0.10) – (3180 ± 40)/(T/K); temp range ~290–345 K (Antoine eq., combined torsion-weighing effusion, Piacente et al. 1985)
9.530 (extrapolated from Antoine eq., Stephenson & Malanowski 1987)
log (P_L/kPa) = 6.36093 – 1857.75/(–76.51 + T/K); temp range 398–573 K (Antoine eq., Stephenson & Malanowski 1987)
log (P/mmHg) = 65.6033 – 5.3779 × 10^3/(T/K) –20.518·log (T/K) + 6.7861 × 10^{-3}·(T/K) + 2.1167 × 10^{-13}·$(T/K)^2$; temp range 263–751 K (vapor pressure eq., Yaws 1994)

Henry's Law Constant (Pa·m^3/mol at 25°C):
0.223 (calculated-P/C)
0.102 (gas stripping-GC, Altschuh et al. 1999)

Octanol/Water Partition Coefficient, log K_{OW}:
1.88 (shake flask-UV, Fujita et al. 1964)
1.88 (Ichikawa et al. 1969)
1.88 (Leo et al. 1971; Hansch & Leo 1979)
1.90 (exptl., Leo et al. 1971; Rekker 1977)
1.98 (calculated-π const., Norrington et al. 1975)
1.73, 1.75; 1.61 (calculated-f const., calculated-π const., Rekker 1977)
1.90, 1.88 (shake flask, Hansch & Leo 1979)
1.57 (HPLC-k′ correlation, Könemann et al. 1979)
1.89 ± 0.01 (HPLC-k′ correlation, Hammers et al. 1982)
2.00 (HPLC-k′ correlation, Hammers et al. 1982)
1.910 ± 0.013 (slow-stirring-GC, De Bruijn et al. 1989)
1.88 (recommended, Sangster 1993)
1.91 ± 0.14, 1.52 ± 0.51 (solvent generated liquid-liquid chromatography SGLLC-correlation, RP-HPLC-k′ correlation, Cichna et al. 1995)
1.88 (recommended, Hansch et al. 1995)

Octanol/Air Partition Coefficient, log K_{OA}:

Bioconcentration Factor, log BCF:
1.06 (zebrafish, Zok et al. 1991)
–0.097 to 0.342 (average for carp, Tsuda et al. 1993)
1.06; 1.55, 0.70, 0.92 (quoted; calculated values, Bintein et al. 1993)

Sorption Partition Coefficient, log K_{OC}:

Environmental Fate Rate Constants, k, or Half-Lives, $t_{½}$:
Volatilization:
Photolysis: direct aqueous photolysis rate constant k = 0.393 ± 0.006 min^{-1} with a calculated $t_{½}$ = 1.76 min (Stegeman et al. 1993).
Oxidation:
Hydrolysis: direct photohydrolysis rate constant k = 0.393 ± 0.006 min^{-1} with a calculated $t_{½}$ = 1.76 min (Stegeman et al. 1993).
Biodegradation: average biodegradation rate of 6.2 mg COD g^{-1} h^{-1} for 97.2% removal (Scow 1982).
Biotransformation: mean bacteria transformation rate constant for all three sites of (2.2 ± 1.7) × 10^{-12} L·organism^{-1}·h^{-1} (Paris & Wolfe 1987; quoted, Steen 1991).
Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants:
k_1 = 19.1 h^{-1} (zebrafish, Zok et al. 1991)
k_2 = 0.21 h^{-1} (carp, Tsuda et al. 1993)

Half-Lives in the Environment:
Biota: $t_{½}$ = 3.3 h in carp with excretion rate k = 0.21 h^{-1} (Tsuda et al. 1993).

TABLE 16.1.3.3.1
Reported vapor pressures of 3-chloroaniline at various temperatures and the coefficients for the vapor pressure equations

$\log P = A - B/(T/K)$ (1) $\ln P = A - B/(T/K)$ (1a)
$\log P = A - B/(C + t/°C)$ (2) $\ln P = A - B/(C + t/°C)$ (2a)
$\log P = A - B/(C + T/K)$ (3)
$\log P = A - B/(T/K) - C\cdot\log (T/K)$ (4)

Kahlbaum 1898		Stull 1947		Piacente et al. 1985			
static method		summary of literature data		torsion-weighing effusion			
t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa
				run 63	average	run 64	average
81.7	400	63.5	133.3	19	8	31	19
89.8	666.6	89.8	666.6	29	17	39	41
102	1333	102	1333	36.5	33	42	50
110.4	2000	116.7	2666	43	49	44	52
116.8	2666	133.6	5333	50	89	45	56
122.0	3333	144.1	7999	57.5	145	46	66
126.2	4000	158	13332	65	250	47	70
129.8	4666	179.5	26664	73	376	49	89
133.2	6333	203.5	53329			50	85
136.2	6000	228.5	101325			51	95
138.8	6666					52	105
149.9	9999	mp/°C	–10.4			53	102
158.0	13332					55	126
179.5	26664					57	146
193.2	53329					59	151
203.5	66661					60.5	170
211.9	79993					62	190
228.5	101325					63	204
						65	240
						69	296
						overall vapor pressure eq.	
						eq. 1	P/kPa
						A	8.86 ± 0.10
						B	3180 ± 40
						$\Delta H_V/(\text{kJ mol}^{-1}) = 60.9 \pm 5$ at 25°C	

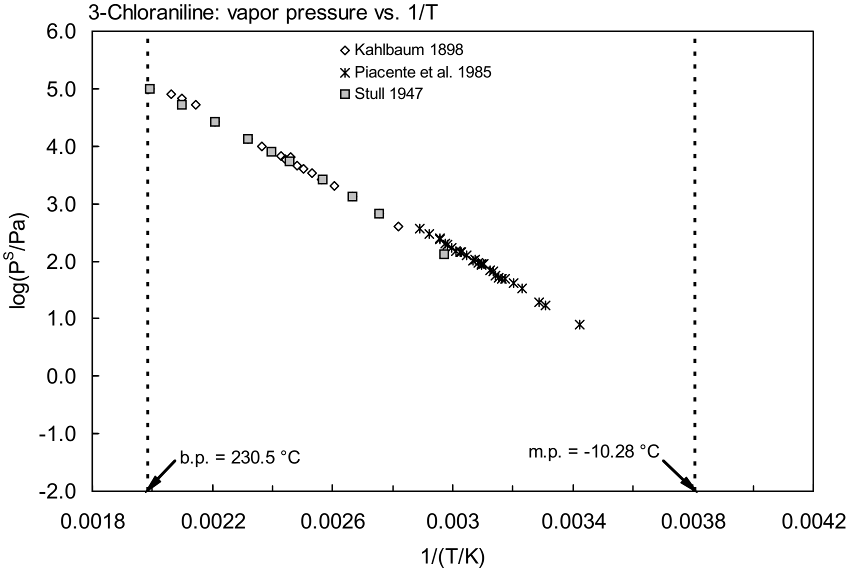
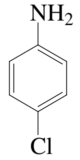


FIGURE 16.1.3.3.1 Logarithm of vapor pressure versus reciprocal temperature for 3-chloroaniline.

16.1.3.4 4-Chloroaniline



Common Name: 4-Chloroaniline
Synonym: 1-amino-4-chlorobenzene, *p*-chloroaniline, 4-chlorophenylamine
Chemical Name: 1-amino-4-chlorobenzene, *p*-chloroaniline, 4-chloroaniline
CAS Registry No: 106-47-8
Molecular Formula: $NH_2C_6H_4Cl$
Molecular Weight: 127.572
Melting Point (°C):
70.5 (Lide 2003)
Boiling Point (°C):
232.0 (Weast 1982–83; Verschueren 1983; Howard 1989)
Density (g/cm^3 at 20°C):
1.429 (19°C, Weast 1982–83)
Molar Volume (cm^3/mol):
131.1 (calculated-Le Bas method at normal boiling point)
Dissociation Constant, pK_a:
3.98 (Perrin 1972; Freitag et al. 1984; quoted, Howard 1989)
4.20 (McLeese et al. 1979)
4.15 (Weast 1982–83)
3.99 (protonated + 1, Dean 1985)
Enthalpy of Vaporization, ΔH_V (kJ/mol):
79 ± 5 (25°C, Piacente et al. 1985)
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
15.69 (Tsonopoulos & Prausnitz 1971)
Entropy of Fusion, ΔS_{fus} (J/mol K):
57.74 (Tsonopoulos & Prausnitz 1971)
Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F: 0.358 (mp at 70.5°C)

Water Solubility (g/m^3 or mg/L at 25°C):
3000 (Philpot et al. 1940)
3900 (Kilzer et al. 1979)
2620 (Schmidt-Bleek et al. 1982; Rott et al. 1982)
2487 (calculated-group contribution method, Kühne et al. 1995)

Vapor Pressure (Pa at 25°C and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):
1.707* (20°C, Knkudsen effusion, measured range 10–30°C, Swan & Mack 1925)
15.19* (extrapolated-regression of tabulated data, temp range 59.3–230.5°C, Stull 1947)
$\log (P/mmHg) = [-0.2185 \times 12832.8/(T/K)] + 8.461034$; temp range 59.3–230.5°C (Antoine eq., Weast 1972–73)
3.173 (effusion method, DePablo 1976)
3.33 (extrapolated, Verschueren 1977)
2.00, 6.67 (20°C, 30°C, quoted, Verschueren 1983)
0.224 (extrapolated-Antoine eq., Boublik et al. 1984)
$\log (P/kPa) = 3.55438 - 521.556/(47.392 + t/°C)$; temp range 90–150°C (Antoine eq. from reported exptl. data, Boublik et al. 1984)
1.636* (torsion-weighing effusion, Piacente et al. 1985)

$\log (P/\text{kPa}) = (11.20 \pm 0.20) - (4170 \pm 60)/(T/\text{K})$; temp range ~298–360 K (Antoine eq., combined torsion-weighing effusion, Piacente et al. 1985)
3.66 (calculated-Antoine eq.-I, Stephenson & Malanowski 1987)
$\log (P_S/\text{kPa}) = 13.448 - 4736/(T/\text{K})$, temp range 283–303 K (Antoine eq.-I, Stephenson & Malanowski 1987)
$\log (P_L/\text{kPa}) = 7.3489 - 2729/(T/\text{K})$, temp range 363–505 K (Antoine eq.-II, Stephenson & Malanowski 1987)
3.33, 32.0 (quoted, calculated-solvatochromic parameters, Banerjee et al. 1990)
$\log (P/\text{mmHg}) = -15.3259 - 2.8592 \times 10^3/(T/\text{K}) + 11.527 \cdot \log (T/\text{K}) - 1.8071 \times 10^{-2} \cdot (T/\text{K}) + 7.2359 \times 10^{-6} \cdot (T/\text{K})^2$; temp range 343–754 K (vapor pressure eq., Yaws 1994)

Henry's Law Constant (Pa m^3/mol at 25°C):
1.0840 (calculated-P/C, Howard 1989)
0.0395 (calculated-P/C, Meylan & Howard 1991)
0.1430 (estimated-bond contribution, Meylan & Howard 1991)

Octanol/Water Partition Coefficient, log K_{OW}:
1.84 (Ichikawa et al. 1969)
1.83 (quoted exptl., Leo et al. 1969, 1971; Hansch & Leo 1985)
1.83 (HPLC-k′ correlation; Carlson et al. 1975)
1.83 (shake flask, Hansch & Leo 1979)
1.57 (HPLC-k′ correlation, Könemann et al. 1979)
1.83, 20.2 (HPLC-k′ correlation, Hammers et al. 1982)
1.64 (inter-laboratory studies, HPLC-RT correlation average, Eadsforth & Moser 1983)
1.88 ± 0.02 (HPLC-RV correlation-ALPM; Garst & Wilson 1984)
2.78 (shake flask, OECD 1981 Guidelines, Geyer et al. 1984)
1.83 (shake flask, Log P Database, Hansch & Leo 1987)
1.83 (RP-HPLC-k′ correlation, Minick et al. 1988)
1.88 ± 0.014 (shake flask/slow-stirring-GC, De Brujin et al. 1989)
1.83 (shake flask, Leahy et al. 1989)
1.80, 1.82 (shake flask, HPLC-RT correlation, Wang et al. 1989)
2.01 (centrifugal partition chromatography CPC-RV correlation, El Tayar et al. 1991)
1.83 (recommended, Sangster 1993)
1.83 (pH 7.4, Hansch et al. 1995)

Octanol/Air Partition Coefficient, log K_{OA}:

Bioconcentration Factor, log BCF:
< 1.30 (golden orfe for 3-d exposure, Körte et al. 1978)
3.08 (green algae for 24-h exposure of dry wt. basis, Körte et al. 1978)
2.42 (green algae for 24-h exposure of wet wt. basis, Körte et al. 1978)
< 1.0, 2.41, 3.11 (golden orfe, algae, activated sludge, Freitag et al. 1982)
2.42 (alga *Chlorella fusca*, wet wt. basis, Geyer et al. 1984)
2.06 (alga *Chlorella fusca*, calculated-K_{OW}, Geyer et al. 1984)
1.11, 2.42, 2.45 (golden ide, algae, activated sludge, Freitag et al. 1985)
0.91 (zebrafish, Zok et al. 1991)
–0.097–0.23 (carp, Tsuda et al. 1993)
0.91; 1.52, 0.63, 0.88 (quoted; calculated values, Bintein et al. 1993)
2.58 (algae *Chlorella fusca*, wet wt basis, Wang et al. 1996)

Sorption Partition Coefficient, log K_{OC}:
2.36–2.67 (five Belgium soils, Van Bladel & Moreale 1977)
1.98–3.18 (five German soils, Rott et al. 1982)
3.74 (colloidal org. matter in ground water, Means 1983)
1.86 (calculated-MCI χ, Sabljic 1987)
2.08 (RP-HPLC-k′ correlation, cyanopropyl column, Hodson & Williams 1988)
1.96, 1.86 (soil, quoted exptl., calculated-MCI χ and fragment contribution, Meylan et al. 1992)

1.61 (calculated-K_{OW}, Kollig 1993)
1.96 (soil, calculated-MCI $^1\chi$, Sabljic et al. 1995)
2.28; 1.86 (HPLC-screening method; calculated-PCKOC fragment method, Müller & Kördel 1996)
3.086, 2.21, 2.48, 2.374, 2.973 (first generation Eurosoils ES-1, ES-2, ES-3, ES-4, ES-5, shake flask/batch equilibrium-HPLC/UV, Gawlik et al. 1998)
2.801, 2.326, 2.145, 2.420 (second generation Eurosoils ES-1, ES-3, ES-4, ES-5, shake flask/batch equilibrium-HPLC/UV and HPLC-k′ correlation, Gawlik et al. 2000)

Environmental Fate Rate Constants, k, or Half-Lives, $t_{1/2}$:

Volatilization: estimated $t_{1/2}$ = 6.4 h from using Henry's law constant for a model river of 1-m deep with 1 m/s current and 3 m/s wind (Lyman et al. 1982; quoted, Howard 1989);
$t_{1/2}$ = 3 d in an experimental pond with spiked 4-chloroaniline (Schauerte et al. 1982; quoted, Howard 1989).
Photolysis:
Oxidation: rate constant k; for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO3} with NO_3 radical and k_{O3} with O_3 or as indicated, *data at other temperatures see reference:
$k_{OH} = (8.3 \pm 0.42) \times 10^{-11}$ cm^3 molecule^{-1} s^{-1} at 295 K (flash photolysis-resonance fluorescence, Wahner & Zetzsch 1983)
k_{OH}(obs.) = 83×10^{-12} cm^3 molecule^{-1} s^{-1}; k_{OH}(calc) = 34.7×10^{-12} cm^3 molecule^{-1} s^{-1} at room temp. in air (Atkinson 1985; Atkinson et al. 1985)
k_{OH}(calc) = 54×10^{-12} cm^3 molecule^{-1} s^{-1}; k_{OH}(obs.) = 83×10^{-12} cm^3 molecule^{-1} s^{-1} at room temp. (SAR, Atkinson 1987)
k_{OH} = (83 to ~44) × 10^{-12} cm^3 molecule^{-1} s^{-1} at 295–296 K (Atkinson 1989)
Hydrolysis:
Biodegradation:
Biotransformation:
Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants:
k_1 = 42.9 h^{-1} (zebrafish, Zok et al. 1991)
k_2 = 0.16 h^{-1} (carp, Tsuda et al. 1993)
k_1 = 17.74 h, k_2 = 0.0465 h (algae *Chlorella fusca*, Wang et al. 1996)

Half-Lives in the Environment:

Air: $t_{1/2}$ = 4.6 h, based on estimated reaction rate with photochemically produced hydroxyl radical of 5×10^5 radicals/cm^3 in atmosphere (Wahner & Zetzsch 1983; quoted, Howard 1989).
Surface water: estimated $t_{1/2}$ = 0.3–3.0 d in river waters in case of a first order reduction process (Zoeteman et al. 1980);
72.1 mg/L total organic carbon (TOC) degraded to 92% TOC after 5 h illumination with a 250 watt tungsten lamp by photo-Fenton reaction in distilled water (Ruppert et al. 1993).
Groundwater: estimated $t_{1/2}$ = 30–300 d in Rhine River (Zoeteman et al. 1980).
Sediment:
Soil:
Biota: $t_{1/2}$ = 4.3 h in carp with excretion rate k = 0.16 h^{-1} (Tsuda et al. 1993).

TABLE 16.1.3.4.1
Reported vapor pressures of 4-chloroaniline at various temperatures and the coefficients for the vapor pressure equations

$\log P = A - B/(T/K)$	(1)	$\ln P = A - B/(T/K)$	(1a)
$\log P = A - B/(C + t/°C)$	(2)	$\ln P = A - B/(C + t/°C)$	(2a)
$\log P = A - B/(C + T/K)$	(3)		
$\log P = A - B/(T/K) - C \cdot \log (T/K)$	(4)		

Swan & Mack 1925		Stull 1947		Piacente et al. 1985			
Knudsen effusion		summary of literature data		torsion-weighing effusion			
t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa
				Run 58	average	Run 66	average
10	0.513	59.3	133.3	26	3.0	52	56
20	1.707	87.9	666.6	31	6.0	56.5	75
30	6.493	102.1	1333	34	8.0	61	128
		117.8	2666	39	13	63	136
		135.0	5333	40	17	65	152
		145.8	7999	43	20	68	238
eq. 4	P/mmHg	159.9	13332	48	31	71	275
A	415.007	182.3	26664	49.5	35	72	316
B	22322	206.6	53329	53	48		
C	138.475	230.5	101325	59	87		
				60.5	100	overall vapor pressure eq.	
$\Delta H_V/(kJ\ mol^{-1}) = 90.37$		mp/°C	70.5	63.5	127	eq. 1	P/kPa
at 20°C				67	170	A	11.20 ± 0.20
				69.5	224	B	4170 ± 60
				82.5	549		
				88.5	832	$\Delta H_V/(kJ\ mol^{-1}) = 70.9 \pm 5$	
						at 25°C	

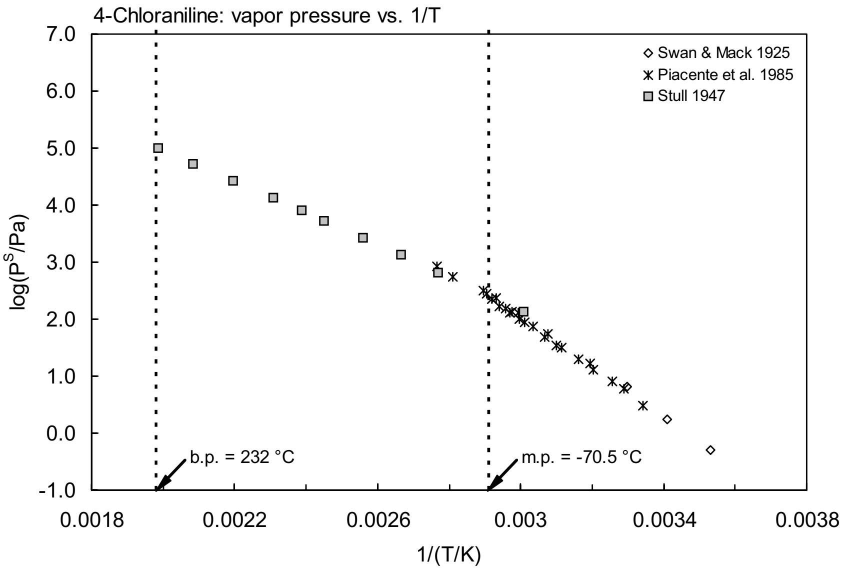
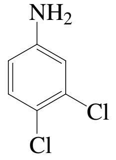


FIGURE 16.1.3.4.1 Logarithm of vapor pressure versus reciprocal temperature for 4-chloroaniline.

16.1.3.5 3,4-Dichloroaniline



Common Name: 3,4-Dichloroaniline
Synonym:
Chemical Name: 3,4-dichloroaniline
CAS Registry No: 95-76-1
Molecular Formula: $C_6H_5Cl_2N$, $C_6H_3NH_2Cl_2$
Molecular Weight: 162.017
Melting Point (°C):
72.0 (Weast 1982–83; Lide 2003)
Boiling Point (°C):
272.0 (Weast 1982–83; Lide 2003)
Density (g/cm^3 at 20°C):
Molar Volume (cm^3/mol):
111.7 (calculated-density, Jaworska & Schultz 1993)
152.0 (calculated-Le Bas method at normal boiling point)
Dissociation Constant, pK_a:
2.968, 3.0 (Perrin 1972)
2.00 (estimated, Wolff & Crossland 1985)
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
Entropy of Fusion, ΔS_{fus} (J/mol K):
Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F: 0.346 (mp at 72°C)

Water Solubility (g/m^3 or mg/L at 25°C):
92.03 (20°C, Wolff & Crossland 1985)
93.2; 740 (quoted exptl.; calculated-group contribution method, Kühne et al. 1995)

Vapor Pressure (Pa at 25°C or as indicated and reported temperature dependence equations):
1.30 (20°C, Wolff & Crossland 1985)
2.27 (extrapolated-Antoine eq., Stephenson & Malanowski 1987)
$\log (P_L/\text{kPa}) = 7.6189 - 3060.03/(T/K)$; temp range 420–545 K (Antoine eq., Stephenson & Malanowski 1987)
$\log (P/\text{mmHg}) = -15.2685 - 3.3857 \times 10^3/(T/K) + 11.926 \cdot \log (T/K) - 1.9227 \times 10^{-2} \cdot (T/K) + 7.4179 \times 10^{-6} \cdot (T/K)^2$; temp range 345–800 K (vapor pressure eq., Yaws 1994)

Henry's Law Constant (Pa·m^3/mol at 25°C):
2.289 (calculated-P/C)

Octanol/Water Partition Coefficient, $\log K_{OW}$:
2.69 (unpublished result, Leo et al. 1971, Hansch & Leo 1979)
2.12 (HPLC-k′ correlation, Könemann et al. 1979)
2.78 (20°C, shake flask-UV, Briggs 1981)
2.69, 2.67 (HPLC-k′ correlation, Hammers et al. 1982)
2.62 (inter-laboratory studies, shake flask average, Eadsforth & Moser 1983)
2.30 (inter-laboratory studies, HPLC-RT correlation average, Eadsforth & Moser 1983)
2.14, 2.63 (HPLC-k′ correlation, Eadsforth 1986)
2.69 (shake flask, Log P Database, Hansch & Leo 1987)
2.68 (recommended, Sangster 1993)
2.69 (recommended, Hansch et al. 1995)
2.69 (LOGPSTAR or CLOGP data, Sabljic et al. 1995)

Octanol/Air Partition Coefficient, log K_{OA}:

Bioconcentration Factor, log BCF:

1.48	(zebrafish, Zok et al. 1991)
1.48; 2.02, 1.88, 1.75	(fish: quoted; calculated values-K_{OW}, Bintein et al. 1993)

Sorption Partition Coefficient, log K_{OC}:

2.29	(20°C, sorption isotherm-GC, converted from K_{OM} multiplied by 1.724, Briggs 1981)
1.40	(calculated-K_{OW}, wet sediment, Wolff & Crossland 1985)
2.29	(Sabljic 1987)
2.05	(soil, quoted, Sabljic 1987)
2.29, 2.08	(soil, quoted, calculated-MCI χ and fragment contribution, Meylan et al. 1992)
2.29	(calculated-MCI $^1\chi$, Sabljic et al. 1995)
2.26, 2.39	(RP-HPLC-k′ correlation including MCI related to non-dispersive intermolecular interactions, hydrogen-bonding indicator variable, Hong et al. 1996)

Environmental Fate Rate Constants, k, or Half-Lives, $t_{½}$:

Volatilization: first order rate constant k(calc) = 5.0×10^{-3} d^{-1} (Wolff & Crossland 1985).

Photolysis: phototransformation rate constant k = 0.12 to 0.20 d^{-1} (Wolff & Crossland 1985).

Oxidation:

Hydrolysis: not expected to occur (Wolff & Crossland 1985).

Biodegradation:

Biotransformation:

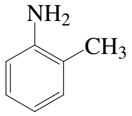
Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants:

k_1 = 78.5 h^{-1} (zebrafish, Zok et al. 1991)

Half-Lives in the Environment:

Surface water: overall rate of loss predicted from outdoor ponds was calculated based on direct phototransformation, and indirect phototransformation k = 0.13 to 0.22 d^{-1} corresponding to $t_{½}$ = 3.2 to 5.3 d; the observed rate of loss varied from 0.11 to 0.17 d^{-1} corresponding to $t_{½}$ = 4.1 – 6.3 d (Wolff & Crossland 1985).

16.1.3.6 *o*-Toluidine (2-Methylbenzeneamine)



Common Name: *o*-Toluidine
Synonym: 2-aminotoluene, *o*-aminotoluene, 2-methylaniline, 2-methylbenzeneamine
Chemical Name: 2-aminotoluene, *o*-methylaniline, *o*-toluidine
CAS Registry No: 95-53-4
Molecular Formula: C_7H_9N, $C_6H_4(CH_3)NH_2$
Molecular Weight: 107.153
Melting Point (°C):
  –14.41 (Lide 2003)
Boiling Point (°C):
  200.3 (Lide 2003)
Density (g/cm^3 at 20°C):
  0.9984, 0.99430 (10, 25°C, Dreisbach 1955, Riddick et al. 1986)
  0.9984 (20°C, Weast 1982–83)
Molar]Volume (cm^3/mol):
  107.3 (20°C, calculated-density, Stephenson & Malanowski 1987)
  132.4 (calculated-Le Bas method at normal boiling point)
Dissociation Constant, pK_a:
  4.40, 4.447, 4.46 (Perrin 1972)
  4.44 (Weast 1982–83)
  4.45 (protonated cation + 1, Dean 1985)
  4.43 (Sangster 1989)
Enthalpy of Vaporization, ΔH_V (kJ/mol):
  56.739, 44.597 (25°C, bp, Riddick et al. 1986)
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
  7.535 (Dreisbach 1955)
Entropy of Fusion, ΔS_{fus} (J/mol K):
Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F: 1.0

Water Solubility (g/m^3 or mg/L at 25°C):
  16330 (20°C, shake flask-GC, Chiou 1981; Chiou & Schmedding 1981; Chiou et al. 1982)
  15000 (quoted, Verschueren 1983)
  16300 (calculated-K_{OW}, Müller & Klein 1992)

Vapor Pressure (Pa at 25°C and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):
  133.3* (48.2°C, static method, measured range 48.2–199.7°C, Kahlbaum 1898)
  42.72* (extrapolated-regression of tabulated data, temp range 44–199.7°C, Stull 1947)
  $\log (P/mmHg) = 7.60681 - 2033.6/(230 + t/°C)$ (Antoine eq., Dreisbach & Martin 1949)
  7605* (118.46°C, ebulliometry, measured range 118.46–200.30°C, Dreisbach & Shrader 1949)
  42.26 (calculated by formula, Dreisbach 1955)
  $\log (P/mmHg) = 7.28896 - 1768.7/(201.0 + t/°C)$; temp range 103–320°C (Antoine eq. for liquid state, Dreisbach 1955)
  $\log (P/atm) = [-0.2185 \times 12663.4/(T/K)] + 8.440371$; temp range 41–203.3°C (Antoine eq., Weast 1972–73)
  42.93 (extrapolated-Cox eq., Chao et al. 1983)
  $\log (P/mmHg) = [1 - 473.369/(T/K)] \times 10\text{^}\{0.907135 - 6.44774 \times 10^{-4}\cdot(T/K) + 4.94693 \times 10^{-7}\cdot(T/K)^2\}$; temp range: 300.0–710.0 K (Cox eq., Chao et al. 1983)
  13.33, 40.0 (20°C, 30°C, quoted, Verschueren 1983)
  33.96 (extrapolated-Antoine eq., Boublik et al. 1984)

log (P/kPa) = 6.20039 – 1623.158/(186.641 + t/°C); temp range 118.5–200.3°C (Antoine eq. from reported exptl. data, Boublik et al. 1984)
43.0 (selected lit., Riddick et al. 1986)
log (P/mmHg) = 6.73171 – 2033.6/(230.0 + t/°C); temp range: not specified (Antoine eq., Riddick et al. 1986)
34.18 (extrapolated-Antoine eq., Dean 1985, 1992)
log (P/mmHg) = 7.08203 – 1627.72/(187.13 + t/°C); temp range 118–200°C (Antoine eq., Dean l985, 1992)
36.46 (extrapolated-Antoine eq., Stephenson & Malanowski 1987)
log (P_L/kPa) = 6.26948 – 1672.87/(–81.47 + T/K); temp range 391–474 K, (Antoine eq., Stephenson & Malanowski 1987)
log (P/mmHg) = 96.5685 – 6.2643 × 10^3/(T/K) – 32.265·log (T/K) + 1.2361 × 10^{-2}·(T/K) + 6.2915 × 10^{-13}·$(T/K)^2$; temp range 249–694 K (vapor pressure eq., Yaws 1994)

Henry's Law Constant (Pa·m^3/mol at 25°C):
0.095 (calculated-P/C)
0.201 (gas stripping-GC, Altschuh et al. 1999)

Octanol/Water Partition Coefficient, log K_{OW}:
1.29 (shake flask-UV, Leo et al. 1971)
1.43 (HPLC-k′ correlation, Carlson et al. 1975)
1.63 (RP-HPLC-RT correlation, Veith et al. 1979a)
1.42 (shake flask-UV at pH 7.5, Martin-Villodre et al. 1986)
1.34 (HPLC-RT correlation, average, Ge et al. 1987)
1.32 (shake flask, Log P Database, Hansch & Leo 1987)
1.32 (recommended, Sangster 1989)
1.44, 1.57 (shake flask, HP:C-RT correlation, Wang et al. 1989)
1.43 (recommended, Sangster 1993)
1.32 (recommended, Hansch et al. 1995)

Octanol/Air Partition Coefficient, log K_{OA}:

Bioconcentration Factor, log BCF:

Sorption Partition Coefficient, log K_{OC}:
1.24 (calculated-K_{OW}, Kollig 1993)

Environmental Fate Rate Constants, k, or Half-Lives, $t_{½}$:
Volatilization:
Photolysis:
Hydrolysis:
Oxidation: rate constant k = 1 × 10^4 M^{-1} s^{-1} for oxidation by RO_2 radicals at 30°C in aquatic systems with $t_{½}$ = 0.8 d (Howard 1972; Hendry et al. 1974; quoted, Mill 1982);
rate constant k < 2 × 10^2 M^{-1} s^{-1} for oxidation by singlet oxygen at 25°C in aquatic systems with $t_{½}$ > 100 yr (Foote 1976; Mill 1979; quoted, Mill 1982);
photooxidation $t_{½}$ = 62.4 – 3480 h in water, based on estimated rate constants for reactions of representative aromatic amines with OH and RO_2 radicals (Mill & Mabey 1985; quoted, Howard et al. 1991);
photooxidation $t_{½}$ = 0.394 – 3.94 h in air, based on estimated rate constant for the reaction with hydroxyl radical in air (Atkinson 1987; quoted, Howard et al. 1991).
Biodegradation: decomposition by a soil microflora in > 64 d (Alexander & Lustigman 1966; quoted, Verschueren 1983);
aqueous aerobic $t_{½}$ = 24 – 168 h, based on aqueous aerobic screening test data (Baird et al. 1977; Sasaki 1978; quoted, Howard et al. 1991);
average biodegradation k = 15.1 mg COD g^{-1} h^{-1} for 97.7% removal (Scow 1982);
aqueous anaerobic $t_{½}$ = 96 – 672 h, based on estimated unacclimated aqueous aerobic biodegradation half-life (Howard et al. 1991).
Biotransformation:

Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants:

Half-Lives in the Environment:

Air: photooxidation $t_{1/2}$ = 0.394 – 3.94 h, based on estimated rate constant for the reaction with hydroxyl radical in air (Atkinson 1987; quoted, Howard et al. 1991);
atmospheric transformation lifetime was estimated to be < 1 d (Kelly et al. 1994).

Surface water: estimated $t_{1/2}$ = 1.0 d for methylaniline in Rhine River in case of a first order reduction process (Zoeteman et al. 1980)
photooxidation $t_{1/2}$ = 62.4 – 3480 h, based on estimated rate constants for reactions of representative aromatic amines with OH and RO_2 radicals (Mill & Mabey 1985; quoted, Howard et al. 1991).

Groundwater: $t_{1/2}$ = 48 – 336 h, based on estimated unacclimated aqueous aerobic biodegradation half-life (Howard et al. 1991).

Sediment:

Soil: $t_{1/2}$ = 24 – 168 h, based on estimated unacclimated aqueous aerobic biodegradation half-life (Howard et al. 1991).

Biota:

TABLE 16.1.3.6.1
Reported vapor pressures of *o*-toluidine at various temperatures

Kahlbaum 1898		Stull 1947		Dreisbach & Shrader 1949	
static method-manometer*		summary of literature data		ebulliometry	
t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa
48.2	133.3	44.0	133.3	118.46	7605
55.3	266.6	69.3	666.6	122.22	8851
61.4	400.0	81.4	1333	125.99	10106
65.7	533.3	95.1	2666	139.0	16500
69.3	666.6	110.0	5333	168.06	42066
81.4	1333.2	119.8	7999	184.80	67661
94.9	2666.4	133.0	13332	200.30	101325
103.6	3999.7	153.0	26664		
110.0	5332.9	170.2	53329		
115.1	6666.1	199.7	101325		
125.4	9999.2				
133.0	13332	mp/°C	–16.3		
154.0	26664				
166.2	39997				
176.2	53329				
183.9	66661				
190.5	79993				
196.2	93326				
199.7	101325				

*complete list see ref.

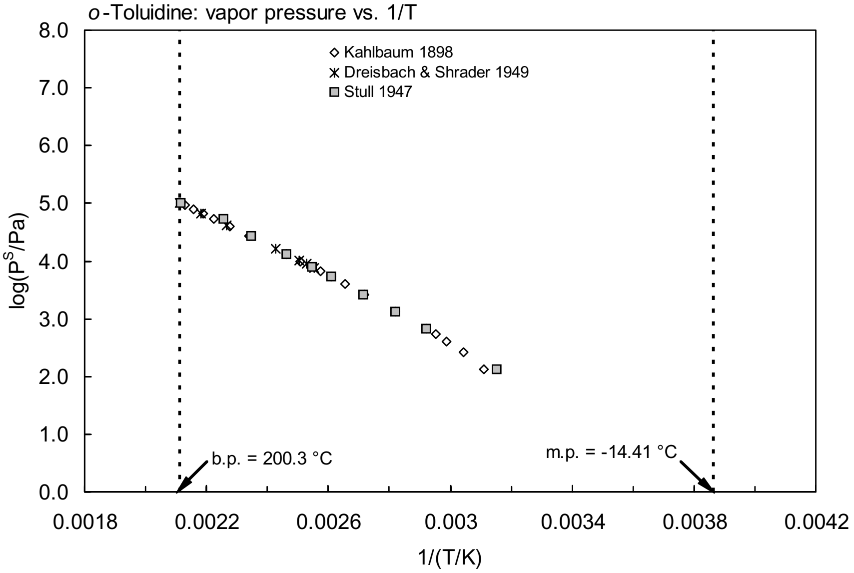
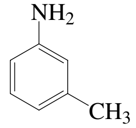


FIGURE 16.1.3.6.1 Logarithm of vapor pressure versus reciprocal temperature for *o*-toluidine.

16.1.3.7 *m*-Toluidine (3-Methylbenzeneamine)



Common Name: *m*-Toluidine
Synonym: 3-aminotoluene, 3-methylbenzeneamine, 3-methylaniline
Chemical Name: 3-aminotoluene, *m*-amino-methylbenzene, *m*-methylaniline, *m*-toluidine
CAS Registry No: 108-44-1
Molecular Formula: $C_6H_4(CH_3)NH_2$
Molecular Weight: 107.153
Melting Point (°C):
–31.3 (Lide 2003)
Boiling Point (°C):
203.3 (Stull 1947; Weast 1982–83; Lide 2003)
Density (g/cm^3 at 20°C):
0.9889 (Dreisbach 1955; Weast 1982–83)
Molar Volume (cm^3/mol):
108.4 (20°C, Stephenson & Malanowski 1987)
132.4 (calculated-Le Bas method at normal boiling point)
Dissociation Constant, pK_a:
4.66, 4.712, 4.72 (Perrin 1972)
4.73 (Weast 1982–83)
4.71 (protonated cation + 1, Dean 1985)
4.70 (Sangster 1989)
Enthalpy of Vaporization, ΔH_V (kJ/mol):
57.283, 44.848 (25°C, bp, Riddick et al. 1986)
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
7.08 (Dreisbach 1955)
3.891 (Riddick et al. 1986)
Entropy of Fusion, ΔS_{fus} (J/mol K):
Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F: 1.0

Water Solubility (g/m^3 or mg/L at 25°C):
15031 (20°C, shake flask-GC, Chiou 1981; Chiou & Schmedding 1981; Chiou et al. 1982)

Vapor Pressure (Pa at 25°C and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):
133.3* (49.8°C, static method, measured range 49.8–203.3°C, Kahlbaum 1898)
49.54* (extrapolated-regression of tabulated data, temp range 41–203.3°C, Stull 1947)
$\log (P/\text{mmHg}) = 7.616512 - 2052.0/(230 + t/°C)$ (Antoine eq., Dreisbach & Martin 1949)
7605* (121.77°C, ebulliometry, measured range 121.77-203.34°C, Dreisbach & Shrader 1949)
36.64 (calculated by formula, Dreisbach 1955)
$\log (P/\text{mmHg}) = 7.27435 - 1772.06/(200.0 + t/°C)$; temp range 105–320°C (Antoine eq. for liquid state, Dreisbach 1955)
$\log (P/\text{mmHg}) = [-0.2185 \times 12104.1/(T/K)] + 8.440371$; temp range 41–203°C (Antoine eq., Weast 1972–73)
33.49 (calculated-Cox eq., Chao et al. 1983)
$\log (P/\text{atm}) = [1 - 476.329/(T/K)] \times 10\text{^}\{0.923479 - 6.91988 \times 10^{-4}\cdot(T/K) + 5.41104 \times 10^{-7}\cdot(T/K)^2\}$; temp range: 280.0–705.0 K (Cox eq., Chao et al. 1983)
27.91 (extrapolated-Antoine eq., Boublik et al. 1984)
$\log (P/\text{kPa}) = 6.21454 - 1620.608/(203.346 + t/°C)$; temp range 121.9–203.4°C (Antoine eq. from reported exptl. data, Boublik et al. 1984)
25.66 (extrapolated-Antoine eq., Dean 1985, 1992)

log (P/mmHg) = 7.09367 – 1631.43/(183.91 + t/°C); temp range 122–203°C (Antoine eq., Dean 1985, 1992)
36.0 (quoted lit., Riddick et al. 1986)
log (P/kPa) = 17.6292 – 3200.9/(T/K) – 3.323·log (T/K), temp range not specified (vapor pressure eq., Riddick et al. 1986)
26.86 (extrapolated-Antoine eq., Stephenson & Malanowski 1987)
log (P_L/kPa) = 6.27299 – 1669.26/(–85.339 + T/K); temp range 394–447 K (Antoine eq., Stephenson & Malanowski 1987)
25.50 (calculated-Cox eq., Chao et al. 1990)
log (P/mmHg) = 7.0317 – 3.2034 × 10^3/(T/K) + 2.3006·log (T/K) – 9.7791 × 10^{-3}·(T/K) + 4.6824 × 10^{-6}·$(T/K)^2$; temp range 243–709 K (vapor pressure eq., Yaws 1994)

Henry's Law Constant (Pa·m^3/mol at 25°C):
0.257 (calculated-P/C)
0.169 (gas stripping-GC, Altschuh et al. 1999)

Octanol/Water Partition Coefficient, log K_{OW}:
1.40 (shake flask-UV, Fujita et al. 1964)
1.43 (HPLC-k′ correlation, Carlson et al. 1975)
1.42 (20°C, shake flask-UV, Briggs 1981)
1.43 (shake flask, Log P Database, Hansch & Leo 1987)
1.40 (recommended, Sangster 1989)
1.49, 1.37 (shake flask, HPLC-RT correlation, Wang et al. 1989)
1.40 (recommended, Hansch et al. 1995)

Octanol/Air Partition Coefficient, log K_{OA}:

Bioconcentration Factor, log BCF:

Sorption Partition Coefficient, log K_{OC}:
1.41 (soil, quoted obs. as log K_{OM}, Sabljic 1987)
1.65 (soil, calculated-MCI $^1\chi$, Sabljic et al. 1995)

Environmental Fate Rate Constants, k, or Half-Lives, $t_{1/2}$:
Volatilization:
Photolysis:
Hydrolysis:
Oxidation: rate constant k = 1 × 10^4 M^{-1} s^{-1} for oxidation by RO_2 radical at 30°C in aquatic systems with $t_{1/2}$ = 0.8 d (Howard 1972; Hendry et al. 1974; quoted, Mill 1982);
k < 2 × 10^2 M^{-1} s^{-1} for oxidation by singlet oxygen at 25°C in aquatic systems with $t_{1/2}$ > 100 yr (Foote 1976; Mill 1979; quoted, Mill 1982).
Biodegradation: decomposition by a soil microflora in 8 d (Alexander & Lustigman 1966; quoted, Verschueren 1983);
average biodegradation rate of 30.0 mg COD g^{-1} h^{-1} for 97.7% removal (Scow 1982).
Biotransformation:
Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants:

Half-Lives in the Environment:
Surface water: estimated $t_{1/2}$ = 1.0 d for methylaniline in Rhine River in case of a first order reduction process (Zoeteman et al. 1980)

TABLE 16.1.3.7.1
Reported vapor pressures of *m*-toluidine at various temperatures

Kahlbaum 1898		Stull 1947		Dreisbach & Shrader 1949	
static method-manometer*		summary of literature data		ebulliometry	
t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa
49.8	133.3	41.0	133.3	121.77	7605
58.9	266.6	68.0	666.6	125.57	8851
64.8	400.0	82.0	1333	129.03	10114
69.3	533.3	96.7	2666	142.27	16500
72.8	666.6	113.5	5333	171.18	42066
85.3	1333.2	123.8	7999	187.87	67661
98.5	2666.4	136.7	13332	203.34	101325
107.1	3999.7	157.6	26664		
113.6	5332.9	180.6	53329		
118.7	6666.1	203.3	101325		
129.0	9999.2				
136.6	13332	mp/°C	–31.5		
157.6	26664				
169.8	39997				
179.8	53329				
187.5	66661				
194.0	79993				
199.8	93326				
203.3	101325				

*complete list see ref.

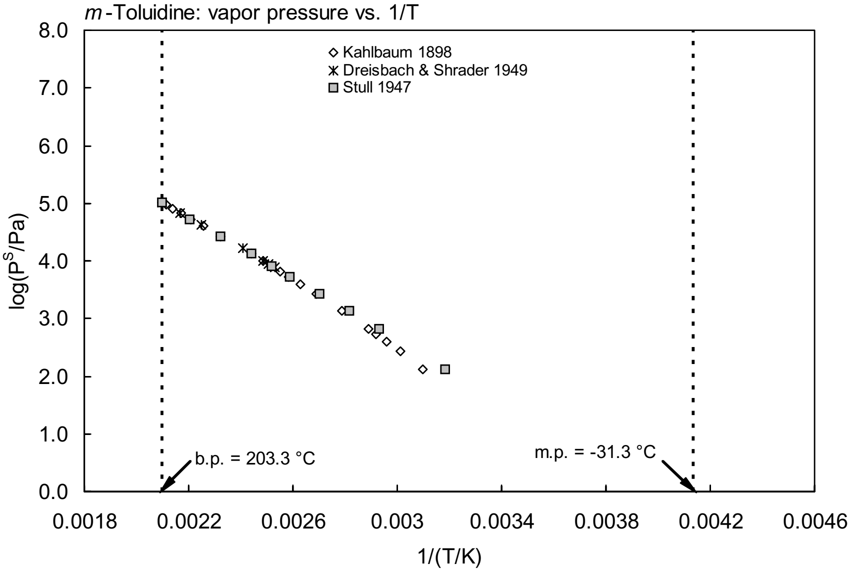
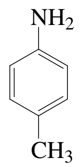


FIGURE 16.1.3.7.1 Logarithm of vapor pressure versus reciprocal temperature for *m*-toluidine.

16.1.3.8 *p*-Toluidine (4-Methylbenzeneamine)



Common Name: *p*-Toluidine
Synonym: 4-aminotoluene, 4-methylaniline, 4-methylbenzenamine
Chemical Name: 4-aminotoluene, *p*-amino-methylbenzene, *p*-methylaniline, *p*-toluidine
CAS Registry No: 106-49-0
Molecular Formula: $C_6H_4(CH_3)NH_2$
Molecular Weight: 107.153
Melting Point (°C):
  43.6 (Lide 2003)
Boiling Point (C):
  200.4 (Lide 2003)
Density (g/cm^3 at 20°C):
  0.9619 (20°C, Weast 1982–83)
  1.043 (Verschueren 1983)
Molar Volume (cm^3/mol):
  132.4 (calculated-Le Bas method at normal boiling point)
Dissociation Constant, pK_a:
  5.02, 5.08, 5.084 (Perrin 1972)
  5.08 (Weast 1982–83; Sangster 1989)
  5.08 (protonated cation + 1, Dean 1985)
  5.17 (shake flask-HPLC/UV, Johnson & Westall 1990)
Enthalpy of Vaporization, ΔH_V (kJ/mol):
  56.195, 44.271 (25°C, bp, Riddick et al. 1986)
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
  17.32 (Tsonopoulos & Prausnitz 1971)
  18.91 (Riddick et al. 1986)
Entropy of Fusion, ΔS_{fus} (J/mol K):
  54.81 (Tsonopoulos & Prausnitz 1971)
  57.61 (observed, Yalkowsky & Valvani 1980)
Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F: 0.657 (mp at 43.6°C)

Water Solubility (g/m^3 or mg/L at 25°C as indicated):
  65400 (20–25°C, shake flask-gravimetric, Dehn 1917)
  8965 (Seidell 1941, 1952)
  7400 (21°C, Verschueren 1983)
  6643, 5370 (20°C, shake flask-UV, calculated, Hashimoto et al. 1984)

Vapor Pressure (Pa at 25°C or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):
  133.3* (46.9°C, static method, measured range 46.9–200.4°C, Kahlbaum 1898)
  log (P/mmHg) = –2597/(T/K) + 8.366 (isoteniscope method, temp range not specified, Kobe et al. 1941)
  46.27* (extrapolated-regression of tabulated data, temp range 42–200.4°C, Stull 1947)
  44.70 (calculated by formula, Dreisbach 1955)
  log (P/mmHg) = 7.25173 – 1755.0/(201.0 + t/°C); temp range 103–330°C (Antoine eq. for liquid state, Dreisbach 1955)
  log (P/atm) = [–0.2185 × 12428.6/(T/K)] + 8.748585; temp range 42–200.4°C (Antoine eq., Weast 1972–73)
  38.13 (calculated-Cox eq., Chao et al. 1983)

$\log (P/\text{mmHg}) = [1 - 473.445/(T/K)] \times 10\text{\^{}}\{0.915691 - 6.57014 \times 10^{-4}\cdot(T/K) + 5.11261 \times 10^{-7}\cdot(T/K)^2\}$; temp range 290.0–700.0 K (Cox eq., Chao et al. 1983)
40.17 (calculated-Antoine eq., Dean 1985, 1992)
$\log (P/\text{mmHg}) = 7.26022 - 1758.55/(201.0 + t/°\text{C})$; temp range not specified (Antoine eq., Dean 1985,1992)
45.0 (quoted lit., Riddick et al. 1986)
$\log (P/\text{kPa}) = 18.2818 - 3269.3/(T/K) - 3.877\cdot\log (T/K)$; temp range not specified (vapor pressure eq., Riddick et al. 1986)
27.03 (extrapolated-Antoine eq., Stephenson & Malanowski 1987)
$\log (P_L/\text{kPa}) = 6.17451 - 1585.0/(-93.44 + T/K)$; temp range 393–474 K (Antoine eq., Stephenson & Malanowski 1987)
$\log (P/\text{mmHg}) = -13.9927 - 2.5795 \times 10^3/(T/K) - 10.823\cdot\log (T/K) - 1.7705 \times 10^{-2}\cdot(T/K) + 7.6741 \times 10^{-6}\cdot(T/K)^2$; temp range 317–693 K (vapor pressure eq., Yaws 1994)

Henry's Law Constant ($\text{Pa}\cdot\text{m}^3$/mol at 25°C):
0.656 (calculated-P/C)
0.0768 (gas stripping-GC, Altschuh et al. 1999)

Octanol/Water Partition Coefficient, log K_{OW}:
1.39 (shake flask-UV, Fujita et al. 1964)
1.41 (HPLC-k′ correlation, Carlson et al. 1975)
1.56 (shake flask-UV, Ezumi & Kubota 1980)
1.40 (20°C, shake flask-UV, Briggs 1981)
1.44 ± 0.03 (HPLC-RV correlation-ALPM, Garst & Wilson 1984)
1.42 (HPLC-k′ correlation, Haky & Young 1984)
1.39 (shake flask-UV at pH 7.5, Martin-Villodre et al. 1986)
1.41 (HPLC-RT correlation, average, Ge et al. 1987)
1.39 (shake flask, Leahy et al. 1989)
1.39 (recommended, Sangster 1989, 1993)
1.38, 1.39 (shake flask, HPLC-RT correlation, Wang et al. 1989)
1.40 (shake flask-HPLC/UV, Johnson & Westall 1990)
1.40 (shake flask-UV, Roberts et al. 1991)
1.40 (32°C, shake flask-UV, pH 7, Takahashi et al.1993)
1.39 (recommended, Hansch et al. 1995)

Octanol/Air Partition Coefficient, log K_{OA}:

Bioconcentration Factor, log BCF:

Sorption Partition Coefficient, log K_{OC}:
2.51, 2.70, 2.71 (Morocco soil, Oakville soil, Milford soil, Graveel et al. 1986)
1.66 (soil, quoted obs. as log K_{OM}, Sabljic 1987)
2.74, 2.22, 2.20 (Podzol soil, Alfisol soil, sediment, von Oepen et al. 1991)
1.24 (calculated-K_{OW}, Kollig 1993)
1.90 (soil, calculated-MCI ${}^1\chi$, Sabljic et al. 1995)
2.21; 1.86 (HPLC-screening method; calculated-PCKOC fragment method, Müller & Kördel 1996)
3.28, 2.01, 2.30, 2.084 (first generation Eurosoils ES-1, ES-2, ES-3, ES-4, shake flask/batch equilibrium-HPLC/UV, Gawlik et al. 1998)
2.138, 2.133, 2.212, 2.041 (second generation Eurosoils ES-1, ES-2, ES-3, ES-4, shake flask-batch equilibrium-HPLC/UV and HPLC-k′ correlation, Gawlik et al. 2000)

Environmental Fate Rate Constants, k, or Half-Lives, $t_{1/2}$:
Volatilization:
Photolysis:
Hydrolysis:

Oxidation: rate constant k = 1 × 10^4 M^{-1} s^{-1} for oxidation by RO_2 radical at 30°C in aquatic systems with $t_{½}$ = 0.8 d (Howard 1972; Hendry et al. 1974; quoted, Mill 1982);

k < 2 × 10^2 M^{-1} s^{-1} for oxidation by singlet oxygen at 25°C in aquatic systems with $t_{½}$ > 100 yr (Foote 1976; Mill 1979; quoted, Mill 1982).

Biodegradation: decomposition by a microflora in 4 d (Alexander & Lustigman 1966; quoted, Verschueren 1983); average biodegradation rate of 20 mg COD g^{-1} h^{-1} for 97.7% removal (Scow 1982).

Biotransformation:

Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants:

Half-Lives in the Environment:

Surface water: estimated $t_{½}$ = 1.0 d for methylaniline in Rhine River in case of a first order reduction process (Zoeteman et al. 1980)

TABLE 16.1.3.8.1
Reported vapor pressures of *p*-toluidine at various temperatures

Kahlbaum 1898		**Stull 1947**	
static method-manometer*		**summary of literature data**	
t/°C	**P/Pa**	**t/°C**	**P/Pa**
46.9	133.3	42.0	133.3
55.9	266.6	68.2	666.6
62.0	400.0	81.8	1333
66.4	533.3	95.8	2666
70.1	666.6	111.5	5333
82.2	1333.2	121.5	7999
95.6	2666.4	133.7	13332
104.3	3999.7	154.0	26664
110.7	5332.9	176.9	53329
115.8	6666.1	200.4	101325
126.1	9999.2		
133.7	13332	mp/°C	44.5
154.7	26664		
166.9	39997		
176.9	53329		
184.6	66661		
191.1	79993		
196.9	93326		
200.4	101325		

*complete list see ref.

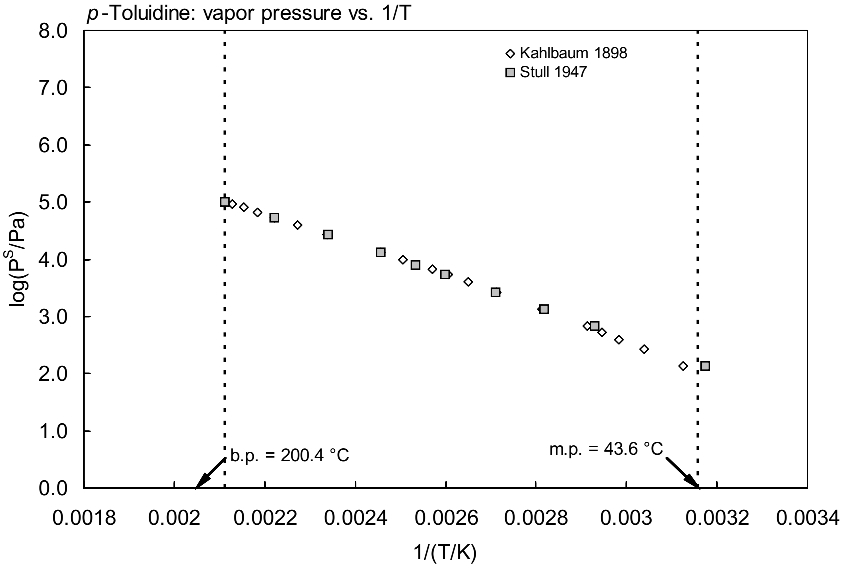
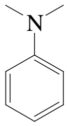


FIGURE 16.1.3.8.1 Logarithm of vapor pressure versus reciprocal temperature for *p*-toluidine.

16.1.3.9 N,N′-Dimethylaniline



Common Name: N,N′-Dimethylaniline
Synonym: N,N′-dimethylbenzenamine
Chemical Name: N,N′-dimethylaniline
CAS Registry No: 121-69-7
Molecular Formula: $C_8H_{11}N$, $C_6H_5N(CH_3)_2$
Molecular Weight: 121.180
Melting Point (°C):
2.42 (Lide 2003)
Boiling Point (°C):
194.0 (Weast 1982–83)
194.15 (Lide 2003)
Density (g/cm^3 at 20°C):
0.9557 (Weast 1982–83)
Molar Volume (cm^3/mol):
154.6 (calculated-Le Bas method at normal boiling point)
Dissociation Constant pK:
5.15 (pK_{BH^+}, Riddick et al. 1986)
5.10 (Sangster 1993)
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
11.42 (Tsonopoulos & Prausnitz 1971)
Entropy of Fusion, ΔS_{fus} (J/mol K):
41.46 (Tsonopoulos & Prausnitz 1971)
Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F: 1.0

Water Solubility (g/m^3 or mg/L at 25°C or as indicated):
1105 (shake flask-GC, Chiou et al. 1982)
1540, 1680 (20, 30°C, shake flask-GC/TC, measured range 0–90°C, Stephenson 1993c)

Vapor Pressure (Pa at 25°C and reported temperature dependence equations):
106.3 (extrapolated-regression of tabulated data, temp range 20.0–193.1°C, Stull 1947)
133.3 (29.5°C, Stull 1947)
83.90 (calculated-Antoine eq., Boublik et al. 1973)
$\log (P/atm) = [-0.2185 \times 11320.4/(T/K)] + 8.197379$; temp range: 29.5–193°C, (Antoine eq., Weast 1972–73)
68.95 (calculated-Cox eq., Chao et al. 1983)
$\log (P/mmHg) = [1 - 466.445/(T/K)] \times 10\hat{}\{0.909397 - 7.07673 \times 10^{-4} \pm (T/K) + 5.69581 \times 10^{-7} \pm (T/K)^2\}$; temp range 275.0–685.0 K (Cox eq., Chao et al. 1983)
84.5 (extrapolated-Antoine eq., Boublik et al. 1984)
$\log (P/kPa) = 6.5031 - 1865.084/(211.171 + t/°C)$; temp range 71.02–196.8°C (Antoine eq. from reported exptl. data, Boublik et al. 1984)
83.91 (extrapolated-Antoine eq., Dean 1985, 1992)
$\log (P/mmHg) = 6.91048 - 946.35/(246.68 + t/°C)$; temp range –87 to 7°C (Antoine eq., Dean 1985, 1992)
670.0 (quoted from Stull 1947, Riddick et al. 1986)
107.0 (extrapolated-Antoine eq., Stephenson & Malanowski 1987)
$\log (P_L/kPa) = 7.07329 - 2301.63/(-12.001 + T/K)$; temp range 302–467 K (liquid, Antoine eq.-I, Stephenson & Malanowski 1987)
$\log (P_L/kPa) = 6.55663 - 1864.075/(-55.854 + T/K)$; temp range 363–418 K (liquid, Antoine eq.-II, Stephenson & Malanowski 1987)

$\log (P/\text{mmHg}) = 2–.177 - 3.1095 \times 10^3/(T/K) - 4.0127 \cdot \log (T/K) + 5.8538 \times 10^{-10} \cdot (T/K) + 3.5387 \times 10^{-7} \cdot (T/K)^2$; temp range 276–687 K (vapor pressure eq., Yaws 1994)

Henry's Law Constant ($Pa \cdot m^3/mol$):

11.73	(calculated-P/C)

Octanol/Water Partition Coefficient, log K_{OW}:

2.31	(shake flask-UV, Fujita et al. 1964)
2.62	(shake flask-UV at pH 7.4, Rogers & Cammarata 1969)
1.66	(shake flask-UV, Leo et al. 1971)
2.29	(shake flask-UV, Yaguzhinskii et al. 1973)
2.30	(shake flask at pH 7, Unger et al. 1978)
2.43	(HPLC-RT correlation, Miyake et al. 1986)
2.28	(RP-HPLC-RT correlation, ODS column with masking agent, Bechalany et al. 1989)
2.32	(CPC correlation, El Tayar et al. 1991)
2.31	(recommended, Sangster 1993)
2.31	(recommended, Hansch et al. 1995)
2.05	(microemulsion electrokinetic chromatography-retention factor correlation, Poole et al. 2000)

Octanol/Air Partition Coefficient, log K_{OA}:

Bioconcentration Factor, log BCF:

Sorption Partition Coefficient, log K_{OC}:

1.99; 2.53; 2.06	(Alfisol soil; Podzol soil; sediment, von Oepen et al. 1991)
2.26, 1.89	(soil, quoted, calculated-MCI χ and fragment contribution, Meylan et al. 1992)
2.26	(soil, calculated-MCI $^1\chi$, Sabljic et al. 1995)

Environmental Fate Rate Constants, k, or Half-Lives, $t_{1/2}$:

Volatilization:

Photolysis:

Oxidation: rate constant k; for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO3} with NO_3 radical and k_{O3} with O_3 or as indicated, *data at other temperatures see reference:

$k = 1 \times 10^4\ M^{-1}\ s^{-1}$ for oxidation by RO_2 radical at 30°C in aquatic systems with $t_{1/2} = 0.8$ d (Howard 1972; Hendry et al. 1974; quoted, Mill 1982)

$k < 2 \times 10^2\ M^{-1}\ s^{-1}$ for oxidation by singlet oxygen at 25°C in aquatic systems with $t_{1/2} > 100$ yr (Foote 1976; Mill 1979; quoted, Mill 1982)

k_{OH}*(exptl) = $(1.48 \pm 0.11) \times 10^{-10}\ cm^3\ molecule^{-1}\ s^{-1}$, measured range 278–464 K; $k_{O3} = (9.1 \pm 1.0) \times 10^{-18}\ cm^3\ molecule^{-1}\ s^{-1}$ at 296 ± 2 K (relative rate method, Atkinson et al. 1987)

$k_{OH} = 1.5 \times 10^{-10}\ cm^3\ molecule^{-1}\ s^{-1}$ with atmospheric lifetimes of 1.9 h in clean troposphere and 1.0 h in moderately polluted atmosphere; $k_{O3} = 9.1 \times 10^{-18}\ cm^3\ molecule^{-1}\ s^{-1}$ with atmospheric lifetimes of 1.8 d in clean troposphere and 14 h in moderately polluted atmosphere at room temp. (Atkinson et al. 1987)

k_{OH}(calc) = $4.66 \times 10^{-10}\ cm^3\ molecule^{-1}\ s^{-1}$, k_{OH}(obs) = $1.48 \times 10^{-10}\ cm^3\ molecule^{-1}\ s^{-1}$, (SAR structure-activity relationship, Atkinson 1987)

k_{OH}(calc) = $1.78 \times 10^{-10}\ cm^3\ molecule^{-1}\ s^{-1}$ (molecular orbital calculations, Klamt 1993)

Hydrolysis:

Biodegradation: aerobic $t_{1/2}$ = 672–4320 h, based on unacclimated aqueous screening test data and anaerobic $t_{1/2}$ = 2880–17280 h, based on estimated unacclimated aqueous aerobic biodegradation half-life (Howard et al. 1991)

Biotransformation:

Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants:

Half-Lives in the Environment:

Air: atmospheric lifetimes of 1.9 h in clean troposphere and 1.0 h in moderately polluted atmosphere, based on the gas-phase reaction with hydroxyl radical in air at room temp.; atmospheric lifetimes of 1.8 d in clean troposphere and 14 h in moderately polluted atmosphere, based on the gas-phase reaction with O_3 in air at room temp. (Atkinson et al. 1987);

$t_{½}$ = 2.7–21 h, based on photooxidation half-life in air (Howard et al. 1991);

atmospheric transformation lifetime was estimated to be < 1 d (Kelly et al. 1994).

Surface water: estimated $t_{½}$ = 2.3 d in Rhine River in case of a first order reduction process (Zoeteman et al. 1980)

$t_{½}$ = 19.3–1925 h, based on reaction with singlet oxygen in aqueous solution (Howard et al. 1991)

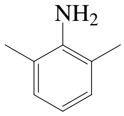
Groundwater: $t_{½}$ = 1344–8640 h, based on estimated unacclimated aqueous aerobic biodegradation half-life (Howard et al. 1991)

Sediment:

Soil: $t_{½}$ = 672–4320 h, based on estimated unacclimated aqueous aerobic biodegradation half-life (Howard et al. 1991)

Biota:

16.1.3.10 2,6-Xylidine (2,6-Dimethylbenzeneamine)



Common Name: 2,6-Xylidine
Synonym: 2,6-dimethylaniline, 2,6-dimethylbenzeneamine
Chemical Name: 2,6-dimethylaniline
CAS Registry No: 87-62-7
Molecular Formula: $C_8H_{11}N$, 2,6-$(CH_3)_2C_6H_3NH_2$
Molecular Weight: 121.180
Melting Point (°C):
    11.20 (Weast 1982–83; Riddick et al. 1986; Lide 2003)
Boiling Point (°C):
    214.0 (at 739 mm Hg, Weast 1982–83; Verschueren 1983)
    215 (Lide 2003)
Density (g/cm^3 at 20°C):
    0.9842 (Weast 1982–83; Riddick et al. 1986)
Molar Volume (cm^3/mol):
    123.1 (20°C, calculated-density)
    154.6 (calculated-Le Bas method at normal boiling point)
Dissociation Constant pK:
    3.95 (pK_{BH^+}, Riddick et al. 1986)
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
Entropy of Fusion, ΔS_{fus} (J/mol K):
Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F: 1.0

Water Solubility (g/m^3 or mg/L at 25°C):
    slightly soluble (Dean 1985; Budavari 1989)

Vapor Pressure (Pa at 25°C and reported temperature dependence equations):
    43.03 (extrapolated-regression of tabulated data, temp range 44–217.9°C, Stull 1947)
    $\log (P/\text{atm}) = [1 - 490.795/(T/K)] \times 10^{\{0.926009 - 6.89676 \times 10^{-4} \cdot (T/K) + 5.31053 \times 10^{-7} \cdot (T/K)^2\}}$; temp range: 285.0–720.0 K (Cox eq., Chao et al. 1983)
    17.33 (Howard et al. 1986)
    670.0 (quoted from Stull 1947, Riddick et al. 1986)
    35.99 (calculated-solvatochromic parameters, Banerjee et al. 1990)

Henry's Law Constant (Pa·m^3/mol at 25°C):
    17.28 (calculated-P/C from selected value)

Octanol/Water Partition Coefficient, log K_{OW}:
    1.96 (calculated, Verschueren 1983)
    1.91 (calculated-CLOGP, Jäckel & Klein 1991)

Octanol/Air Partition Coefficient, log K_{OA}:

Bioconcentration Factor, log BCF:

Sorption Partition Coefficient, log K_{OC}:

Environmental Fate Rate Constants, k, or Half-Lives, $t_{½}$:

Volatilization:

Photolysis:

Oxidation: rate constant $k = 1 \times 10^4\ M^{-1}\ s^{-1}$ for oxidation by RO_2 radical at 30°C in aquatic systems with $t_{½} = 0.8$ d (Howard 1972; Hendry et al. 1974; quoted, Mill 1982);

$k < 2 \times 10^2\ M^{-1}\ s^{-1}$ for oxidation by singlet oxygen at 25°C in aquatic systems with $t_{½} > 100$ yr (Foote 1976; Mill 1979; quoted, Mill 1982);

photooxidation $t_{½} = 0.33–3.3$ h in air, based on estimated reaction rate constant with OH radical (Atkinson 1987; selected, Howard et al. 1991) and photooxidation $t_{½} = 62.4–3480$ h in water, based on reaction rate constants of amine class with $RO_2\cdot$ and OH radicals in water (Güesten et al. 1981; Mill & Mabey 1985; selected, Howard et al. 1991).

Hydrolysis: no hydrolyzable group (Howard et al. 1991).

Biodegradation: aqueous aerobic biodegradation $t_{½} = 672–4320$ h, based on a biological screening study (Baird et al. 1977; selected Howard et al. 1991) and a soil degradation study (Bollag et al. 1978; selected, Howard et al. 1991); aqueous anaerobic biodegradation $t_{½} = 2688–17280$ h, based on estimated aqueous biodegradation half-lives (Howard et al. 1991).

Biotransformation:

Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants:

Half-Lives in the Environment:

Air: $t_{½} = 0.33–3.3$ h, based on estimated photooxidation half-lives in air from estimated reaction rate constant with OH radical in air (Atkinson 1987; selected, Howard et al. 1991).

Surface water: estimated $t_{½} = 2.0$ d for dimethylaniline in Rhine River in case of a first order reduction process (Zoeteman et al. 1980)

$t_{½} = 62.4–3480$ h, based on photooxidation half-life in water (Howard et al. 1991).

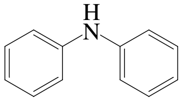
Groundwater: $t_{½} = 1344–8640$ h, based on estimated aqueous aerobic biodegradation half-lives (Howard et al. 1991).

Sediment:

Soil: $t_{½} = 72–7584$ h, based on soil persistence and soil biodegradation studies (Bollag et al. 1978; Medvedev & Davidov 1981; selected, Howard et al. 1991).

Biota:

16.1.3.11 Diphenylamine



Common Name: Diphenylamine
Synonym: N-diphenylamine, N-phenyl aniline, DPA
Chemical Name: N-diphenylamine, diphenylamine
CAS Registry No: 122-39-4
Molecular Formula: $C_{12}H_{11}N$, $C_6H_5NHC_6H_5$
Molecular Weight: 169.222
Melting Point (°C):
53.2 (Lide 2003)
Boiling Point (°C):
302.0 (Stull 1947; Weast 1982–83; Verschueren 1983; Dean 1985; Lide 2003)
Density (g/cm^3 at 20°C):
1.160 (Weast 1982–83; Dean 1985)
Molar Volume (cm^3/mol):
145.9 (20°C calculated-density)
200.3 (calculated-Le Bas method at normal boiling point)
Dissociation Constant, pK_a:
0.89 (Perrin 1972)
0.90 (protonated cation + 1, Dean 1985)
0.78 (Sangster 1989)
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
17.53 (Tsonopoulos & Prausnitz 1971)
Entropy of Fusion, ΔS_{fus} (J/mol K):
53.56 (Tsonopoulos & Prausnitz 1971)
54.81; 56.5 (exptl., calculated, Yalkowsky & Valvani 1980)
Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F: 0.529 (mp at 53.2°C)

Water Solubility (g/m^3 or mg/L at 25°C as indicated):
150 (20–25°C, shake flask-gravimetric method, Dehn 1917)
308 (Briggs 1981)
48 (20°C, shake flask and membrane filter-fluorophotometric, Hashimoto et al. 1982)
52, 54 (20°C, shake flask and glass fiber filters-fluorophotometric, Hashimoto et al. 1982)
300 (Verschueren 1983)
53 (20°C, Yalkowsky et al. 1987)

Vapor Pressure (Pa at 25°C and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):
0.5682* (extrapolated-regression of tabulated data, temp range 108.3–302°C, Stull 1947)
$\log (P/\text{mmHg}) = [-0.2185 \times 14920.3/(T/K)] + 8.564067$; temp range 108.3–302°C (Antoine eq., Weast 1972–73)
$\log (P/\text{atm}) = [1 - 575.114/(T/K)] \times 10^{\{0.936992 - 6.17195 \times 10^{-4}\cdot(T/K) + 4.32696 \times 10^{-7}\cdot(T/K)^2\}}$; temp range 335.0–670.0 K (Cox eq., Chao et al. 1983)
0.0612 (calculated-Antoine eq.-I, Stephenson & Malanowski 1987)
$\log (P_S/\text{kPa}) = 12.704 - 5043.9/(T/K)$; temp range 298–323 K (solid, Antoine eq.-I, Stephenson & Malanowski 1987)
$\log (P_L/\text{kPa}) = 7.15045 - 2778.28/(-35.102 + T/K)$; temp range 381–575 K (liquid, Antoine eq.-II, Stephenson & Malanowski 1987)
$\log (P_L/\text{kPa}) = 6.5746 - 2430.7/(-41.15 + T/K)$; temp range 573–673 K (liquid, Antoine eq.-III, Stephenson & Malanowski 1987)
$\log (P/\text{mmHg}) = 9.7736 - 3.9008 \times 10^3/(T/K) + 0.91207\cdot\log (T/K) - 5.898 \times 10^{-3}\cdot(T/K) + 2.3012 \times 10^{-6}\cdot(T/K)^2$; temp range 326–817 K (vapor pressure eq., Yaws 1994)

Henry's Law Constant (Pa m^3/mol at 25°C):

0.285	(calculated-P/C, Meylan & Howard 1991)
0.106	(estimated-bond contribution, Meylan & Howard 1991)
0.035	(calculated-P/C from selected values)

Octanol/Water Partition Coefficient, log K_{OW}:

3.23	(shake flask-UV, pH 7.4, Rogers & Cammarata 1969)
3.34	(unpublished result, Leo et al. 1971)
3.34, 3.50, 3.72	(unpublished results, Rekker 1977)
2.37	(RP-HPLC-RT correlation, Veith et al. 1979a)
3.45	(Hansch & Leo 1979)
3.42	(shake flask-UV, Briggs 1981)
3.37	(inter-laboratory shake flask average, Eadsforth & Moser 1983)
3.72 ± 0.03	(HPLC-RV correlation-ALPM, Garst & Wilson 1984)
2.69	(HPLC-RT correlation, average, Ge et al. 1987)
3.42	(shake flask, Log P Database, Hansch & Leo 1987)
3.50	(recommended, Sangster 1989, 1993)
3.70, 3.68	(shake flask, HPLC-RT correlation, Wang et al. 1989)
3.50	(recommended, Hansch et al. 1995)
2.99, 3.13, 3.04, 3.18	(HPLC-k′ correlation, different combinations of stationary and mobile phases under isocratic conditions, Makovskaya et al. 1995)
3.35	(microemulsion electrokinetic chromatography-retention factor correlation, Poole et al. 2000)

Octanol/Air Partition Coefficient, log K_{OA}:

7.64	(calculated-S_{oct} and vapor pressure P, Abraham et al. 2001)

Bioconcentration Factor, log BCF:

1.48	(fathead minnow, Veith et al. 1979b)
1.48, 2.10	(quoted, calculated-K_{OW}, Mackay 1982)

Sorption Partition Coefficient, log K_{OC}:

2.78	(sorption isotherm-GC, converted from K_{OM} organic matter-water in various soils, Briggs 1981)
2.78, 3.28	(soil, calculated-MCI χ and fragment contribution, Meylan et al. 1992)
3.30	(calculated-K_{OW}, Kollig 1993)
2.70	(soil, calculated-MCI $^1\chi$, Sabljic et al. 1995)
2.80, 2.93	(RP-HPLC-k′ correlation including MCI related to non-dispersive intermolecular interactions, hydrogen-bonding indicator variable, Hong et al. 1996)

Environmental Fate Rate Constants, k, or Half-Lives, $t_{1/2}$:

Volatilization:

Photolysis:

Oxidation: rate constant $k = 1 \times 10^4\ M^{-1}\ s^{-1}$ for oxidation by RO_2 radical at 30°C in aquatic systems with $t_{1/2} = 0.8$ d (Howard 1972; Hendry et al. 1974; quoted, Mill 1982);

$k < 2 \times 10^2\ M^{-1}\ s^{-1}$ for oxidation by singlet oxygen at 25°C in aquatic systems with $t_{1/2} > 100$ yr (Foote 1976; Mill 1979; quoted, Mill 1982);

photooxidation $t_{1/2}$ = 31–1740 h in water, based on photooxidation rate constants with OH and RO_2 radicals for the amine class (Mill & Mabey 1985; Güesten et al. 1981; selected, Howard et al. 1991);

photooxidation $t_{1/2}$ = 0.247–2.47 h, based on estimated rate data for the reaction with hydroxyl radicals in air (Atkinson 1987; selected, Howard et al. 1991).

Hydrolysis: rate constant $k = 1.2 \times 10^{10}$ L mol^{-1} s^{-1} for reactions with hydroxyl radical in aqueous solution, (Buxton et al. 1986; quoted, Armbrust 2000);

measured hydroxy radical rate constant $k = 4.9 \times 10^{13}\ M^{-1}\cdot h^{-1}$ (Armbrust 2000)

Biodegradation: aqueous aerobic $t_{1/2}$ = 168–672 h, based on estimated aqueous aerobic biodegradation screening test data (Malaney 1960; quoted, Howard et al. 1991);

aqueous anaerobic $t_{1/2}$ = 672–2688 h, based on estimated aqueous aerobic biodegradation half-life (Howard et al. 1991).

Biotransformation:

Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants:

Half-Lives in the Environment:

Air: photooxidation $t_{1/2}$ = 0.247–2.47 h, based on estimated rate data for the reaction with hydroxyl radical in air (Atkinson 1987; selected, Howard et al. 1991).

Surface water: photooxidation $t_{1/2}$ = 31–1740 h in water, based on photooxidation rate constants with OH and RO_2 radicals for the amine class (Mill & Mabey 1985; Güesten et al. 1981; selected, Howard et al. 1991); $t_{1/2}$ = 31–672 h, based on estimated unacclimated aqueous aerobic degradation half-life and photooxidation half-life in water (Howard et al. 1991).

Groundwater: $t_{1/2}$ = 336–1344 h, based on estimated aqueous aerobic biodegradation half-life (Howard et al. 1991).

Sediment:

Soil: $t_{1/2}$ = 168–672 h, based on estimated aqueous aerobic biodegradation half-life (Howard et al. 1991).

Biota:

TABLE 16.1.3.11.1
Reported vapor pressures of diphenylamine at various temperatures

Stull 1947	
summary of literature data	
t/°C	**P/Pa**
108.3	133.3
141.7	666.6
157.0	1333
175.2	2666
194.3	5333
206.9	7999
222.9	13332
247.5	26664
274.1	53329
302.0	101325
mp/°C	52.9

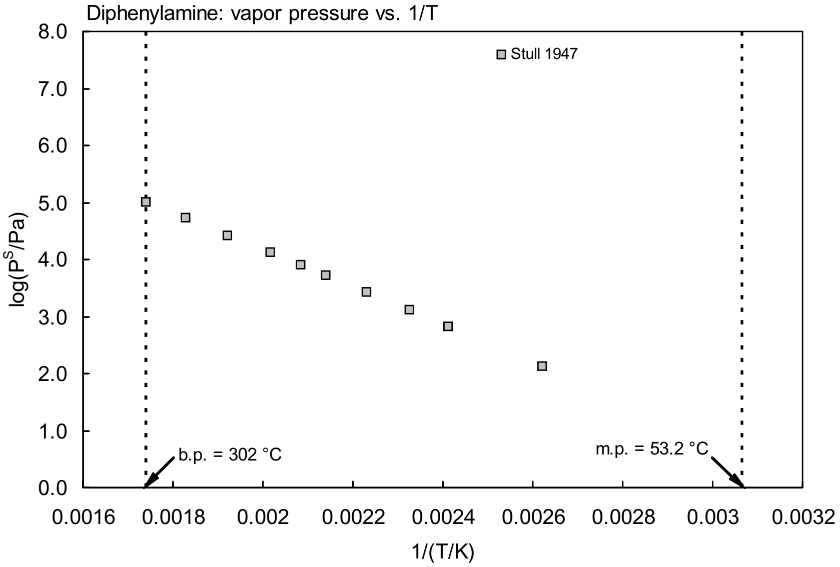
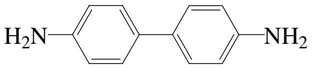


FIGURE 16.1.3.11.1 Logarithm of vapor pressure versus reciprocal temperature for diphenylamine.

16.1.3.12 Benzidine



Common Name: Benzidine
Synonym: *p,p′*-bianiline, 4,4′-diaminobiphenyl, 4,4′-biphenyldiamine, (1,1′-biphenyl)-4,4′-diamine
Chemical Name: *p*-benzidine
CAS Registry No: 92-87-5
Molecular Formula: $C_{12}H_{12}N_2$, $NH_2C_6H_4C_6H_4NH_2$
Molecular Weight: 184.236
Melting Point (°C):
128 (Weast 1982–83)
120 (Lide 2003)
Boiling Point (°C):
400 (Weast 1982–83)
401 (Lide 2003)
Density (g/cm³ at 20°C):
1.250 (Verschueren 1983)
Molar Volume (cm³/mol):
213.0 (calculated-Le Bas method at normal boiling point)
Dissociation Constant, pK_a:
4.66 (pK_1), 3.57 (pK_2) (30°C, Perrin 1965; quoted, Mabey et al. 1982; Howard 1989)
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
Entropy of Fusion, ΔS_{fus} (J/mol K):
Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F: 0.117 (mp at 120°C)

Water Solubility (g/m³ or mg/L at 25°C as indicated):
400 (12°C, Verschueren 1977, 1983)
520 (Shriner et al. 1978)
360 (24°C at pH 5.9, shake flask-LSC, Means et al. 1980)
276 (20°C, Schmidt-Bleek et al. 1982)
359 (Gerstl & Helling 1987)

Vapor Pressure (Pa at 25°C):
0.724 (calculated-Trouton's rule, Mabey et al. 1982)
1.0×10^{-6} (20°C, Schmidt-Bleek et al. 1982)

Henry's Law Constant (Pa·m³/mol at 25°C or as indicated):
3.93×10^{-6} (estimated, Hine & Mookerjee 1975)
0.0394 (calculated-P/C at 12°C, Mabey et al. 1982)
4.60×10^{-7} (calculated-P/C, this work)

Octanol/Water Partition Coefficient, log K_{OW}:
1.34 (shake flask, Korenman 1971)
1.34 (recommended, Sangster 1993)
1.34 (recommended, Hansch et al. 1995)

Octanol/Air Partition Coefficient, log K_{OA}:

Bioconcentration Factor, log BCF:
1.74, 2.66, 2.81, 3.4 (fish, mosquitoes, snail, algae; Lu et al. 1977)
1.60 (bluegills, USEPA 1980; quoted, Howard 1989)
1.00 (microorganisms-water, calculated-K_{OW}, Mabey et al. 1982)

1.90, 2.93, 3.08 (golden ide, algae, activated sludge, Freitag et al. 1985)

Sorption Partition Coefficient, log K_{OC}:

1.66	(soil/sediment, equilibrium sorption isotherm by shake flask-LSC at pH 5.9, Means et al. 1980)
1.02	(sediment-water, calculated-K_{OW}, Mabey et al. 1982)
5.95; 5.68; 5.35; 5.91	(Russell soil; Chalmers soil; Kokomo soil; Milford soil, Graveel et al. 1986)
3.00	(calculated-MCI χ, Gerstl & Helling 1987)
3.46, 3.44	(soil, quoted, calculated-MCI χ and fragment contribution, Meylan et al. 1992)
1.26	(calculated-K_{OW}, Kollig 1993)
3.46	(soil, calculated-MCI $^1\chi$, Sabljic et al. 1995)

Environmental Fate Rate Constants, k, or Half-Lives, $t_{1/2}$:

Volatilization:

Photolysis:

Hydrolysis:

Oxidation: aqueous oxidation rate constants for singlet oxygen $k < 4 \times 10^7$ M^{-1} h^{-1} and for peroxy radical of 1.1×10^8 M^{-1} h^{-1} at 25°C (Mabey et al. 1982);

photooxidation $t_{1/2}$ = 0.312–3.12 h, based on estimated rate constant for the reaction with hydroxyl radical in air (Atkinson 1987; quoted, Howard et al. 1991).

Biodegradation: aqueous aerobic $t_{1/2}$ = 48–192 h, based on aerobic soil die-away test data (Lu et al. 1977; quoted, Howard et al. 1991);

overall biodegradation $t_{1/2}$ = 76 d, when in sludge was applied to a sandy loam soil in a biological soil reactor and worked into the top 20 cm of soil (Kincannon & Lin 1985; quoted, Howard 1989);

aqueous aerobic $t_{1/2}$ = 192–768 h, based on estimated unacclimated aqueous aerobic biodegradation half-life (Howard et al. 1991).

Biotransformation: rate constant for bacterial transformation of 1×10^{-10} $mL \cdot cell^{-1} \cdot h^{-1}$ in water (Mabey et al. 1982).

Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants:

Half-Lives in the Environment:

Air: $t_{1/2}$ = 0.312–3.12 h, based on estimated rate constant for the reaction with hydroxyl radical in air (Atkinson 1987; quoted, Howard et al. 1991);

estimated $t_{1/2}$ ~ 1 d for the reaction with hydroxyl radical and ozone (Howard 1989);

atmospheric transformation lifetime was estimated to be < 1 d (Kelly et al. 1994).

Surface water: estimated $t_{1/2}$ ~ 1 d for the reaction with radicals and redox reactions with naturally occurring cations, etc. and perhaps with photodegradation (Howard 1989);

$t_{1/2}$ = 31.2–192 h, based on estimated photooxidation half-life in water and estimated unacclimated aqueous aerobic biodegradation half-life (Howard et al. 1991).

Ground water: $t_{1/2}$ = 96–484 h, based on estimated unacclimated aqueous aerobic biodegradation half-life (Howard et al. 1991).

Sediment:

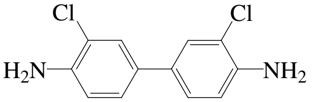
Soil: $t_{1/2}$ < 10 d in soil (USEPA 1979; quoted, Ryan et al. 1988);

$t_{1/2}$ = 48–192 h, based on aerobic soil die-away test data (Lu et al. 1977; quoted, Howard et al. 1991);

overall biodegradation $t_{1/2}$ = 76 d, when in sludge was applied to a sandy loam soil in a biological soil reactor and worked into the top 20 cm of soil (Kincannon & Lin 1985; quoted, Howard 1989).

Biota: depuration $t_{1/2}$ ~ 7 d from bluegills (Lu et al. 1977; quoted, Howard 1989).

16.1.3.13 3,3′-Dichlorobenzidine



Common Name: 3,3′-Dichlorobenzidine
Synonym: 3,3′-dichloro-4,4′-diamino(1,1′-biphenyl), DCB
Chemical Name: 3,3′-dichlorobenzidine
CAS Registry No: 91-94-1
Molecular Formula: $C_{12}H_{10}Cl_2N_2$, $NH_2C_6H_3(Cl)C_6H_3(Cl)NH_2$
Molecular Weight: 253.126
Melting Point (°C):
132.5 (Lide 2003)
Boiling Point (°C):
Density (g/cm^3 at 20°C):
Molar Volume (cm^3/mol):
254.8 (calculated-Le Bas method at normal boiling point)
Dissociation Constant, pK_b:
11.7 (Kollig 1993)
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
Entropy of Fusion, ΔS_{fus} (J/mol K):
Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F: 0.0882 (mp at 132.5°C)

Water Solubility (g/m^3 or mg/L at 25°C or as indicated):
4.00 (22°C, as dihydrochloride, Banerjee et al. 1978)
3.99 (22°C, at pH 6.9 as DCB.2HCl, quoted, Verschueren 1983)
3.11 (shake flask-UV/LSC, Banerjee et al. 1980)

Vapor Pressure (Pa at 25°C):
0.00133 (estimated, Mabey et al. 1982)

Henry's Law Constant (Pa·m^3/mol at 25°C):
0.0811 (calculated-P/C, Mabey et al. 1982)

Octanol/Water Partition Coefficient, log K_{OW}:
3.02 (calculated as per Leo et al.1971)
3.51 (23°C, shake flask, Banerjee et al. 1980)
3.35 (calculated-activity coeff. γ from UNIFAC, Banerjee & Howard 1988)
3.51 (recommended, Sangster 1993)
3.51 (recommended, Hansch et al. 1995)

Octanol/Air Partition Coefficient, log K_{OA}:

Bioconcentration Factor, log BCF:
2.70 (bluegill sunfish, Appleton & Sikka 1980)
2.97 (microorganisms-water, calculated-K_{OW}, Mabey et al. 1982)
2.79, 2.97, 3.49 (fish, algae, activated sludge, Freitag et al. 1985)

Sorption Partition Coefficient, log K_{OC}:
3.19 (sediment-water, calculated-K_{OW}, Mabey et al. 1982)
4.35, 3.87 (soil: quoted, calculated-MCI χ and fragment contribution, Meylan et al. 1992)
3.30 (calculated-K_{OW}, Kollig 1993)
4.35 (soil, calculated-MCI $^1\chi$, Sabljic et al. 1995)

Environmental Fate Rate Constants, k, or Half-Lives, $t_{½}$:

Volatilization:

Photolysis:

direct aqueous photolysis rate constant $k = 2.1 \times 10^{-6}$ h^{-1} in summer at 40°N latitude (Mabey et al. 1982);

both aqueous and atmospheric photolysis $t_{½}$ = 0.025–0.075 h, based on direct photolysis in distilled water in midday summer sunlight (Banerjee et al. 1978; Sikka et al. 1978; quoted, Callahan et al. 1979; Howard et al. 1991) and approximate winter sunlight direct photolysis half-life (Banerjee et al. 1978; Sikka et al. 1978; Lyman et al. 1982; quoted, Howard et al. 1991).

Hydrolysis:

Oxidation: aqueous oxidation rate constants for singlet oxygen $k < 4 \times 10^7$ M^{-1} h^{-1} and for peroxy radical $k < 4 \times 10^7$ M^{-1} h^{-1} at 25°C (Mabey et al. 1982);

photooxidation $t_{½}$ = 31.2 – 1740 h in water, based on estimated rate constants for reactions with OH and RO_2 radicals in water (Mill & Mabey 1985; quoted, Howard et al. 1991);

photooxidation $t_{½}$ = 0.905 – 9.05 h in air, based on estimated rate constant for the reaction with hydroxyl radical in air (Atkinson 1987; quoted, Howard et al. 1991)

Biodegradation: aqueous aerobic $t_{½}$ = 672 – 4320 h, based on lake die-away study test data (Appleton et al. 1978; quoted, Howard et al. 1991) and a soil die-away test (Boyd et al. 1984; quoted, Howard et al. 1991);

aqueous anaerobic $t_{½}$ = 2688 – 17280 h, based on estimated unacclimated aqueous aerobic biodegradation half-life (Howard et al. 1991).

Biotransformation: rate constant for bacterial transformation $k = 3 \times 10^{-12}$ $mL\cdot cell^{-1}\cdot h^{-1}$ in water (Mabey et al. 1982).

Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants:

Half-Lives in the Environment:

Air: $t_{½}$ = 0.905 – 9.05 h, based on estimated rate constant for the reaction with hydroxyl radical in air (Atkinson 1987; quoted, Howard et al. 1991);

estimated $t_{½}$ ~ 1 d for the reaction with hydroxyl radical and ozone (Howard 1989);

atmospheric transformation lifetime by photolysis was estimated to be < 1 d (Kelly et al 1994).

Surface water: $t_{½}$ = 0.025 – 0.075 h, based on direct photolysis in distilled water in midday summer sunlight (Banerjee et al. 1978; Sikka et al. 1978; quoted, Howard et al. 1991) and approximate winter sunlight direct photolysis half-life (Banerjee et al. 1978; Sikka et al. 1978; Lyman et al. 1982; quoted, Howard et al. 1991).

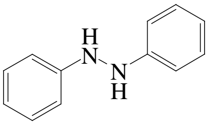
Ground water: $t_{½}$ = 1344 – 8640 h, based on estimated unacclimated aqueous aerobic biodegradation half-life (Howard et al. 1991).

Sediment: $t_{½}$ = 30 min by suspended microcrystalline clays may be considered the most important fate process in the aquatic environment (Callahan et al. 1979).

Soil: $t_{½}$ = 672 – 4320 h, based on estimated unacclimated aqueous aerobic biodegradation half-life (Howard et al. 1991).

Biota:

16.1.3.14 N,N′-Bianiline



Common Name: N,N′-Bianiline
Synonym: 1,2-diphenylhydrazine, hydrazobenzene
Chemical Name: 1,2-diphenylhydrazine, hydrazobenzene
CAS Registry No: 122-66-7
Molecular Formula: $C_{12}H_{12}N_2$, $C_6H_5NHNHC_6H_5$
Molecular Weight: 184.236
Melting Point (°C):
131 (Weast 1982–83; Lide 2003)
Boiling Point (°C):
293 (as azobenzene, IARC 1975)
Density (g/cm^3 at 20°C):
1.158 (16°C, Weast 1982–83)
Molar Volume (cm^3/mol):
213.0 (calculated-Le Bas method at normal boiling point)
Dissociation constant pK_b:
13.2 (Kollig 1993)
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
Entropy of Fusion, ΔS_{fus} (J/mol K):
Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F: 0.0912 (mp at 131°C)

Water Solubility (g/m^3 or mg/L at 25°C):
0.252 (20°C, as azobenzene, Takagishi et al. 1968)

Vapor Pressure (Pa at 25°C or as indicated and reported temperature dependence equations):
0.00347 (quoted, Mabey et al. 1982)
$\log (P/mmHg) = 16.8982 - 5.0039 \times 10^3/(T/K) - 0.35846 \cdot \log (T/K) - 9.9629 \times 10^{-3} \cdot (T/K) + 4.2938 \times 10^{-6} \cdot (T/K)^2$;
temp range 404–573 K (vapor pressure eq., Yaws 1994)

Henry's Law Constant (Pa·m^3/mol at 25°C):
3.45×10^{-4} (calculated-P/C, Mabey et al. 1982)

Octanol/Water Partition Coefficient, log K_{OW}:
3.82 (shake flask-UV as for azobenzene, Fujita et al. 1964)
3.03 (calculated as per Leo et al. 1971, Callahan et al. 1979)
2.94 (shake flask, Hansch & Leo 1979; 1987)
2.94 (recommended, Sangster 1993)
2.94 (recommended, Hansch et al. 1995)

Octanol/Air Partition Coefficient, log K_{OA}:

Bioconcentration Factor, log BCF:
2.46 (microorganisms-water, calculated-K_{OW}, Mabey et al. 1982)

Sorption Partition Coefficient, log K_{OC}:
2.62 (sediment-water, calculated-K_{OW}, Mabey et al. 1982)
1.40 (calculated-K_{OW}, Kollig 1993)

Environmental Fate Rate Constants, k, or Half-Lives, $t_{½}$:

Volatilization:

Photolysis:

Hydrolysis:

Oxidation: aqueous oxidation rate constants for singlet oxygen $k < 4 \times 10^7$ M^{-1} h^{-1} and for peroxy radical, $k < 1 \times 10^9$ M^{-1} h^{-1} at 25°C (Mabey et al. 1982);

photooxidation $t_{½}$ = 31 – 1740 h, based on photooxidation rate constants with OH and RO_2 radicals for the amine class (Güesten et al. 1981; Mill & Mabey 1985; quoted, Howard et al. 1991);

photooxidation $t_{½}$ = 0.3 – 3.0 h in air, based on estimated rate data for the reaction with hydroxyl radical in air (Atkinson 1987; quoted, Howard et al. 1991).

Biodegradation: aqueous aerobic $t_{½}$ = 672 – 4320 h, based on acclimated aerobic aqueous screening test data (Malaney 1960; quoted, Howard et al. 1991); aqueous anaerobic $t_{½}$ = 2880 – 17280 h, based on estimated unacclimated aqueous aerobic biodegradation half-life (Howard et al. 1991).

Biotransformation: bacterial transformation $k = 1 \times 10^{-10}$ $mL \cdot cell^{-1} \cdot h^{-1}$ in water (Mabey et al. 1982).

Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants:

Half-Lives in the Environment:

Air: photooxidation $t_{½}$ = 0.3 – 3.0 h, based on estimated rate data for the reaction with hydroxyl radical in air (Atkinson 1987; quoted, Howard et al. 1991);

atmospheric transformation lifetime was estimated to be < 1 d (Kelly et al. 1994).

Surface water: photooxidation $t_{½}$ = 31 – 1740 h, based on photooxidation rate constants with OH and RO_2 radicals for the amine class (Güesten et al. 1981; Mill & Mabey 1985; quoted, Howard et al. 1991).

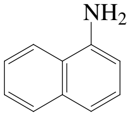
Groundwater: $t_{½}$ = 1344 – 8640 h, based on estimated unacclimated aqueous aerobic biodegradation half-life (Howard et al. 1991).

Sediment:

Soil: $t_{½}$ = 672 – 4320 h, based on estimated aqueous aerobic biodegradation half-life (Howard et al. 1991).

Biota:

16.1.3.15 α-Naphthylamine (1-Aminonaphthalene)



Common Name: 1-Naphthylamine
Synonym: 1-naphthalenamine, α-naphthylamine, 1-NA, 1-aminonaphthalene, naphthalidine
Chemical Name: 1-naphthalenamine
CAS Registry No: 134-32-7
Molecular Formula: $C_{10}H_7NH_2$
Molecular Weight: 143.185
Melting Point (°C):
  49.2 (Lide 2003)
Boiling Point (°C):
  300.7 (Lide 2003)
Density (g/cm^3 at 20°C):
  1.1229 (25°C, Weast 1982–8)
  1.123 (Dean 1985)
Molar Volume (cm^3/mol):
  161.8 (calculated-Le Bas method at normal boiling point)
Dissociation Constant pK_a:
  3.92 (Sangster 1993)
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
  14.23 ± 0.105 (Tsonopoulos & Prausnitz 1971)
Entropy of Fusion, ΔS_{fus} (J/mol K):
  44.35 ± 3.35 (Tsonopoulos & Prausnitz 1971)
Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F: 0.579 (mp at 49.2°C)

Water Solubility (g/m^3 or mg/L at 25°C):
  1700 (Verschueren 1983)
  590 parts in water (Budavari 1989)

Vapor Pressure (Pa at 25°C and reported temperature dependence equations):
  0.803 (extrapolated-regression of tabulated data, temp range 104.3–300.8°C, Stull 1947)
  $\log (P/\text{mmHg}) = [-0.2185 \times 14529.5/(T/K)] + 8.29900$; temp range 104.3–300.8°C (Antoine eq., Weast 1972–73)
  0.557 (extrapolated-Cox eq., Chao et al. 1983)
  $\log (P/\text{atm}) = [1 - 574.066/(T/K)] \times 10\text{^}\{0.822931 - 2.94554 \times 10^{-4}\cdot(T/K) + 2.19845 \times 10^{-7}\cdot(T/K)^2\}$; temp range: 325.0–645.0 K (Cox eq., Chao et al. 1983)
  0.446 (extrapolated, liquid, Antoine eq., Stephenson & Malanowski 1987)
  $\log (P_L/\text{kPa}) = 6.88407 - 2570.55/(-46.989 + T/K)$; temp range 377–574 K (Antoine eq., Stephenson & Malanowski 1987)

Henry's Law Constant (Pa·m^3/mol at 25°C):
  6.197 (gas stripping-GC, Altschuh et al. 1999)

Octanol/Water Partition Coefficient, log K_{OW}:
  2.23 (Leo et al. 1969)
  2.25 (shake flask, Hansch & Leo 1979)
  2.27 (shake flask-UV at pH 7.5, Martin-Villodre et al. 1986)
  2.33 (HPLC-k′ correlation, Minick et al. 1988)
  2.25 (recommended, Sangster 1993)
  2.25 (recommended, Hansch et al. 1995)
  2.34 (microemulsion electrokinetic chromatography-retention factor correlation, Poole et al. 2000)

Octanol/Air Partition Coefficient, log K_{OA}:

Bioconcentration Factor, log BCF:

Sorption Partition Coefficient, log K_{OC}:

3.58, 3.43, 3.50	(Milford soil, Morocco soil, Oakville soil, Graveel et al. 1986)
2.63, 2.68, 3.15	(sediment, Alfisol soil, Podzol soil, von Oepen et al. 1991)
3.51, 3.48	(soil, quoted exptl., calculated-MCI χ, Meylan et al. 1992)
3.51	(soil, calculated-MCI $^1\chi$, Sabljic et al. 1995)
2.0–2.65	(5 soils, pH 2.8–7.4, batch equilibrium-sorption isotherm, Li et al. 2000)

Environmental Fate Rate Constants, k, or Half-Lives, $t_{1/2}$:

Volatilization:

Photolysis:

Oxidation: rate constant $k = 1 \times 10^4\ M^{-1}\ s^{-1}$ for oxidation by RO_2 radical at 30°C in aquatic systems with $t_{1/2} = 0.8$ d (Howard 1972; Hendry et al. 1974; quoted, Mill 1982);

rate constant $k < 2 \times 10^2\ M^{-1}\ s^{-1}$ for oxidation by singlet oxygen at 25°C in aquatic systems with $t_{1/2} > 100$ yr (Foote 1976; Mill 1979; quoted, Mill 1982);

atmospheric $t_{1/2} = 0.292$–2.92 h, based on estimated rate constants for the reaction with OH radical in air and aqueous photooxidation $t_{1/2} = 62.4$–3480 h, based on estimated rate constants for reaction of representative aromatic amines with OH and RO_2 radicals in aqueous solution (Howard et al. 1991);

photooxidation $t_{1/2} = 0.08$–0.13 h under sunlight and $t_{1/2} = 0.25$–9.1 h under UV light when adsorbed on silica; $t_{1/2} = 0.10$–0.15 h under sunlight and $t_{1/2} = 0.15$–10.5 h under UV light when adsorbed on alumina on the TLC plates under simulated atmospheric conditions (Hasegawa et al. 1993).

Hydrolysis:

Biodegradation: aqueous aerobic biodegradation $t_{1/2} = 672$–4320 h and aqueous anaerobic biodegradation $t_{1/2} = 2688$–17280 h, based on slow biodegradation observed in aerobic soil die-away test study and aerobic activated sludge screening tests (Howard et al. 1991).

Biotransformation:

Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants:

Half-Lives in the Environment:

Air: $t_{1/2} = 0.292$–2.92 h, based on estimated photooxidation half-life in air (Howard et al. 1991).

Surface water: $t_{1/2} = 0.62.4$–3840 h, based on estimated rate constants for reactions of aromatic amines with OH and RO_2 radicals in aqueous solutions (Howard et al. 1991).

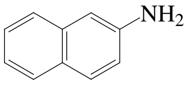
Groundwater: $t_{1/2} = 1344$–8640 h, based on slow biodegradation observed in an aerobic soil die-away test study and aerobic activated sludge screening tests (Howard et al. 1991).

Sediment:

Soil: $t_{1/2} = 672$–4320 h, based on slow biodegradation observed in an aerobic soil die-away test study and aerobic activated sludge screening tests (Howard et al. 1991).

Biota:

16.1.3.16 β-Naphthylamine (2-Aminonaphthalene)



Common Name: 2-Naphthylamine
Synonym: 2-naphthalenamine, β-naphthylamine, 2-NA, 2-aminonaphthalene, naphthalidine
Chemical Name: 2-naphthalenamine
CAS Registry No: 91-59-8
Molecular Formula: $C_{10}H_7NH_2$
Molecular Weight: 143.185
Melting Point (°C):
    113 (Weast 1982–83; Lide 2003)
Boiling Point (°C):
    306.2 (Lide 2003)
Density (g/cm^3):
    1.0614 (at 98°C, Weast 1982–83; Verschueren 1983; Dean 1985)
Molar Volume (cm^3/mol):
    161.8 (calculated-Le Bas method at normal boiling point)
Dissociation Constant pK_a:
    4.15 (Sangster 1993)
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
    21.97 (Tsonopoulos & Prausnitz 1971)
Entropy of Fusion, ΔS_{fus} (J/mol K):
    57.32 (Tsonopoulos & Prausnitz 1971)
Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F: 0.137 (mp at 113°C)

Water Solubility (g/m^3 or mg/L at 25°C or as indicated):
    6.40 (18°C, Ciusa 1922; quoted, Tsonopoulos & Prausnitz 1971)
    0.19 (18–20°C, Neish 1948; quoted, Tsonopoulos & Prausnitz 1971)

Vapor Pressure (Pa at 25°C and reported temperature dependence equations):
    0.634 (extrapolated-regression of tabulated data, temp range 108–306.1°C, Stull 1947)
    $\log (P/\text{atm}) = [-0.2185 \times 14679.6/(T/K)] + 8.435133$; temp range 108–306.1°C (Antoine eq., Weast 1972–73)
    0.369 (extrapolated-Cox eq., Chao et al. 1983)
    $\log (P/\text{atm}) = [1 - 579.422/(T/K)] \times 10\text{\^{}}\{0.860256 - 4.44286 \times 10^{-4}\cdot(T/K) + 3.71453 \times 10^{-7}\cdot(T/K)^2\}$; temp range: 385.0–645.0 K (Cox eq., Chao et al. 1983)
    0.035 (Howard et al. 1986)
    0.035 (interpolated, solid, Antoine eq., Stephenson & Malanowski 1987)
    0.362 (extrapolated, liquid, Antoine eq., Stephenson & Malanowski 1987)
    $\log (P_S/\text{kPa}) = 8.4859 - 3859/(T/K)$, temp range: 283–323 K, (Antoine eq.-I, Stephenson & Malanowski 1987)
    $\log (P_L/\text{kPa}) = 6.88978 - 2604.31/(-46.068 + T/K)$, temp range 388–579 K (Antoine eq.-II, Stephenson & Malanowski 1987)
    0.340 (calculated-solvatochromic parameters, Banerjee et al. 1990)

Henry's Law Constant (Pa·m^3/mol at 25°C):

Octanol/Water Partition Coefficient, log K_{OW}:
    2.28 (shake flask, Hansch & Leo 1979)
    2.26 (20°C, shake flask, Korenman & Polumestnaya, 1982)
    2.40 (calculated-UNIFAC activity coeff., Campbell & Luthy 1985)
    2.40 (shake flask-AS, pH 7.5, Martin-Villodre et al. 1986)
    2.34 (recommended, Sangster 1993)
    2.28 (recommended, Hansch et al. 1995)

Octanol/Air Partition Coefficient, log K_{OA}:

Bioconcentration Factor, log BCF:

Sorption Partition Coefficient, log K_{OC}:

1.77 (calculated-K_{OW}, Kollig 1993)

Environmental Fate Rate Constants, k, or Half-Lives, $t_{½}$:

Volatilization:

Photolysis:

Oxidation: rate constant k = 1 × 10^4 M^{-1} s^{-1} for oxidation by RO_2 radicals at 30°C in aquatic systems with $t_{½}$ = 0.8 d (Howard 1972; Hendry et al. 1974; quoted, Mill 1982);

rate constant k < 2 × 10^2 M^{-1} s^{-1} for oxidation by singlet oxygen at 25°C in aquatic systems with $t_{½}$ > 100 yr (Foote 1976; Mill 1979; quoted, Mill 1982);

photooxidation $t_{½}$ = 0.30–2.90 h in air, based on estimated rate constant for the vapor-phase reaction with hydroxyl radical in air (Atkinson 1987; quoted, Howard et al. 1991);

aqueous photooxidation $t_{½}$ = 62–3480 h, based on estimated rate constants for reaction of representative aromatic amines with OH and RO_2 radicals in aqueous solution (Güesten et al. 1981; Mill & Mabey 1985; quoted, Howard et al. 1991);

photooxidation $t_{½}$ = 0.05–0.14 h under sunlight and 0.20–10.0 h under UV light when adsorbed on silica and $t_{½}$ = 0.16–0.19 h under sunlight and $t_{½}$ = 0.22–10.8 h under UV light when adsorbed on alumina TLC plates under simulated atmospheric conditions (Hasegawa et al. 1993).

Hydrolysis:

Biodegradation: aqueous aerobic biodegradation $t_{½}$ = 672–4320 h, based on unacclimated aerobic screening test data (Fochtman & Eisenberg 1979; quoted, Howard et al. 1979) and unacclimated soil grab sample data (Medvedev & Davidov 1981; quoted, Howard et al. 1991); aqueous anaerobic biodegradation $t_{½}$ = 2880–17280 h, based on estimated unacclimated aqueous aerobic biodegradation half-life (Howard et al. 1991).

Biotransformation:

Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants:

Half-Lives in the Environment:

Air: photooxidation $t_{½}$ = 0.30–2.90 h, based on estimated rate constant for the vapor-phase reaction with hydroxyl radical in air (Atkinson 1987; quoted, Howard et al. 1991).

Surface water: $t_{½}$ = 62.0–3840 h, based on estimated rate constants for reactions of aromatic amines with OH and RO_2 radicals in aqueous solutions (Güesten et al. 1981; Mill & Mabey 1985; quoted, Howard et al. 1991).

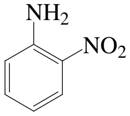
Groundwater: $t_{½}$ = 1344–8640 h, based on estimated unacclimated aqueous aerobic biodegradation half-life (Howard et al. 1991).

Sediment:

Soil: $t_{½}$ = 672–4320 h, based on unacclimated aerobic screening test data (Fochtman & Eisenberg 1979; quoted, Howard et al. 1991) and unacclimated aerobic soil grab sample data (Medvedev & Davidov 1981; quoted, Howard et al. 1981).

Biota:

16.1.3.17 2-Nitroaniline



Common Name: 2-Nitroaniline
Synonym: 1-amino-2-nitrobenzene, *o*-aminonitrobenzene, *o*-nitroaniline, 2-nitrophenylamine, 2-nitrobenzeneamine
Chemical Name: 1-amino-2-nitrobenzene, *o*-nitroaniline, 2-nitroaniline
CAS Registry No: 88-74-4
Molecular Formula: $C_6H_6N_2O_2$, $C_6H_4NH_2NO_2$
Molecular Weight: 138.124
Melting Point (°C):
71.0 (Lide 2003)
Boiling Point (°C):
284 (Lide 2003)
Density (g/cm^3 at 20°C):
1.442 (15°C, Weast 1982–83; Verschueren 1983; Dean 1985)
Molar Volume (cm^3/mol):
138.7 (calculated-Le Bas method at normal boiling point)
Dissociation Constant, pK_a:
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
16.11 (Tsonopoulos & Prausnitz 1971)
Entropy of Fusion, ΔS_{fus} (J/mol K):
46.86 (Tsonopoulos & Prausnitz 1971)
Fugacity Ratio at 25°C (assuming ΔSfus = 56 J/mol K), F: 0.354 (mp at 71.0°C)

Water Solubility (g/m^3 or mg/L at 25°C or as indicted):
1212, 2423 (25, 40°C, synthetic method-shake flask-titration, Collet & Johnson 1926)
1740 (calculated-K_{OW}, Yalkowsky & Morozowich 1980)
1260 (Verschueren 1983)

Vapor Pressure (Pa at 25°C and reported temperature dependence equations):
log (P/mmHg) = 8.81842 – 3336.52/(T/K); measured range 150–215°C (isoteniscope, Berliner & May 1925)
log (P/mmHg) = 9.55950 – 4037.7/(T/K); measured range 190–250°C (isoteniscope, Berliner & May 1925)
0.620 (extrapolated-regression of tabulated data, temp range 104–284.5°C, Stull 1947)
0.072 (Knudsen method, calculated-Antoine eq., Hoyer & Peperle 1958)
log (P/mmHg) = 12.50 – 4701/(T/K), temp range 0–50°C (Knudsen effusion method, Hoyer & Peperle 1958)
log (P/mmHg) = [–0.2185 × 15284.0/(T/K)] + 8.868383; temp range 104–284.5°C (Antoine eq., Weast 1972–73)
< 13.3 (30°C, Verschueren 1983)
0.650 (extrapolated-Antoine eq., Dean 1985, 1992)
log (P/mmHg) = 8.8684 – 3336.5/(T/K); temp range 150–260°C (Antoine eq., Dean 1985, 1992)
log (P_S/kPa) = 11.625 – 4701/(T/K); temp range 273–323 K (Antoine eq.-I, Stephenson & Malanowski 1987)
log (P_L/kPa) = 11.3629 – 7444.3/(240.83 + T/K); temp range 423–553 K (Antoine eq.-II, Stephenson & Malanowski 1987)
log (P/mmHg) = $-112.5774 - 1.5945 \times 10^3/(T/K) + 54.577 \cdot \log(T/K) - 7.6775 \times 10^{-2} \cdot (T/K) + 3.6152 \times 10^{-5} \cdot (T/K)^2$; temp range 345–558 K (vapor pressure eq., Yaws 1994)

Henry's Law Constant (Pa·m^3/mol):

Octanol/Water Partition Coefficient, log K_{OW}:
1.44 (shake flask-UV, Fujita et al. 1964)
1.83 (shake flask-UV, Hansch & Anderson 1967)
1.62 (HPLC-RT correlation, Carlson et al. 1975)
1.81 (Hansch & Leo 1979)

1.72 (shake flask, Eadsforth & Moser 1983)
1.67 (calculated-HPLC-k′ correlation, Deneer et al. 1987)
1.50 (calculated-linear extrapolation exptl. log k at various solvent compositions, Deneer et al. 1987)
1.93, 1.73 (25°C, 60°C, shake flask-UV, Kramer & Henze 1990)
1.85 (recommended, Sangster 1993)
1.80 ± 0.14, 1.35 ± 0.51 (solvent generated liquid-liquid chromatography SGLLC-correlation, RP-HPLC-k′ correlation, Cichna et al. 1995)
1.85 (recommended, Hansch et al. 1995)

Octanol/Air Partition Coefficient, log K_{OA}:

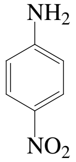
Bioconcentration Factor, log BCF:
0.91; 1.49, 0.55, 0.83 (quoted exptl.; calculated values-K_{OW}, Bintein et al. 1993)

Sorption Partition Coefficient, log K_{OC}:

Environmental Fate Rate Constants, k, or Half-Lives, $t_{½}$:

Half-Lives in the Environment:
Surface water: estimated $t_{½}$ = 1.4 d in Rhine River in case of a first order reduction process (Zoeteman et al. 1980)

16.1.3.18 4-Nitroaniline



Common Name: 4-Nitroaniline
Synonym: 1-amino-4-nitrobenzene, *p*-aminonitrobenzene, *p*-nitroaniline, 4-nitrobenzenamine, 4-nitrophenylamine
Chemical Name: 1-amino-4-nitrobenzene, *p*-nitroaniline, 4-nitroaniline
CAS Registry No: 100-01-6
Molecular Formula: $C_6H_6N_2O_2$, $C_6H_4NH_2NO_2$
Molecular Weight: 138.124
Melting Point (°C):
147.5 (Lide 2003)
Boiling Point (°C):
332 (Lide 2003)
Density (g/cm^3 at 20°C):
1.424 (Weast 1982–83; Verschueren 1983)
1.4370 (14°C, Dean 1985)
Molar Volume (cm^3/mol):
138.7 (calculated-Le Bas method at normal boiling point)
Dissociation Constant, pK_a:
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
21.09 (Tsonopoulos & Prausnitz 1971)
Entropy of Fusion, ΔS_{fus} (J/mol K):
50.21 (Tsonopoulos & Prausnitz 1971)
Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F: 0.0628 (mp at 147.5°C)

Water Solubility (g/m^3 or mg/L at 25°C or as indicated):
568, 1157 (25, 40°C, synthetic method-shake flask-titration, Collet & Johnson 1926)
728 (30°C, shake flask-interferometry, Gross et al. 1931)
603 (calculated-K_{OW}, Yalkowsky & Morozowich 1980)
380 (20°C, shake flask-membrane filter-fluorophotometry, Hashimoto et al. 1982)
390, 400 (20°C, shake flask-glass fiber filters-fluorophotometry, Hashimoto et al. 1982)
800; 22000 (19°C, 100°C, Verschueren 1983)
800 (Dean 1985)

Vapor Pressure (Pa at 25°C and reported temperature dependence equations):
$\log(P/\text{mmHg}) = 9.55950 - 4037.7/(T/K)$; measured range 190–250°C (isoteniscope, Berliner & May 1925)
0.035 (extrapolated-regression of tabulated data, temp range 142.4–336°C, Stull 1947)
$\log(P/\text{mmHg}) = 13.69 - 5707/(T/K)$, temp range 30–90°C, (Knudsen effusion method, Hoyer & Peperle 1958)
$\log(P/\text{mmHg}) = [-0.2185 \times 17220.2/(T/K)] + 9.041879$; temp range 142.4–336°C (Antoine eq., Weast 1972–73)
0.200, 0.933 (20°C, 30°C, Verschueren 1983)
0.014 (extrapolated-Antoine eq., Dean 1985)
$\log(P/\text{mmHg}) = 9.5595 - 4039.73/(T/K)$; temp range 190–260°C (Antoine eq., Dean 1985, 1992)
$\log(P_S/\text{kPa}) = 11.1109 - 5093/(T/K)$; temp range 346–366 K (solid, Antoine eq.-I, Stephenson & Malanowski 1987)
$\log(P_L/\text{kPa}) = 8.7988 - 4071.3/(T/K)$; temp range 473–538 K (liquid, Antoine eq.-II., Stephenson & Malanowski 1987)
$\log(P/\text{mmHg}) = 56.1642 - 5.3655 \times 10^3/(T/K) - 17.958\cdot\log(T/K) + 9.092 \times 10^{-3}\cdot(T/K) + 7.0305 \times 10^{-10}\cdot(T/K)^2$; temp range 421–609 K (vapor pressure eq., Yaws 1994)

Henry's Law Constant (Pa·m^3/mol):

Octanol/Water Partition Coefficient, log K_{OW}:

1.39	(shake flask-UV, Fujita et al. 1964; Hansch & Leo 1979)
0.59	(calculated-activity coeff. γ from UNIFAC, Campbell & Luthy 1985)
1.16	(HPLC-k′ correlation, Deneer et al. 1987)
1.10	(calculated-linear extrapolation exptl. values of log k at various solvent compositions, Deneer et al. 1987)
1.15	(HPLC-RT correlation, Wang et al. 1989)
1.51, 1.36	(25°C, 60°C, shake flask-UV, Kramer & Henze 1990)
1.30	(CPC-RV correlation, Tsai et al. 1991)
1.30	(CPC-RV correlation, El Tayar et al. 1991)
1.35	(recommended, Sangster 1993)
1.39 ± 0.14, 0.75 ± 0.48	(solvent generated liquid-liquid chromatography SGLLC-correlation, RP-HPLC-k′ correlation, Cichna et al. 1995)
1.37	(recommended, Hansch et al. 1995)

Octanol/Air Partition Coefficient, log K_{OA}:

Bioconcentration Factor, log BCF:

Sorption Partition Coefficient, log K_{OC}:

2.26; 2.66; 2.12 (Alfisol soil; Podzol soil; sediment, von Oepen et al. 1991)

0.64; 1.25, –0.18, 0.41 (quoted exptl.; calculated values-K_{OW}, Bintein et al. 1993)

2.16, 2.22, 2.19 (RP-HPLC-k′ correlation on 3 different stationary phases, Szabo et al. 1995)

1.86, 1.84 (RP-HPLC-k′ correlation including MCI related to non-dispersive intermolecular interactions, hydrogen-bonding indicator variable, Hong et al. 1996)

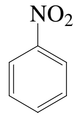
Environmental Fate Rate Constants, k, or Half-Lives, $t_{1/2}$:

Half-Lives in the Environment:

Surface water: estimated $t_{1/2}$ = 2.3 d in Rhine River in case of a first order reduction process (Zoeteman et al. 1980)

16.1.4 NITROAROMATIC COMPOUNDS

16.1.4.1 Nitrobenzene



Common Name: Nitrobenzene
Synonym: nitrobenzol, oil of mirbane
Chemical Name: nitrobenzene
CAS Registry No: 98-95-3
Molecular Formula: $C_6H_5NO_2$
Molecular Weight: 123.110
Melting Point (°C):
5.7 (Stull 1947; Dreisbach 1955; Weast 1982–83; Howard 1989; Lide 2003)
Boiling Point (°C):
210.8 (Weast 1982–83; Lide 2003)
Density (g/cm^3 at 20°C):
1.2032, 1.1982 (20°C, 25°C, Dreisbach 1955)
1.2036 (20°C, Weast 1982–83)
Molar Volume (cm^3/mol):
102.0 (calculated from density, Rohrschneider 1973; Chiou 1985)
112.0 (calculated-Le Bas method at normal boiling point)
Dissociation Constant pK_a:
Enthalpy of Vaporization, ΔH_V (kJ/mol):
55.186, 43.421 (25°C, bp, Dreisbach 1961)
55.013, 40.769 (25°C, bp, Riddick et al. 1986)
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
11.59 (Dreisbach 1955)
12.13 (Tsonopoulos & Prausnitz 1971)
11.63 (Riddick et al. 1986)
Entropy of Fusion, ΔS_{fus} (J/mol K):
43.51 (Tsonopoulos & Prausnitz 1971)
Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F: 1.0

Water Solubility (g/m^3 or mg/L at 25°C or as indicated. Additional data at other temperatures designated * are compiled at the end of this section):
1780, 2050 (15, 30°C, shake flask-interferometry, Gross et al. 1931)
2060* (30°C, shake flask-interferometry and titration, measured range 0–60°C, Vermillion et al. 1941)
1204 (shake flask-centrifuge, Booth & Everson 1948)
1930 (Seidell 1941)
2018 (shake flask-interferometry, Donahue & Bartell 1952)
1950 (Deno & Berkheimer 1960)
2259 (35°C, shake flask-UV spectrophotometry, Hine et al. 1963)
2060 (Hansch et al. 1968)
1900 (20°C, Verschueren 1977, 1983)
2093 (shake flask-LSC, Banerjee et al. 1980)
2090 (shake flask-radioactive analysis, Veith et al. 1980)
2043 (20–27°C, shake flask-GC, Chiou 1985)
1900 (20°C, Riddick et al. 1986; quoted, Howard 1989)
1930* (20°C, shake flask-UV spectrophotometry, measured range 10–40°C, Beneš & Dohnal 1999)

Vapor Pressure (Pa at 25°C or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):

133.3* (53.1°C, static-manometer, measured range 53.1–208.3°C, Kahlbaum 1898)
38.80 (saturated vapor density-gas saturation, Puck & Wise 1946)
42.06* (extrapolated-regression of tabulated data, temp range 44.4–210.6°C, Stull 1947)
10063* (134.1°C, ebulliometry, measured range 134.1–210.629°C, Brown 1952)
37.86 (calculated by formula, Dreisbach 1955; quoted, Hine & Mookerjee 1975)
$\log (P/\text{mmHg}) = 7.08283 - 1722.2/(199.0 + t/°\text{C})$; temp range 108–300°C (Antoine eq. for liquid state, Dreisbach 1955)
32.3* (23.14°C, gas saturation, measured range 6.09–23.14°C, Lynch & Wilke 1960)
$\log (P/\text{mmHg}) = 7.545 - 2064/(t/°\text{C} + 230)$; temp range 6.09–23.14°C (gas saturation, Lynch & Wilke 1960)
80.0 (35°C, gas saturation-gravitational or UV spectrophotometry, Hine et al. 1963)
$\log (P/\text{mmHg}) = [-0.2185 \times 12168.2/(T/K)] + 8.416268$; temp range 44.4–210.6°C (Antoine eq., Weast 1972–73)
34.60 (extrapolated-Antoine eq., Boublik et al. 1973)
$\log (P/\text{mmHg}) = 7.11562 - 1746.585/(201.783 + t/°\text{C})$, temp range 134–210.6°C (Antoine eq. from reported exptl. data, Boublik et al. 1973)
20.00 (20°C, Verschueren 1977, 1983)
28.37 (calculated-bp, Mackay et al. 1982)
34.36 (extrapolated-Antoine eq., Boublik et al. 1984)
$\log (P/\text{kPa}) = 6.23424 - 1741.779/(201.257 + t/°\text{C})$; temp range 134–210.6°C (Antoine eq. from reported exptl. data, Boublik et al. 1984)
$\log (P/\text{kPa}) = 4.06596 - 323.457/(-58.276 + t/°\text{C})$; temp range 239–291°C (Antoine eq. from reported exptl. data, Boublik et al. 1984)
34.63 (extrapolated-Antoine eq., Dean 1985; 1992)
$\log (P/\text{mmHg}) = 6.91048 - 946.35/(246.68 + t/°\text{C})$; temp range –87 to 7°C (Antoine eq., Dean 1985, 1992)
37.0 (quoted lit., Riddick et al. 1986)
$\log (P/\text{kPa}) = 6.670 - 2064.0/(230.0 + t/°\text{C})$, temp range not specified (Antoine eq., Riddick et al. 1986)
37.65 (extrapolated-Antoine eq.-II, Stephenson & Malanowski 1987)
$\log (P_L/\text{kPa}) = 6.22069 - 1732.222/(-72.886 + T/K)$; temp range 407–484 K (Antoine eq.-I, Stephenson & Malanowski 1987)
$\log (P_L/\text{kPa}) = 6.6699 - 2064/(-43.15 + T/K)$; temp range 279–296 K (Antoine eq.-II, Stephenson & Malanowski 1987)
33.33 (Howard et al. 1986)
$\log (P/\text{mmHg}) = -54.4937 - 2.1123 \times 10^3/(T/K) + 29.321 \cdot \log (T/K) - 4.4839 \times 10^{-2} \cdot (T/K) + 2.0162 \times 10^{-5} \cdot (T/K)^2$; temp range 279–719 K (vapor pressure eq., Yaws 1994)

Henry's Law Constant (Pa·m³/mol at 25°C):

2.367, 4.51, 4.723 (exptl., calculated-group contribution, calculated-bond contribution, Hine & Mookerjee 1975)
1.327 (calculated-P/C, Mabey et al. 1982)
2.472 (estimated, Lyman et al. 1982)
5.06 (calculated-molecular structure, Russell et al. 1992)
0.868 (gas stripping-GC, Altschuh et al. 1999)

Octanol/Water Partition Coefficient, log K_{OW}:

1.85 (shake flask-UV, Fujita et al. 1964; Hansch et al. 1968; Leo et al. 1969, 1971; Hansch & Leo 1979, 1985;)
1.74 (Neely et al. 1974)
1.85, 1.84 (Hansch & Leo 1979)
1.82 (HPLC-RT correlation, Veith et al. 1979a)
1.83 (shake flask-LSC, Banerjee et al. 1980)
1.98, 1.78 (HPLC-k′ correlation, McDuffie 1981)
1.85 (generator column-HPLC, Wasik et al. 1981; Tewari et al. 1982;)
1.88 (shake flask-UV, Unger & Chiang 1981)
1.99 (RP-HPLC-k′ correlation, Miyake & Terada 1982)
1.83, 1.84 (calculated-activity coeff. γ from UNIFAC, octanol and water solubility considered; calculated-activity coeff. γ from UNIFAC, octanol and water solubility not considered, Arbuckle 1983)
1.85, 1.88 (lit. values, Verschueren 1983)

1.83 ± 0.02 (HPLC-RV correlation-ALPM, Garst & Wilson 1984)
1.84 (calculated-activity coefficient γ from UNIFAC, Campbell & Luthy 1985)
1.87 (Lu et al. 1986)
1.85 (RP-HPLC-k′ correlation, Minick et al. 1988)
1.89 (HPLC-k′ correlation, Deneer et al. 1987)
1.84 (calculated-activity coeff. γ from UNIFAC, Banerjee & Howard 1988)
1.70 (RP-HPLC-RT correlation, ODS column with masking agent, Bechalany et al. 1989)
1.828 ± 0.001 (shake flask/slow-stirring-GC, De Bruijn et al. 1989)
1.85 (recommended, Sangster 1989, 1993)
1.836 ± 0.051; 1.828 ± 0.001 (average values, stir-flask method by BRE; by RITOX, Brooke et al. 1990)
1.83, 1.85, 1.88 (CPC-retention volume correlation; Gluck & Martin 1990)
1.94, 2.25 (25°C, 60°C, shake flask-UV, Kramer & Henze 1990)
1.57 (shake flask-UV, Nakagawa et al. 1992)
1.85 (shake flask-GC, Alcron et al. 1993)
1.85 (recommended, Hansch et al. 1995)
2.25, 2.12, 2.20, 2.23 (HPLC-k′ correlation, different combinations of stationary and mobile phases under isocratic conditions, Makovskaya et al. 1995)
1.88 (shake flask-dialysis tubing-HPLC/UV, both phases, Andersson & Schrăder 1999)
1.93 (microemulsion electrokinetic chromatography-retention factor correlation, Poole et al. 2000)

Octanol/Air Partition Coefficient, log K_{OA}:

Bioconcentration Factor, log BCF:
1.18 (fathead minnows, Veith et al. 1979b)
0.06 (calculated-K_{OW}, Veith et al. 1980)
< 1.0; 1.36 (golden orfe; green algae, Freitag et al. 1982)
1.38; 1.42 (alga *Chlorella fusca*, wet wt. basis; calculated-K_{OW}, Geyer et al. 1984)
0.78 (*P. reticulata*, Canton et al. 1985; quoted, Howard 1989)
< 1.0, 1.38, 1.60 (golden orfe, algae, activated sludge, Freitag et al. 1982)
< 1.0, 1.30, 1.60 (golden ide, algae, activated sludge, Freitag et al. 1985)
1.47 ± 0.12 (guppy-fat wt. basis, Deneer et al. 1987)

Sorption Partition Coefficient, log K_{OC}:
1.94 (20°C, sorption isotherm-GC, converted from K_{OM} multiplied by 1.724, Briggs 1981)
2.30 (Lincoln fine sand, calculated exptl. value, Wilson et al. 1981)
2.23, 2.57 (Danish subsoils, Loekke 1985)
1.63, 1.84 (two Norwegian organic soils, Seip et al. 1986)
1.70 (soil, quoted, Sabljic 1987)
1.95 ± 0.84, 2.02 ± 1.18; 1.99 (Captina slit loam, McLaurin sandy loam; weighted mean, batch equilibrium-sorption isotherm, Walton et al. 1992)
1.43 (predicted-K_{OW}, Walton et al. 1992)
1.51 (calculated-K_{OW}, Kollig 1993)
2.20 (soil, calculated-QSAR MCI ${}^1\chi$, Sabljic et al. 1995)
2.05, 2.16, 2.15 (RP-HPLC-k′ correlation on 3 different stationary phases, Szabo et al. 1995)
1.99, 1.84 (RP-HPLC-k′ correlation including MCI related to non-dispersive intermolecular interactions, hydrogen-bonding indicator variable, Hong et al. 1996)
2.20; 2.28 (HPLC-screening method; calculated-PCKOC fragment method, Müller & Kördel 1996)
2.51, 2.03, 2.26, 2.09, 1.90 (soil: calculated-K_{OW}; HPLC-screening method using LC-columns of different stationary phases, Szabo et al. 1999)

Environmental Fate Rate Constants, k, or Half-Lives, $t_{1/2}$:
Volatilization: $t_{1/2}$(calc) ≈ 200 h from water bodies (Mackay & Leinonen 1975; quoted, Callahan et al. 1979)
$t_{1/2}$ = 45 d was estimated in a model river 1 m deep with a 1.0 m/s current and a 3 m/s wind (Lyman et al. 1982; quoted, Howard 1989).

Photolysis: aqueous photolysis $t_{½}$ = 67–200 d, based on measured photolysis rate constant in distilled water under midday sun at 40°N latitude (Simmons & Zepp 1986; Howard 1989; Howard et al. 1991);

atmospheric photolysis $t_{½}$ = 67–200 d, based on measured photolysis rate constant in distilled water under midday sun at 40°N latitude (Simmons & Zepp 1986; quoted, Howard 1989; Howard et al. 1991);

rate constant k = 2.37×10^{-3} h^{-1} with H_2O_2 under photolysis at 25°C in F-113 solution and with HO- in the gas (Dilling et al. 1988).

Hydrolysis:

Oxidation: rate constant k, for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO3} with NO_3 radical and k_{O3} with O_3 or as indicated *data at other temperatures see reference:

photooxidation $t_{½}$ = 125 d to 22 yr in water, based on measured rate constant for reaction with hydroxyl radical in water (Dorfman & Adams 1973; Anbar & Neta 1967; quoted, Howard et al. 1991)

k << 360 M^{-1} h^{-1} for singlet oxygen, k << 1.0 M^{-1} h^{-1} for peroxy radical at 25°C (Mabey et al. 1982)

k = (0.09 ± 0.02) M^{-1} s^{-1} for 5–10 mM to react with ozone in water using 50–1000 mM of *t*-BuOH as scavenger at pH 2 and 20–23°C (Hoigné & Bader 1983)

k_{OH}(obs.) = 0.15×10^{-12} cm^3 $molecule^{-1}$ s^{-1} at 296 K (Becker et al. 1984; quoted, Carlier et al. 1986)

k_{OH} = 0.21×10^{-12} cm^3 $molecule^{-1}$ s^{-1} at room temp. (Zetzsch 1982)

k_{OH}(calc) = 0.30×10^{-12} cm^3 $molecule^{-1}$ s^{-1} and 0.27×10^{-12} cm^3 $molecule^{-1}$ s^{-1} at room temp. (Atkinson 1985; Atkinson et al. 1985)

k_{OH}* = 0.137×10^{-12} cm^3 $molecule^{-1}$ s^{-1} at 299 K, measured range 259–362 K (flash photolysis-resonance fluorescence, Witte et al. 1986)

k_{OH}(calc) = 1.1×10^{-13} cm^3 $molecule^{-1}$ s^{-1}, 1.7×10^{-13} cm^3 $molecule^{-1}$ s^{-1} (addition of OH for different positions of the electrophilic attack, Witte et al. 1986)

k_{O3} < 7×10^{-21} cm^3 $molecule^{-1}$ s^{-1} at 296 ± 2 K (relative rate method, Atkinson et al. 1987)

k_{OH} = 1.3×10^{-13} cm^3 $molecule^{-1}$ s^{-1} with atmospheric lifetimes τ = 180 d in clean troposphere and 90 d in moderately polluted atmosphere; k_{O3} < 7×10^{-21} cm^3 $molecule^{-1}$ s^{-1} with atmospheric lifetimes τ > 6 yr in clean troposphere and τ > 2 yr in moderately polluted atmosphere at room temp. (Atkinson et al. 1987)

k_{OH}(calc) = 2.5×10^{-13} $cm^3 \cdot molecule^{-1}$ s^{-1}, k_{OH}(obs.) = 1.4×10^{-13} $cm^3 \cdot molecule^{-1}$ s^{-1} (SAR structure-activity relationship, Atkinson 1987)

k_{OH} = (0.16 – < 0.90) × 10^{-12} cm^3 $molecule^{-1}$ s^{-1} at 296 K (review, Atkinson 1989)

phototransformation decay rate constant of 0.17 min^{-1} on 0.20 g/L of TiO_2, 8.8 min^{-1} on 0.20 g/L of ZnO and 3.1 min^{-1} on 1.0 g/L of Al_2O_3 (Minero et al. 1994)

Abiotic Transformation: Degradation in reductive environment:

k = 0.187 min^{-1} with solute concn of 50 μM in a 19 day-old 0.2g/L magnetite suspension at pH 7 and 1.5 mM Fe(II) at 25°C (Klusen et al. 1995)

k = (7.39 ± 1.28) × 10^{-2} M^{-1} s^{-1} in H_2S with (mercapto)juglone (an abiotic reductant found in natural systems) solution at pH 6.65 (Wang & Arnold 2003)

Biodegradation:

decomposition by a soil microflora in more than 64 d (Alexander & Lustigman 1966; quoted, Verschueren 1983)

$t_{½}$(aq. anaerobic) = 48–300 h, based on anaerobic natural die-away test data for 2,4-dinitrotoluene (Spanggord et al. 1980; quoted, Howard et al. 1991)

k = 14 mg COD g^{-1} h^{-1} average biodegradation rate for 98% removal (Scow 1982)

$t_{½}$(aq. aerobic) = 322–4728 h, based on aerobic soil column biodegradation study data (Kincannon & Lin 1985; quoted, Howard et al. 1991)

$t_{½}$(aerobic) = 13 d, $t_{½}$(anaerobic) = 2 d in natural waters (Capel & Larson 1995)

Biotransformation: first-order rate constant of 0.7 d^{-1} corresponding to a half-life of 1 d in adopted activated sludge under aerobic conditions (Mills et al. 1982); rate constant for bacterial transformation of 3×10^{-9} mL $cell^{-1}$ h^{-1} in water (Mabey et al. 1982).

Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants:

Half-Lives in the Environment:

Air: atmospheric lifetimes: τ = 180 d in clean troposphere and τ = 90 d in moderately polluted atmosphere, based on gas-phase reaction with OH radical in atmosphere at room temp. and atmospheric lifetimes τ > 6 yr in clean troposphere and τ > 2 yr in moderately polluted atmosphere, based on gas-phase reaction with O_3 (estimated rate constant) in atmosphere at room temp. (Atkinson et al. 1987);

photooxidation $t_{1/2}$ = 0.544 – 5.44 h, based on measured rate constant for reaction with hydroxyl radical in air (Atkinson et al. 1987; quoted, Howard 1989; Howard et al. 1991);

atmospheric transformation lifetime was estimated to be > 5 d (Kelly et al. 1994).

Surface water: photooxidation $t_{1/2}$ = 125 d to 22 yr, based on measured rate constant for reaction with hydroxyl radical in water (Dorfman & Adams 1973; Anbar & Neta 1967; quoted, Howard et al. 1991);

estimated $t_{1/2}$ = 0.3 – 3.0 d in rivers (Zoeteman et al. 1980);

$t_{1/2}$ = 322 – 4728 h, based on estimated unacclimated aqueous aerobic biodegradation half-life (Howard et al. 1991)

$t_{1/2}$(aerobic) = 13 d, $t_{1/2}$(anaerobic) = 2 d in natural waters (Capel & Larson 1995).

Groundwater: estimated $t_{1/2}$ = 1.0 d in Rhine River in case of a first order reduction process (Zoeteman et al. 1980)

$t_{1/2}$ = 48 – 9456 h, based on estimated unacclimated aqueous anaerobic biodegradation half-life for 2,4-dinitrotoluene and estimated unacclimated aqueous aerobic biodegradation half-life (Howard et al. 1991).

Sediment:

Soil: estimated degradation $t_{1/2}$ = 625 d in activated sludge (Freitag et al. 1985; quoted, Anderson et al. 1991)

$t_{1/2}$ = 322 – 4728 h, based on aerobic soil column biodegradation study data (Kincannon & Lin 1985; quoted, Howard et al. 1991);

calculated $t_{1/2}$ = 9.1 d from first-order kinetic of degradation rate in sterilized soils (Anderson et al. 1991).

Biota:

TABLE 16.1.4.1.1
Reported aqueous solubilities of nitrobenzene at various temperatures

Gross et al. 1931		Vermillion et al. 1941		Beneš & Dohnal 1999	
shake flask-interferometry		interferometry		shake flask-UV	
t/°C	S/g·m^{-3}	t/°C	S/g·m^{-3}	t/°C	S/g·m^{-3}
15	1780	0	1660	10	1770
30	2050	6	1700	20	1930
		30	2060	30	2060
		60	3120	40	2200
		titration		ΔH_{sol}/(kJ mol^{-1}) =5.4 ± 0.2	
		30	2060		at 25°C.
		50	2640		

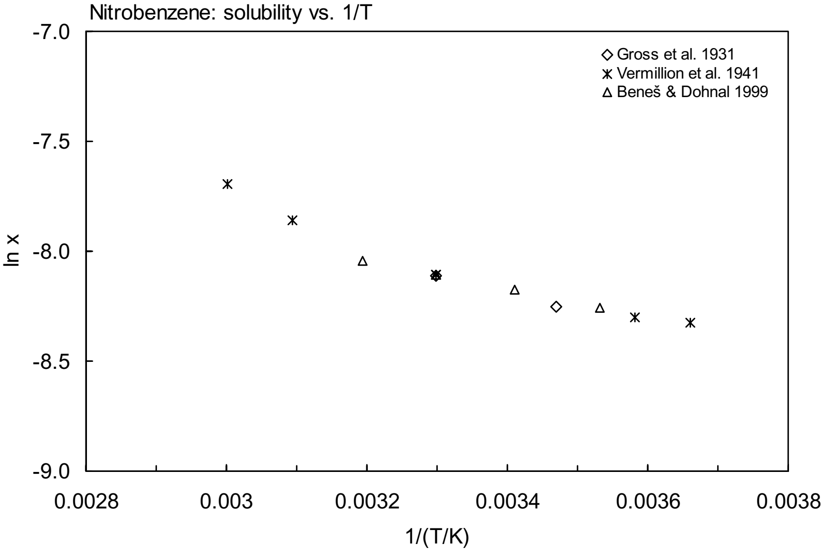


FIGURE 16.1.4.1.1 Logarithm of mole fraction solubility (ln *x*) versus reciprocal temperature for nitrobenzene.

TABLE 16.1.4.1.2
Reported vapor pressures of nitrobenzene at various temperatures and the coefficients for the vapor pressure equations

$\log P = A - B/(T/K)$ (1) $\ln P = A - B/(T/K)$ (1a)
$\log P = A - B/(C + t/°C)$ (2) $\ln P = A - B/(C + t/°C)$ (2a)
$\log P = A - B/(C + T/K)$ (3)
$\log P = A - B/(T/K) - C \cdot \log (T/K)$ (4)

Kahlbaum 1898*		Stull 1947		Lynch & Wilke 1960		Brown 1952	
static-manometer		summary of literature data		gas saturation		ebulliometry	
t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa
53.1	133.3	44.4	133.3	6.09	8.799	134.1	10063
59.8	266.6	71.6	666.6	12.57	14.80	139.75	13372
64.9	400.0	84.9	1333	12.67	13.33	143.17	16084
69.2	533.3	99.3	2666	14.67	16.93	149.73	18692
72.9	666.6	115.4	5333	14.72	17.73	154.61	21866
85.4	1333.2	125.8	7999	21.37	29.06	159.77	25704
99.1	2666.4	139.9	13332	21.54	29.33	164.45	29641
108.2	3999.7	161.2	26664	23.12	32.26	168.72	33649
114.9	5332.9	185.8	53329	23.14	32.26	172.96	38002
120.0	6666.1	210.6	101325			176.48	44455
131.1	9999.2			bp/°C	210.8	182.07	49014
139.9	13332	mp/°C	5.7			185.70	54019
160.5	26664			eq. 2	P/mmHg	188.90	58839
174.5	39997			A	7.545	196.63	65426
184.5	53329			B	2064	200.41	71843
192.5	66661			C	230	203.88	78997
199.5	79993					206.62	86075
205.0	93326					209.49	92023
208.3	101325					210.626	101322
						210.629	101330

*complete list see ref.

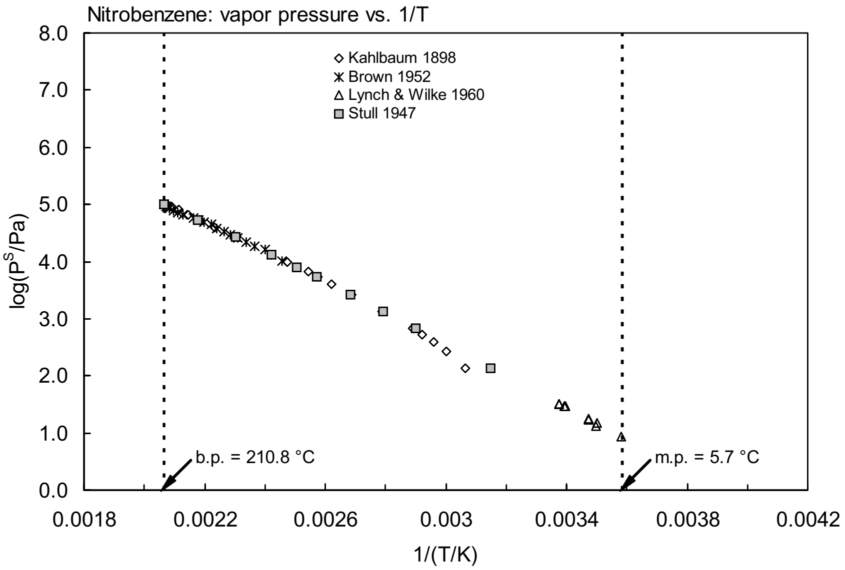
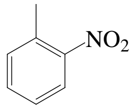


FIGURE 16.1.4.1.2 Logarithm of vapor pressure versus reciprocal temperature for nitrobenzene.

16.1.4.2 2-Nitrotoluene



Common Name: 2-Nitrotoluene
Synonym: 1-methyl-2-nitrobenzene, *o*-nitrotoluene, 2-methylnitrobenzene
Chemical Name: 2-nitrotoluene, *o*-nitrotoluene
CAS Registry No: 88-72-2
Molecular Formula: $C_7H_7NO_2$, $CH_3C_6H_4NO_2$
Molecular Weight: 137.137
Melting Point (°C):
  –10.4 (Lide 2003)
Boiling Point (°C):
  222 (Lide 2003)
Density (g/cm^3 at 20°C):
  1.15693, 1.15232 (20°C, 25°C, Dreisbach & Martin 1949)
  1.1629 (Weast 1982–83)
Molar Volume (cm^3/mol):
  117.9 (20°C, Stephenson & Malanowski 1987)
  153.0 (calculated-Le Bas method at normal boiling point)
Dissociation Constant pK_a:
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
Entropy of Fusion, ΔS_{fus} (J/mol K):
Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F: 1.0

Water Solubility (g/m^3 or mg/L at 25°C. Additional data at other temperatures designated * are compiled at the end of this section):
  652 (30°C, shake flask-interferometer, Gross et al. 1933)
  656 (quoted, Deno & Berkheimer 1960)
  < 233 (shake flask-centrifuge, Booth & Everson 1948)
  324 (Hansch et al. 1968)
  656, 2076 (quoted, predicted-K_{OW}, Valvani et al. 1981)
  652 (30°C, Verschueren 1983)
  656, 771 (quoted, calculated-fragment const., Wakita et al. 1986)
  641; 444 (quoted exptl.; calculated-group contribution method, Kühne et al. 1995)
  609* (20°C, shake flask-UV spectrophotometry, measured range 10–40°C, Beneš & Dohnal 1999)

Vapor Pressure (Pa at 25°C and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):
  23.97* (extrapolated-regression of tabulated data, Kahlbaum 1898)
  27.69* (extrapolated-regression of tabulated data, temp range 50–222.3°C, Stull 1947)
  $\log(P/mmHg) = 7.49454 - 2086.1/(230 + t/°C)$ (Antoine eq., Dreisbach & Martin 1949)
  3640* (115.842°C, ebulliometry, measured range 115.842–174.744°C, Dreisbach & Shrader 1949)
  $\log(P/mmHg) = [-0.2185 \times 12239.7/(T/K)] + 8.286642$; temp range 50–222.3°C (Antoine eq., Weast 1972–73)
  13.33 (20°C, Verschueren 1983)
  1.670 (extrapolated-Antoine eq., Boublik et al. 1984)
  $\log(P/kPa) = 5.01415 - 967.744/(99.208 + t/°C)$; temp range 129.31–222.2°C (Antoine eq. from reported exptl. data, Boublik et al. 1984)
  1.440 (extrapolated-Antoine eq., Dean 1985, 1992)
  $\log(P/mmHg) = 5.851 - 946/(96 + t/°C)$, temp range 129–222°C (Antoine eq., Dean 1985, 1992)
  $\log(P_L/kPa) = 6.32043 - 1827.66/(-71.63 + T/K)$; temp range 402–496 K (Antoine eq., Stephenson & Malanowski 1987)

24.80* (ebulliometry, average from extrapolated-Antoine eq., Aim 1994)
$\log (P/\text{mmHg}) = 7.8266 - 2.9906 \times 10^3/(T/K) + 1.1064 \cdot \log (T/K) - 4.9168 \times 10^{-3} \cdot (T/K) + 2.2375 \times 10^{-6} \cdot (T/K)^2$; temp range 270–720 K (vapor pressure eq., Yaws 1994)

Henry's Law Constant (Pa·m^3/mol at 25°C):
5.811 (exptl., Hine & Mookerjee 1975)
4.723, 4.616 (calculated-group contribution, calculated-bond contribution, Hine & Mookerjee 1975)

Octanol/Water Partition Coefficient, log K_{OW}:
2.30 (Leo et al. 1971; Hansch & Leo 1985)
2.30 (HPLC-k′ correlation, Deneer et al. 1987)
2.30 (unpublished data quoted from CLOGP Database and recommended, Sangster 1989)
2.39, 2.43, 2.58 (CPC-RV correlation, Gluck & Martin 1990)
2.46, 2.60; 2.30 (25°C, 60°C, shake flask-UV; quoted lit. value, Kramer & Henze 1990)
2.13 (shake flask-UV, Nakagawa et al. 1992)
2.30 (recommended, Sangster 1993)
2.40 ± 0.15, 2.21 ± 0.53 (solvent generated liquid-liquid chromatography SGLLC-correlation, RP-HPLC-k′ correlation, Cichna et al. 1995)
2.30 (recommended, Hansch et al. 1995)

Octanol/Air Partition Coefficient, log K_{OA}:

Bioconcentration Factor, log BCF:
< 2.0 (*carprinus carpio*, Sasaki 1978; Kawasaki 1980)
1.52, 1.20 (calculated-K_{OW}, S, Lyman et al. 1982; quoted, Howard 1989)
2.28 ± 0.06 (guppy-fat basis, Deneer et al. 1987)

Sorption Partition Coefficient, log K_{OC}:
2.63, 2.09 (soil, calculated-K_{OW}, S, Lyman et al. 1982; quoted, Howard 1989)

Environmental Fate Rate Constants, k, or Half-Lives, $t_{½}$:
Volatilization: estimated $t_{½}$ = 21 h using Henry's law constant for a model river 1-m deep flowing 1 m/s with a wind speed of 3 m/s (Lyman et al. 1982; quoted, Howard 1989).
Photolysis:
Oxidation: rate constant k =3.0×10^{-11} cm^3 molecules^{-1} s^{-1} for the reaction with 8×10^{-5} molecules/cm^3 photochemically produced hydroxyl radical in air (GEMS 1986; quoted, Howard 1989); rate constant k = 7.0×10^{-11} cm^3 molecule^{-1} s^{-1} for the gas-phase reactions with OH radical at 298 K (Atkinson 1989).
Hydrolysis:
Abiotic Transformation: Degradation in reductive environment:
k = 0.141 min^{-1} with solute concn of 50 μM in a 19 day-old 0.2g/L magnetite suspension at pH 7 and 1.5 mM Fe(II) at 25°C (Klusen et al. 1995)
Biodegradation: average biodegradation rate of 32.5 mg COD g^{-1} h^{-1} for 98% removal (Scow 1982).
Biotransformation:
Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants:

Half-Lives in the Environment:
Air: $t_{½}$ = 8 h, based on a rate constant k = 3.0×10^{-11} cm^3 molecules^{-1} s^{-1} for the reaction with 8×10^{-5} molecules/cm^3 photochemically produced hydroxyl radical in air (GEMS 1986; quoted, Howard 1989).
Surface water: estimated $t_{½}$ = 3.2 d in Rhine River in case of a first order reduction process (Zoeteman et al. 1980)
midday $t_{½}$(calc) = 45 min in Aucilla River water due to indirect photolysis using an experimentally determined reaction rate constant k = 0.92 h^{-1} (Zepp et al. 1984; quoted, Howard 1989);
estimated $t_{½}$ = 3.2 d for a river 4 to 5 m deep, based on monitoring data (Zoeteman et al. 1980; quoted, Howard 1989).
Ground water:
Sediment:
Soil:
Biota:

TABLE 16.1.4.2.1
Reported aqueous solubilities of 2-nitrotoluene at various temperatures

Gross et al. 1931		Beneš & Dohnal 1999	
shake flask-interferometry		shake flask-UV	
t/°C	$S/g \cdot m^{-3}$	t/°C	$S/g \cdot m^{-3}$
15	-	10	531
30	652	20	609
		30	688
		40	773
		$\Delta H_{sol}/(kJ\ mol^{-1}) = 9.4 \pm 0.1$ 25°C	

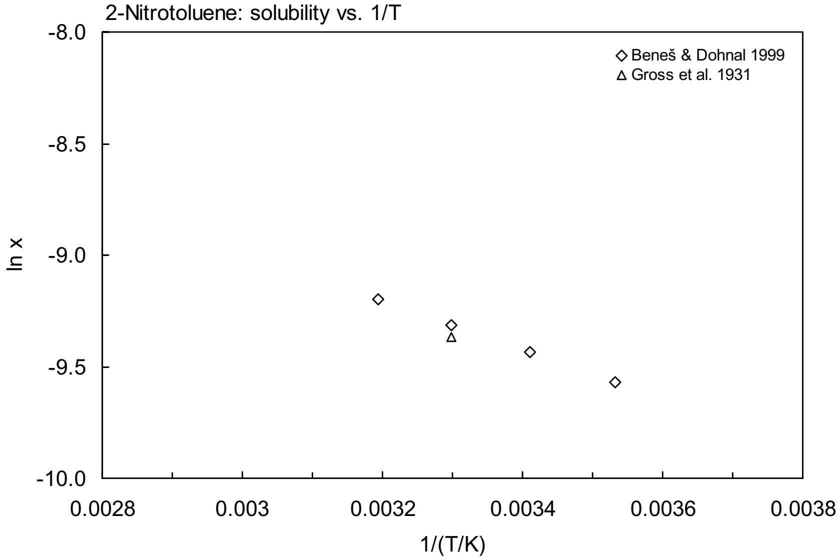


FIGURE 16.1.4.2.1 Logarithm of mole fraction solubility (ln *x*) versus reciprocal temperature for 2-nitrotoluene.

TABLE 16.1.4.2.2
Reported vapor pressures of 2-nitrotoluene at various temperatures and the coefficients for the vapor pressure equations

$\log P = A - B/(T/K)$ (1) $\ln P = A - B/(T/K)$ (1a)
$\log P = A - B/(C + t/°C)$ (2) $\ln P = A - B/(C + t/°C)$ (2a)
$\log P = A - B/(C + T/K)$ (3)
$\log P = A - B/(T/K) - C \cdot \log (T/K)$ (4)

Kahlbaum 1898		Stull 1947		Dreisbach & Shrader 1949		Aim 1994	
static method		summary of literature data		ebulliometry		comparative ebulliometry	
t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa
81.8	666.6	50.0	133.3	129.31	6287	115.842	3640
94.8	1333.2	79.1	666.6	134.51	7605	115.847	3639
109.6	2666.4	93.8	1333	138.75	8851	127.245	5773
114.8	3333.1	109.6	2666	142.43	10114	127.268	5778

TABLE 16.1.4.2.2 (*Continued*)

Kahlbaum 1898		Stull 1947		Dreisbach & Shrader 1949		Aim 1994	
static method		summary of literature data		ebulliometry		comparative ebulliometry	
t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa
119.2	3999.7	126.3	5333	156.61	16500	137.028	8376
122.8	4666.3	137.6	7999	185.48	42077	137.052	8375
126.1	5333	151.5	13332	205.48	67661	144.838	11104
131.7	6666	173.7	26664	222.15	101325	151.379	13955
150.6	13332	197.7	53329			151.415	13946
172.4	26664	222.3	101325	bp/°C	222.15	157.004	16843
186.1	39997					157.028	16827
196.0	53329	mp/°C	–4.1			162.792	20322
204.2	66661					162.840	20311
211.3	79993					168.856	24597
217.5	93326					168.917	24587
220.4	101325					174.744	29405
						mp/°C	–2.90
						bp/°C	222.946
						eq. 3	P/kPa
						A	6.45342
						B	1906.532
						C	65.441
						for temp range: 115–175°C	

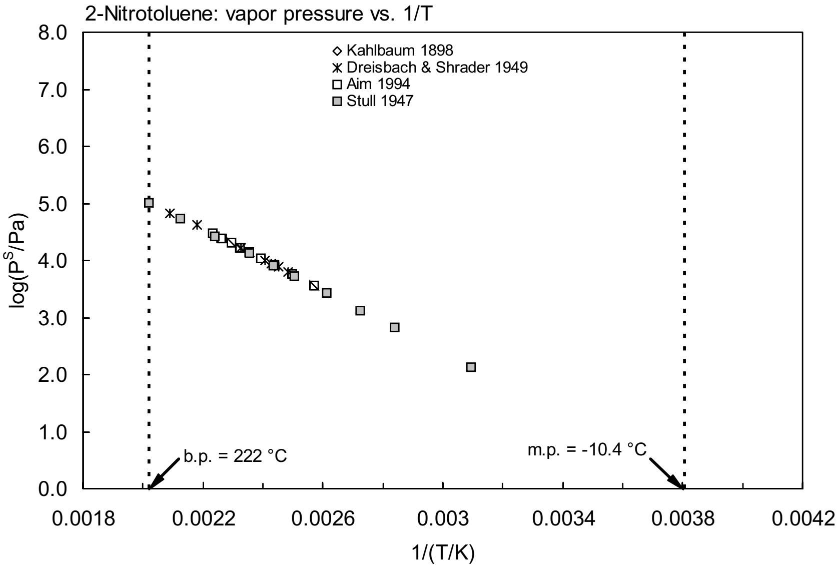
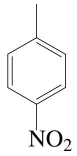


FIGURE 16.1.4.2.2 Logarithm of vapor pressure versus reciprocal temperature for 2-nitrotoluene.

16.1.4.3 4-Nitrotoluene



Common Name: 4-Nitrotoluene
Synonym: 1-methyl-4-nitrobenzene, *p*-nitrotoluene, 4-methylnitrobenzene
Chemical Name: 4-nitrotoluene, *p*-nitrotoluene
CAS Registry No: 99-99-0
Molecular Formula: $CH_3C_6H_4NO_2$
Molecular Weight: 137.137
Melting Point (°C):
51.63 (Lide 2003)
Boiling Point (°C):
238.3 (Stull 1947; Weast 1982–83; Dean 1985; Howard 1989)
Density (g/cm^3 at 20°C):
1.16278, 1.15799 (20°C, 25°C, Dreisbach & Martin 1949)
1.392 (Dean 1985)
Molar Volume (cm^3/mol):
124.2 (75°C, Stephenson & Malanowski 1987)
153.0 (calculated-Le Bas method at normal boiling point)
Dissociation Constant, pK:
–11.27 (Perrin 1972)
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
17.15 (Tsonopoulos & Prausnitz 1971)
Entropy of Fusion, ΔS_{fus} (J/mol K):
50.21 (Tsonopoulos & Prausnitz 1971)
Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F: 0.548 (mp at 51.63°C)

Water Solubility (g/m^3 or mg/L at 25°C or as indicated. Additional data at other temperatures designated * are compiled at the end of this section):
442 (30°C, shake flask-interferometer, Gross et al. 1933)
< 278 (shake flask-centrifuge, Booth & Everson 1948)
302 (Tsonopoulos & Prausnitz 1971)
442 (30°C, Verschueren 1983)
288 (20°C, shake flask-UV spectrophotometry, Hashimoto et al. 1984)
307 (calculated-group contribution method, Kühne et al. 1995)
242* (20°C, shake flask-UV spectrophotometry, measured range 10–40°C, Beneš & Dohnal 1999)

Vapor Pressure (Pa at 25°C or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):
13.98* (extrapolated-regression of tabulated data, measured range 92–237°C, Kahlbaum 1898)
log (P/mmHg) = –2630/(T/K) + 8.025 (isoteniscope method, temp range not specified, Kobe et al. 1941)
22.81* (extrapolated-regression of tabulated data, temp range 53.7–238.2°C, Stull 1947)
log (P/mmHg) = 7.52323 – 2150.6/(230 + t/°C) (Antoine eq., Dreisbach & Martin 1949)
8851* (147.71°C, ebulliometry, measured range 147.71–233.25°C, Dreisbach & Shrader 1949)
0.622* (23.886°C, Knudsen effusion, measured range 297.036–309.518 K, Lenchitz & Velicky 1970)
log (P/mmHg) = 11.5424 – 4130.0708/(T/K); temp range 297–310 K (Knudsen effusion, Lenchitz & Velicky 1970)
log (P/mmHg) = [–0.2185 × 11915.0/(T/K)] + 7.965025; temp range 53.7–238.3°C (Antoine eq., Weast 1972–73)
5.50* (ebulliometry, fitted to Antoine eq., measured range 144–239°C, Ambrose & Gundry 1980)
9.50 (extrapolated-supercooled liq., Ambrose & Gundry 1980)

13.33 (20°C, Verschueren 1983; quoted, Howard 1989)
8.347 (extrapolated-Antoine eq., Boublik et al. 1984)
$\log (P/kPa) = 6.11507 - 1716.897/(184.543 + t/°C)$; temp range 147.7–233.3°C (Antoine eq. from reported exptl. data, Boublik et al. 1984)
8.38 (extrapolated-Antoine eq., Dean 1985, 1992)
$\log (P/mmHg) = 6.9948 - 1720.39/(184.9 + t/°C)$; temp range 148–233°C (Antoine eq., Dean l985, 1992)
0.653 (interpolated-Antoine eq.-I, Stephenson & Malanowski 1987)
$\log (P_S/kPa) = 10.6673 - 4130.07/(T/K)$; temp range 296–310 K (solid, Antoine eq.-I, Stephenson & Malanowski 1987)
$\log (P_L/kPa) = 7.40605 - 2889.12/(23.37 + T/K)$; temp range 423–512 K (liquid, Antoine eq.-II, Stephenson & Malanowski 1987)
15.18* (ebulliometry, average of extrapolated-Antoine eq., Aim 1994)
$\log (P/mmHg) = 9.9641 - 2.6549 \times 10^3/(T/K) - 0.80182\cdot\log (T/K) + 5.3926 \times 10^{-4}\cdot(T/K) - 4.109 \times 10^{-14}\cdot(T/K)^2$; temp range 325–736 K (vapor pressure eq., Yaws 1994)

Henry's Law Constant ($Pa\cdot m^3/mol$ at 25°C):
5.065 (calculated, Hine & Mookerjee 1975)

Octanol/Water Partition Coefficient, log K_{OW}:
2.37 (shake flask-UV, Fujita et al. 1964)
2.40 (unpublished result, Leo et al. 1971)
2.34 (HPLC-k′ correlation, Deneer et al. 1987)
2.42 (recommended, Sangster 1989)
2.10, 2.05 (25°C, 60°C, shake flask-UV, Kramer & Henze 1990)
2.61 (shake flask-UV, Nakagawa et al. 1992)
2.37 (recommended, Sangster 1993)
2.37 ± 0.15 (solvent generated liquid-liquid chromatography SGLLC-correlation, Cichna et al. 1995)
2.42 (recommended, Hansch et al. 1995)
2.18 (microemulsion electrokinetic chromatography-retention factor correlation, Poole et al. 2000)

Octanol/Air Partition Coefficient, log K_{OA}:

Bioconcentration Factor, log BCF:
< 2.0 (*Carprinus carpio*, Sasaki 1978; Kawasaki 1980)
1.57, 1.30 (calculated-K_{OW}, S, Lyman et al. 1982; quoted, Howard 1989)
2.37 ± 0.05 (guppy-fat basis, Deneer et al. 1987)

Sorption Partition Coefficient, log K_{OC}:
2.67, 2.18 (soil, calculated-K_{OW}, S, Lyman et al. 1982; quoted, Howard 1989)

Environmental Fate Rate Constants, k, or Half-Lives, $t_{½}$:
Volatilization: based on Henry's law constant an estimated $t_{½} = 25$ h was obtained for a model river of 1- m deep with a current of 1 m/s and wind speed of 3 m/s (Lyman et al. 1982; quoted, Howard 1989).
Photolysis:
Oxidation: photooxidation $t_{½} = 8.0$ h in air, based on measured rate constant $k = 3 \times 10^{-11}$ cm^3 $molecule^{-1}$ s^{-1} at 25°C for the reaction with photochemically produced 8×10^5 $molecules/cm^3$ hydroxyl radical (GEMS 1986; quoted, Howard 1989).
Hydrolysis:
Abiotic Transformation: Degradation in reductive environment:
$k = 0.101$ min^{-1} with solute concn of 50 μM in a 19 d-old 0.2g/L magnetite suspension at pH 7 and 1.5 mM Fe(II) at 25°C (Klusen et al. 1995)
Biodegradation: average biodegradation rate of 32.5 mg COD g^{-1} h^{-1} for 98% removal (Scow 1982).
Biotransformation:
Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants:

Half-Lives in the Environment:

Air: photooxidation $t_{½}$ = 8.0 h, based on measured rate constant of 3×10^{-11} cm^3 $molecule^{-1}$ s^{-1} at 25°C for the reaction with photochemically produced 8×10^5 molecules/cm^3 hydroxyl radical (GEMS 1986; quoted, Howard 1989).

Surface water: estimated $t_{½}$ = 2.7 d in Rhine River in case of a first order reduction process (Zoeteman et al. 1980) estimated $t_{½}$ = 2.7 d, based on monitoring data for a river of 4 to 5-m deep (Zoeteman et al. 1980; quoted, Howard 1989).

Groundwater:

Sediment:

Soil:

Biota:

TABLE 16.1.4.3.1
Reported aqueous solubilities of 4-nitrotoluene at various temperatures

Gross et al. 1931		Beneš & Dohnal 1999	
shake flask-interferometry		shake flask-UV	
t/°C	S/g·m^{-3}	t/°C	S/g·m^{-3}
15	-	10	179
30	442	20	242
		30	322
		40	418
		ΔH_{sol}/(kJ mol^{-1}) = 21.1 ± 0.1 25°C	

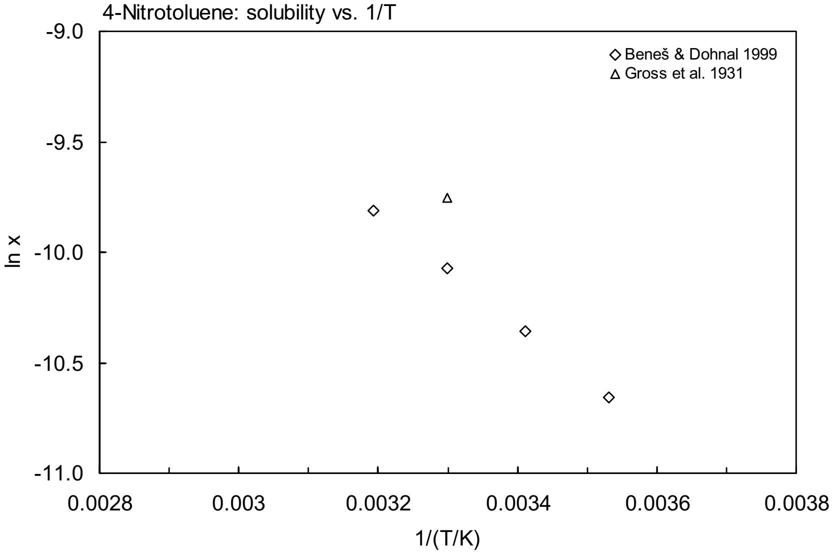


FIGURE 16.1.4.3.1 Logarithm of mole fraction solubility (ln *x*) versus reciprocal temperature for 4-nitrotoluene.

TABLE 16.1.4.3.2
Reported vapor pressures of 4-nitrotoluene at various temperatures and the coefficients for the vapor pressure equations

log P = A – B/(T/K)	(1)	ln P = A – B/(T/K)	(1a)
log P = A – B/(C + t/°C)	(2)	ln P = A – B/(C + t/°C)	(2a)
log P = A – B/(C + T/K)	(3)		
log P = A – B/(T/K) – C·log (T/K)	(4)		

1.

Kahlbaum 1898		Stull 1947		Dreisbach & Shrader 1949		Lenchitz & Velicky 1970	
static method-manometer		summary of literature data		ebulliometry		Knudsen effusion	
t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa
92.3	666.6	53.7	133.3	147.71	8851	23.886	0.6218
105.6	1333.2	85.0	666.6	151.43	10114	23.888	0.6283
120.3	2666.4	100.5	1333	165.98	16500	26.042	0.7311
125.7	3333	117.7	2666	197.75	42077	26.06	0.7330
130.4	3999.7	136.0	5333	216.17	67661	28.029	0.9426
134.4	4666	147.9	7999	233.25	101325	28.065	0.8994
137.9	5333	163.0	13332			30.205	1.0348
143.8	6666	186.7	26664	bp/°C	233.25	30.207	1.0423
164.0	13332	212.5	53329			32.012	1.3291
186.5	26664	238.3	101325			32.033	1.2987
201.2	39997					34.16	1.6681
212.2	53329	mp/°C	51.9			34.165	1.6551
220.8	66661					35.348	2.3313
228.4	79993					35.358	2.2839
234.8	93326					36.368	2.3087
237.7	101325						
						mp/°C	51.5
						enthalpy of sublimation: ΔH_{sub} = 43.095 kJ mol^{-1} at 25°C	
						eq. 1	P/mmHg
						A	11.5424
						B	4130.0828

2.

Ambrose & Gundry 1980		Aim 1994	
bubble-cap ebulliometer		comparative ebulliometry	
t/°C	P/Pa	t/°C	P/Pa
143.498	5649	128.161	3639
148.11	7742	128.167	3639
153.159	9254	140.078	5776
158.081	10956	140.132	5787
163.205	12999	150.293	8378
168.438	15403	150.369	8400
173.494	18066	158.455	11107
180.103	22110	158.487	11118
185.757	26135	165.32	13946

(*Continued*)

TABLE 16.1.4.3.2 (*Continued*)

Ambrose & Gundry 1980		Aim 1994	
bubble-cap ebulliometer		comparative ebulliometry	
t/°C	P/Pa	t/°C	P/Pa
192.227	31460	165.32	13967
198.564	37505	171.181	16823
205.643	44864	171.225	16845
212.568	54256	171.236	16848
218.948	63659	177.246	20306
225.722	75033	177.30	20332
233.058	89121	183.698	24639
238.685	101268		
239.269	102565	mp/°C	51.5
		bp/°C	238.343
tp/°C	51.64		
bp/°C	238.675	eq. 2	P/kPa
ΔH_{fus} = 16.81 kJ mol^{-1}		A	6.36793
ΔH_V = 46.60 kJ mol^{-1}, at bp		B	1931.718
		C	68.661
eq. 3	P/kPa	for temp range: 128–184°C	
A	6.27217		
B	1682,295		
C	–75.321		
for temp range: 416 to 513 K			
vapor pressure eq. for solid:			
eq. 1	P/kPa		
A	32.2514		
B	9018.0		
at triple pt	P = 67.72 Pa		
at 298.15 K	P = 5.5Pa		

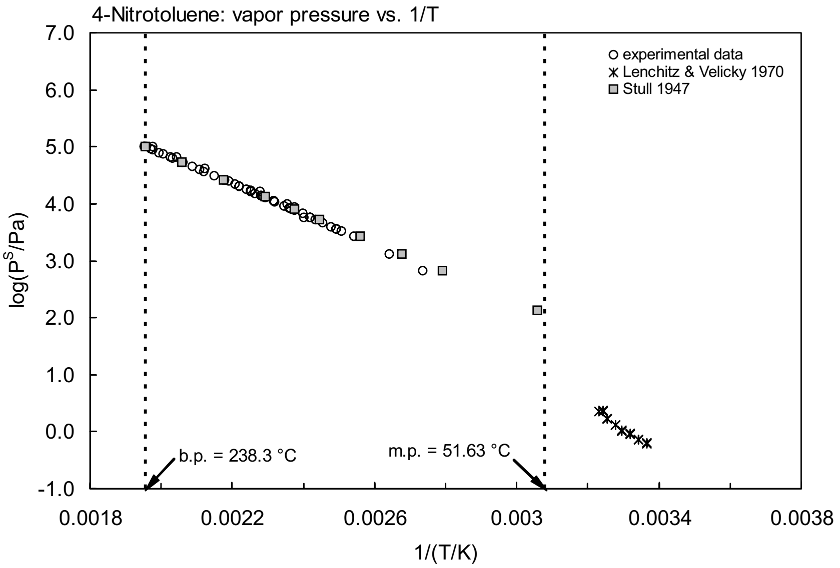
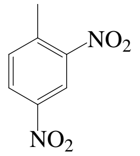


FIGURE 16.1.4.3.2 Logarithm of vapor pressure versus reciprocal temperature for 4-nitrotoluene.

16.1.4.4 2,4-Dinitrotoluene (DNT)



Common Name: 2,4-Dinitrotoluene
Synonym: dinitrotoluol, 1-methyl-2,4-dinitrobenzene, DNT
Chemical Name: 2,4-dinitrotoluene, 1-methyl-2,4-dinitrobenzene
CAS Registry No: 121-14-2
Molecular Formula: $C_7H_6N_2O_4$, $CH_3C_6H_3(NO_2)_2$
Molecular Weight: 182.134
Melting Point (°C):
 70.5 (Lide 2003)
Boiling Point (°C):
 300 dec. (Weast 1982–83; Lide 2003)
Density (g/cm^3 at 20°C):
 1.521 (15°C, Verschueren 1983)
Molar Volume (cm^3/mol):
 175.2 (calculated-Le Bas method at normal boiling point)
Dissociation Constant, pK:
 –13.53 (Perrin 1972)
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
Entropy of Fusion, ΔS_{fus} (J/mol K):
 58.99 (Yalkowsky & Valvani 1980)
Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F: 0.358 (mp at 70.5°C)

Water Solubility (g/m^3 or mg/L at 25°C or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):

270	(22°C, Verschueren 1977, 1983)
300	(22°C, Dunlap 1981)
276; 145	(quoted exptl.; calculated-group contribution method, Kühne et al. 1995)
199	(25.2°C, shake flask-HPLC/UV, Phelan & Barnett 2001)
188*	(22°C, shake flask-HPLC/UV, measured range 12.4–61.8°C, Phelan & Barnett 2001)

Vapor Pressure (Pa at 25°C and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):

0.133* (59°C, Knudsen effusion, measured range 59–69°C, Lenchitz & Velicky 1970)
0.00321 (extrapolated-Antoine eq., Lenchitz & Velicky 1970)
log (P/mmHg) = 12.6177 – 5139.058/(T/K); temp range 331.913–342.277 K (Knudsen effusion, Lenchitz & Velicky 1970)
0.0177* (20°C, gas saturation-GC/ECD, measured range 277.5–344.15 K, Pella 1977)
0.0290 (gas saturation-GC/ECD, interpolated-Antoine eq., measured range 277.5–344.15 K Pella 1977)
log (P/mmHg) = (13.08 ± 0.19) – (4992 ± 59)/(T/K); temp range 277.5–344.15 K (gas saturation, Pella 1977)
0.0147 (20°C, Spanggord et al. 1980)
0.6800 (quoted, Mabey et al. 1982)
log (P/kPa) = 5.06336 – 1216.523/(76.54 + t/°C); temp range 100–199°C (Antoine eq. from reported exptl. data, Boublik et al. 1984)
0.0296, 0.0032 (extrapolated-Antoine eq.-I, eq.-II, Stephenson & Malanowski 1987)
log (P_S/kPa) = 12.27361 – 5009.432/(T/K); temp range 277–343 K (solid, Antoine eq.-I, Stephenson & Malanowski 1987)
log (P_S/kPa) = 11.7426 – 5139.058/(T/K); temp range 331–342 K (solid, Antoine eq.-II, Stephenson & Malanowski 1987)

log (P_L/kPa) = 7.1423 – 3039/(T/K); temp range 473–572 K (liquid, Antoine eq.-III, Stephenson & Malanowski 1987)

log (P_L/kPa) = 6.04898 – 1956.095/(–108.183 + T/K); temp range 344–572 K (liquid, Antoine eq.-IV, Stephenson & Malanowski 1987)

log (P/mmHg) = 5.798 – 1118/(61.8 + t/°C); temp range 200–299°C (Antoine eq., Dean 1992)

log (P/mmHg) = 11.5966 – 3.0079×10^3/(T/K) –1.6468·log (T/K) + 1.5949×10^{-3}·(T/K) – 1.8722×10^{-14}·$(T/K)^2$; temp range 343–814 K (vapor pressure eq., Yaws 1994)

Henry's Law Constant (Pa·m³/mol at 25°C):

0.0160	(calculated-P/C, Smith et al. 1981)
0.4560	(calculated-P/C, Mabey et al. 1982)
0.0878	(Smith et al. 1983; quoted, Howard 1989)
32.23	(quoted from WERL Treatability database, Ryan et al. 1988)

Octanol/Water Partition Coefficient, log K_{OW}:

1.98	(shake flask, Hansch & Leo 1985)
2.04	(HPLC-k′ correlation, Deneer et al. 1987)
1.98	(recommended, Sangster 1993)
1.98	(recommended, Hansch et al. 1995)

Octanol/Air Partition Coefficient, log K_{OA}:

Bioconcentration Factor, log BCF:

1.59	(microorganisms-water, calculated-K_{OW}, Mabey et al. 1982)
1.11, 1.76	(*daphnia magna, lumbriculus variegatus*, Liu et al. 1983)
> 3.30	(*selanastrum capricornutum*, Liu et al. 1983)
1.89, 0.602	(bluegill sunfish in viscera, bluegill sunfish in muscle, Liu et al. 1983)
2.31 ± 0.03	(guppy-fat basis, Deneer et al. 1987)

Sorption Partition Coefficient, log K_{OC}:

1.65	(sediment-water, calculated-K_{OW}, Mabey et al. 1982)
1.68	(calculated-K_{OW}, Kollig 1993)

Environmental Fate Rate Constants, k, or Half-Lives, $t_{1/2}$:

Volatilization: half-life of approximately 100 d (Mills et al. 1982).

Photolysis: direct photolysis rate constant k = 1.6×10^{-2} h^{-1} for summer at 40°N latitude in water (Mabey et al. 1982);

aqueous photolysis $t_{1/2}$ = 23–72 h, based on measured photolysis rates in water (Mill & Mabey 1985; Simmons & Zepp 1986; quoted, Howard et al. 1991);

atmospheric transformation lifetime τ ~ 1–5 d (Kelly et al. 1994).

Hydrolysis:

Oxidation: aqueous oxidation rate constants k << 360 M^{-1} h^{-1} for singlet oxygen and k = 144 M^{-1} h^{-1} for peroxy radical at 25°C (Mabey et al. 1982);

photooxidation $t_{1/2}$ = 284 – 2840 h in air, based on estimated rate constant for the reaction with hydroxyl radical in air (Atkinson 1987; quoted, Howard et al. 1991);

photooxidation $t_{1/2}$ = 3–33 h, based on measured photooxidation rates in natural waters (Spanggord et al. 1980; Simmons & Zepp 1986; quoted, Howard et al. 1991).

Biodegradation: aqueous anaerobic $t_{1/2}$ = 48–240 h, based on anaerobic natural water die-away test data (Spanggord et al. 1980; quoted, Howard et al. 1991); aqueous aerobic $t_{1/2}$ = 672–4320 h, based on aerobic natural water die-away test data (Spanggord et al. 1981; quoted, Howard et al. 1991).

Biotransformation: rate constant of 1×10^{-7} mL $cell^{-1}$ h^{-1} for bacterial transformation in water (Mabey et al. 1982).

Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants:

Half-Lives in the Environment:

Air: photooxidation $t_{½}$ = 284–2840 h, based on estimated rate constant for the reaction with hydroxyl radical in air (Atkinson 1987; quoted, Howard et al. 1991);
atmospheric transformation lifetime τ ~ 1–5 d (Kelly et al. 1994).

Surface water: photooxidation $t_{½}$ = 3–33 h, based on measured photooxidation rates in natural waters (Spanggord et al. 1980; Simmons & Zepp 1986; quoted, Howard et al. 1991);
estimated $t_{½}$ = 1.7 d in Rhine River in case of a first order reduction process (Zoeteman et al. 1980)
sunlight photolysis $t_{½}$ ~ 42 h in pure water but ranged from 3 h to 10 h in three natural waters (Mabey et al. 1982).

Groundwater: $t_{½}$ = 48 – 8640 h, based on estimated unacclimated aqueous anaerobic and aerobic biodegradation half-life (Howard et al. 1991).

Sediment:

Soil: $t_{½}$ = 672 – 4320 h, based on estimated unacclimated aqueous aerobic biodegradation half-life (Howard et al. 1991).

Biota:

TABLE 16.1.4.4.1

Reported aqueous solubilities and vapor pressures of 2,4-dinitrotoluene at various temperatures and the coefficients for the vapor pressure equations

$\log P = A - B/(T/K)$ (1) $\ln P = A - B/(T/K)$ (1a)
$\log P = A - B/(C + t/°C)$ (2) $\ln P = A - B/(C + t/°C)$ (2a)
$\log P = A - B/(C + T/K)$ (3)
$\log P = A - B/(T/K) - C \cdot \log (T/K)$ (4)

Aqueous solubility		Vapor pressure			
Phelan & Barnett 2001		Lenchitz & Velicky 1970		Pella 1977	
shake flask-HPLC/UV		Knudsen effusion		gas saturation-GC	
t/°C	S/g·m^{-3}	t/°C	P/Pa	t/°C	P/Pa
12.4	129	58.765	0.1731	4.0	0.00164
22.0	188	59.927	0.2073	10.0	0.0038
21.7	182	59.927	0.2138	20.0	0.0177
32.0	269	60.883	0.2328	30.0	0.0453
42.0	410	62.926	0.2568	40.0	0.171
51.0	608	62.824	0.3192	50.0	0.695
61.8	975	64.002	0.3450	60.0	1.663
41.2	397	65.115	0.3836	71.0	5.295
25.2	199	67.023	0.4380		
		68.10	0.4952	mp/°C	69.75–70.95
		69.127	0.5202		
				eq. 1	P/mmHg
		mp/°C	71.1	A	13.08
				B	4992
		enthalpy of sublimation:			
		ΔH_{subl} = 98.324 kJ mol^{-1} (at 25°C)		enthalpy of sublimation: ΔH_{subl} = 95.81 kJ mol^{-1}	
		eq. 1	P/mmHg		
		A	12.6177		
		B	5139.058		

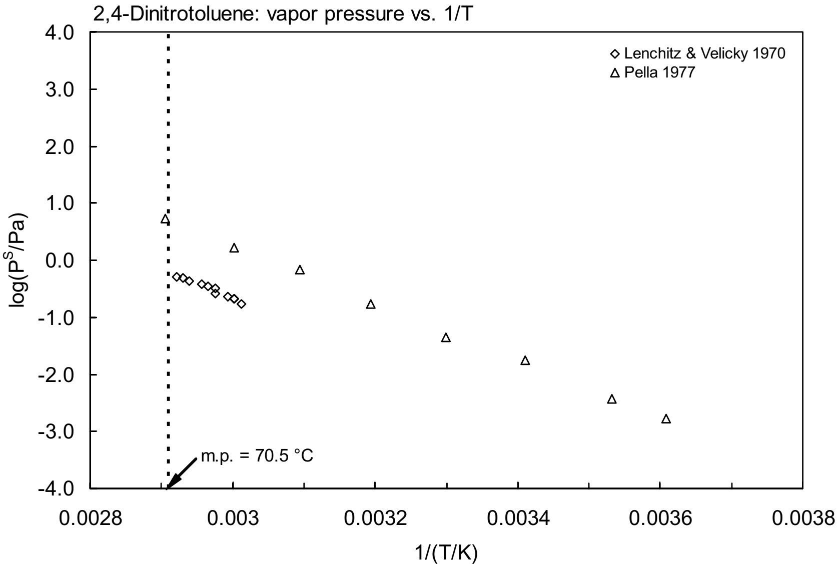
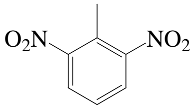


FIGURE 16.1.4.4.1 Logarithm of vapor pressure versus reciprocal temperature for 2,4-dinitrotoluene.

16.1.4.5 2,6-Dinitrotoluene



Common Name: 2,6-Dinitrotoluene
Synonym: dinitrotoluol, 1-methyl-2,6-dinitrobenzene, 2-methyl-1,3-dinitrobenzene
Chemical Name: 2,6-dinitrotoluene, 1-methyl-2,6-dinitrobenzene
CAS Registry No: 606-20-2
Molecular Formula: $C_7H_6N_2O_4$, $CH_3C_6H_3(NO_2)_2$
Molecular Weight: 182.134
Melting Point (°C):
66.0 (Weast 1982–83; Howard 1989; Lide 2003)
Boiling Point (°C):
285 (Verschueren 1977; Callahan et al. 1979; Howard 1989; Lide 2003)
Density (g/cm^3 at 20°C):
1.2833 (111°C, Weast 1982–83; Dean 1985)
Molar Volume (cm^3/mol):
141.9 (111°C, Stephenson & Malanowski 1987)
175.2 (calculated-Le Bas method at normal boiling point)
Dissociation Constant pK_a:
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
Entropy of Fusion, ΔS_{fus} (J/mol K):
Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F: 0.396 (mp at 66.0°C)

Water Solubility (g/m^3 or mg/L at 25°C or as indicated.):
180 (20°C, estimated, Mabey et al. 1982)
300 (selected, Mills et al. 1982)
182; 155 (quoted exptl.; calculated-group contribution method, Kühne et al. 1995)

Vapor Pressure (Pa at 25°C and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):
2.40 (29°C, Mabey et al. 1982)
0.0756* (gas saturation-GC/ECD, fitted to Antoine eq., temp range 277.5–323.15 K, Pella 1977)
$\log (P/mmHg) = (13.99 \pm 0.18) - (5139 \pm 52)/(T/K)$, temp range 277.5–323.15 K (gas saturation, Pella 1977)
0.0756 (Howard et al. 1986; quoted, Banerjee et al. 1990)
0.0767 (interpolated-Antoine eq.-I, Stephenson & Malanowski 1987)
$\log (P_S/kPa) = 11.9436 - 4446.22/(-21.279 + T/K)$; temp range 277–323 K (solid, Antoine eq.-I, Stephenson & Malanowski 1987)
$\log (P_L/kPa) = 7.329 - 2971/(T/K)$; temp range 423–523 K (liquid, Antoine eq.-II, Stephenson & Malanowski 1987)
$\log (P_L/kPa) = 6.70024 - 2160.968/(-93.282 + T/K)$; temp range 330–533 K (liquid, Antoine eq.-III, Stephenson & Malanowski 1987)
0.0756, 1.008 (quoted, calculated-solvatochromic parameters, Banerjee et al. 1990)
$\log (P/mmHg) = 4.372 - 380/(-43.6 + t/°C)$; temp range 150–260°C (Antoine eq., Dean 1992)
$\log (P/mmHg) = -14.5673 - 4.2746 \times 10^3/(T/K) + 12.904\cdot\log (T/K) - 2.380 \times 10^{-2}\cdot(T/K) + 9.4513 \times 10^{-6}\cdot(T/K)^2$; temp range 339–770 K (vapor pressure eq., Yaws 1994)

Henry's Law Constant (Pa·m^3/mol at 25°C)
0.800 (calculated-P/C, Mabey et al. 1982)
32.23 (quoted from WERL Treatability database, Ryan et al. 1988)
0.022 (SOGC 1987; quoted, Howard 1989)

Octanol/Water Partition Coefficient, log K_{OW}:

1.72	(shake flask, Hansch & Leo 1985)
2.02	(HPLC-k′ correlation, Deneer et al. 1987)
2.02	(shake flask-HPLC, Leggett et al. 1992)
2.07	(shake flask-UV, Nakagawa et al. 1992)
2.06	(recommended, Sangster 1993)
2.10	(recommended, Hansch et al. 1995)

Octanol/Air Partition Coefficient, log K_{OA}:

Bioconcentration Factor, log BCF:

3.72	(algal biomass, Davis et al. 1981)
1.71	(microorganisms-water, calculated-K_{OW}, Mabey et al. 1982)
1.08	(calculated-K_{OW}, Lyman et al. 1982; quoted, Howard 1989)
2.44 ± 0.04	(guppy-fat basis, Deneer et al. 1987)

Sorption Partition Coefficient, log K_{OC}:

1.96	(sediment-water, calculated-K_{OW}, Mabey et al. 1982)
2.31	(soil, calculated-K_{OW}, Lyman et al. 1982; quoted, Howard 1989)
1.40	(calculated-K_{OW}, Kollig 1993)

Environmental Fate Rate Constants, k, or Half-Lives, $t_{½}$:

Volatilization: $t_{½}$ ~ 100 d (Mills et al. 1982).

Photolysis: aqueous photolysis $t_{½}$ = 17–25 h, based on measured photolysis rates in water (Simmons & Zepp 1986; Mill & Mabey 1985; quoted, Howard et al. 1991)

89% was photo-transformed in 24 h and none left after 72 h from seawater solution under UV light (Nipper et al. 2004).

Hydrolysis:

Oxidation: aqueous oxidation rate constants k << 360 M^{-1} ± h^{1} for singlet oxygen and k = 144 M^{-1} h^{-1} for peroxy radical at 25°C (Mabey et al. 1982);

photooxidation $t_{½}$ = 2–17 h in water, based on measured photooxidation rates in natural waters (Simmons & Zepp 1986; quoted, Howard et al. 1991);

photooxidation $t_{½}$ = 284–2840 h, based on estimated rate constant for the reaction with hydroxyl radical in air (Atkinson 1987; quoted, Howard et al. 1991).

Biodegradation: aqueous anaerobic $t_{½}$ = 48–300 h, based on anaerobic natural water die-away test data for 2,4-dinitrotoluene; aqueous aerobic $t_{½}$ = 672–4320 h, based on aerobic natural water die-away test data (Spanggord et al. 1981; quoted, Howard et al. 1991).

Biotransformation: k = 1 × 10^{-10} mL $cell^{-1}$ h^{-1} for bacterial transformation in water (Mabey et al. 1982)

Biotransformation in marine sediments: all broken down in 28 d when incubated at 10°C, and in 7 d when incubated at 20°C in the sandy sediment; degraded by days 7 and 3 for incubation at 10 and 20°C, respectively, in fine-grained sediment (Nipper et al. 2004).

Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants:

Half-Lives in the Environment:

Air: estimated atmospheric $t_{½}$ = 8 h, based on the vapor phase reaction with hydroxyl radical in air (GEMS 1985; quoted, Howard 1989); photooxidation $t_{½}$ = 284 – 2840 h, based on estimated rate constant for the reaction with hydroxyl radical in air (Atkinson 1987; quoted, Howard et al. 1991).

Surface water: midday $t_{½}$ ~ 12 min in Aucilla river due to indirect photolysis using experimentally determined rate constant k = 3.6 h^{-1} (Zepp et al. 1984);

photooxidation $t_{½}$ = 2 – 17 h in water, based on measured photooxidation rates in natural waters (Simmons & Zepp 1986; quoted, Howard et al. 1991)

89% was photo-transformed in 24 h and none left after 72 h from seawater solution under UV light (Nipper et al. 2004).

Ground water: $t_{½}$ = 48 – 8640 h, based on estimated unacclimated aqueous anaerobic biodegradation half-life 2,4-dinitrotoluene and estimated unacclimated aqueous aerobic biodegradation half-life (Howard et al. 1991).

Sediment: degraded by days 28 and 7 for incubation at 10 and 20°C, respectively, in sandy marine sediment; degraded by days 7 and 3 for incubation at 10 and 20°C, respectively, in fine-grain sediment (Nipper et al. 2004)

Soil: $t_{1/2}$ = 672 – 4320 h, based on estimated unacclimated aqueous aerobic biodegradation half-life (Howard et al. 1991).

TABLE 16.1.4.5.1
Reported vapor pressures of 2,6-dinitrotoluene at various temperatures

Pella 1977	
gas saturation-GC	
t/°C	P/Pa
4.0	0.00342
10.0	0.0107
20.0	0.0383
30.0	0.147
40.0	0.483
50.0	1.718
mp/°C	57.25–57.75
eq. 1	P/mmHg
log P = A – B/(T/K)	
A	13.99
B	5139
enthalpy of sublimation:	
$\Delta H_{subl} = 98.324$ kJ mol^{-1}	

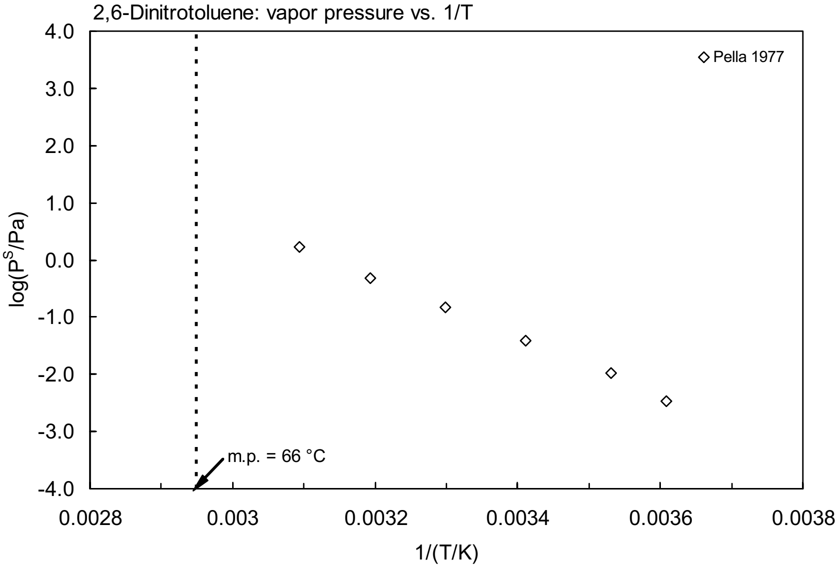
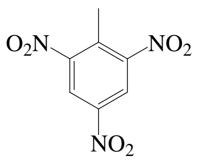


FIGURE 16.1.4.5.1 Logarithm of vapor pressure versus reciprocal temperature for 2,6-dinitrotoluene.

16.1.4.6 2,4,6-Trinitrotoluene (TNT)



Common Name: 2,4,6-Trinitrotoluene
Synonym: TNT
Chemical Name: 2,4,6-trinitrotoluene
CAS Registry No: 118-96-7
Molecular Formula: $C_7H_5N_3O_6$, $(NO_2)_3C_6H_2CH_3$
Molecular Weight: 227.131
Melting Point (°C):
 80.5 (Lide 2003)
Boiling Point (°C):
 240 explodes (Weast 1982–83; Dean 1992; Lide 2003)
Density (g/cm^3):
 1.654 (20°C, Weast 1982–83; Dean 1992)
Dissociation Constant, pK_a:
Molar Volume (cm^3/mol):
 137.3 (20°C, calculated-density)
 187.1 (calculated-Le Bas method at normal boiling point)
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
Entropy of Fusion, ΔS_{fus} (J/mol K):
Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F: 0.285 (mp at 80.5°C)

Water Solubility (g/m^3 or mg/L at 25°C or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):
 120* (20°C, shake flask, measured range 0.30–99.5°C, Taylor & Rinkenbach 1923)
 85.8 (21°C, Hale et al. 1979)
 104* (20°C, temp range 10–30°C, Spanggord et al. 1983)
 200 (15°C, Verschueren 1983)
 100 (Dean 1992)
 101.5* (average value at pH < 9.1, shake flask-HPLC/UV, measured range 6–42°C, Ro et al. 1996)
 101.6, 100.5, 110.5 (pH 3.5, pH 6.8, pH 9.1, shake flask-HPLC/UV spectrophotometry, Ro et al. 1996)
 $\ln [S/(mg\ L^{-1})] = 16.12 - 3413/(T/K)$, temp range 6–42°C, (pH < 8, shake flask-HPLC/spec., Ro et al. 1996)
 115* (23.02°C, shake flask-HPLC/UV, measured range 13.6–61°C, Phelan & Barnett 2001)
 99.85* 97.7* 99.9* (20°C, pH 4.2, 5.7, 6.2, shake flask-HPLC/UV, measured range 2.3–38°C, Lynch et al. 2001)
 $\ln [S/(mg\ L^{-1})] = 16.981 - 3607.5/(T/K)$; temp range 2.3–38°C (composite solubility prediction correlation, shake flask-HPLC/UV measurements, Lynch et al. 2001)

Vapor Pressure (Pa at 25°C or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):
 0.352* (53°C, Knudsen effusion, measured range 50–143°C, Edwards 1950)
 $\log (P_S/cmHg) = 14.34 - 6180/(T/K)$; range 50–81°C (solid, Knudsen effusion, Edwards 1950)
 $\log (P_L/cmHg) = 10.90 - 4960/(T/K)$; range 81–143°C (liquid, Knudsen effusion, Edwards 1950)
 0.0568* (54.756°C, Knudsen effusion, measured range 55–76°C, Lenchitz & Velicky 1970)
 $\log (P/mmHg) = 13.0776 - 5400.536/(T/K)$; temp range 55–76°C (Knudsen effusion, Lenchitz & Velicky 1970)
 0.00107* (gas saturation-GC/ECD, measured range 287.15–329.65 K, Pella 1977)
 $\log (P/mmHg) = (12.31 \pm 0.34) - (5175 \pm 105)/(T/K)$, temp range 287.15–329.65 K (gas saturation, Pella 1977)
 $\log (P/kPa) = 7.36331 - 3199.923/(248.004 + t/°C)$; temp range 230–250°C (liquid, Antoine eq. from reported exptl. data, Boublik et al. 1984)
 0.00078 (interpolated-Antoine eq.-I, Stephenson & Malanowski 1987)

log (P_S/kPa) = 13.596 – 5874.238/(T/K); temp range 293–353 K (solid, Antoine eq.-I, Stephenson & Malanowski 1987)
log (P_S/kPa) = 12.2025 – 5400.536/(T/K); temp range 337–350 K (solid, Antoine eq-II., Stephenson & Malanowski 1987)
log (P_L/kPa) = 6.40336 – 2191.85/(–121.43 + T/K); temp range 353–523 K (liquid, Antoine eq.-III, Stephenson & Malanowski 1987)
log (P/mmHg) = 7.67152 – 2669.4/(205.6 + t/°C); temp range 230–250°C (Antoine eq., Dean 1992)
log (P/mmHg) = 6.3156 – 2.6756×10^3/(T/K) – 4.6215·log (T/K) + 6.1747×10^{-9}·(T/K) – 2.3743×10^{-12}·$(T/K)^2$; temp range 354–518 K (vapor pressure eq., Yaws 1994)

Henry's Law Constant (Pa·m^3/mol at 25°C):

Octanol/Water Partition Coefficient, log K_{OW}:

1.60	(shake flask, Log P Database, Hansch & Leo 1987)
1.8	(shake flask-HPLC, Leggett et al. 1992)
1.73	(recommended, Sangster 1993)
2.05	(estimated-SPARC, Elovitz & Weber 1999)

Octanol/Air Partition Coefficient, log K_{OA}:

Bioconcentration Factor, log BCF or log K_B:

1.09	(aquatic oligochaete *Tubifex tubifex*, Conder et al. 2004)

Sorption Partition Coefficient, log K_{OC}:

Environmental Fate Rate Constants, k, and Half-Lives, $t_{½}$:
Volatilization:
Photolysis: $t_{½}$ = 14 h in summer, $t_{½}$ = 22–84 h in winter in pure water and photolyzed very rapidly in natural waters (Mabey et al. 1983)
photocatalytic degradation rates of TNT in a circular photocatalytic reactor using a UV lamp as a light source and TiO_2 as a photocatalyst: 1) at different initial TNT concns: k = 0.0989 min^{-1} with $t_{½}$ = 7.07 min at initial concn of 10 mg/L; k = 0.0644 min^{-1} with $t_{½}$ = 10.76 min at initial concn of 20 mg/L; k = 0.0405 min^{-1} with $t_{½}$ = 17.11 min at initial concn of 30 mg/L; k = 0.0269 min^{-1} with $t_{½}$ = 25.77 min at initial concn of 50 mg/L; and k = 0.0165 min^{-1} with $t_{½}$ = 42.01 min at initial concn of 100 mg/L. 2) at different pH: k = 0.0173 min^{-1} with $t_{½}$ = 27.6 min at pH 3.0; k = 0.0422 min^{-1} with $t_{½}$ = 20.1 min at pH 7.0 and k = 0.0451 min^{-1} with $t_{½}$ = 21.5 min at pH 11.0 (Son et al. 2004)
Photooxidation:
Hydrolysis:
Biodegradation: 95% disappearance within 2 h under aerobic conditions, and complete loss within 10 min under anaerobic conditions in sediment-water systems (Elovitz & Weber 1999)
Biotransformation: 100 % biotransformed when incubated at both 10 and 20°C in 7 d in fine-grain sediment; in sandy sediment although some picric acid could still be measured after 28 d of incubation at 10°C, none left after 56 d of incubation at 20°C (Nipper 2004)
Bioconcentration and Uptake and Elimination Rate Constants (k_1 and k_2):

Half-Lives in the Environment:
Air:
Surface water: photolysis $t_{½}$ = 14 h in summer, $t_{½}$ = 22–84 h in water in pure water, less than 1/2 h in some natural waters (Mabey et al. 1983)
photocatalytic degradation $t_{½}$ = 7.07 min to 42.1 min for different initial concn of TNT from 10- 100 mg/L, and $t_{½}$ = 27.1 – 21.5 min at pH 3.0–7.0 in a circular reactor, using a UV lamp as a light source and TiO_2 as a photocatalyst (Son et al. 2004)
Ground water:
Sediment: rapid disappearance 95% within 2 h, of TNT in an aerobic sediment-water system; under anaerobic conditions, TNT loss was complete within 10 min (Elovitz & Weber 1999)

100 % biotransformed when incubated at both 10 and 20°C in 7 d in fine-grain sediment; in sandy sediment although some picric acid could still be measured after 28 d of incubation at 10°C, none left after 56 d of incubation at 20°C (Nipper 2004)

Soil:

Biota: steady-state concn reached within 1-h in uptake experiments, and TNT depuration after a 24-h exposure occurred completely by 3 h (aquatic oligochaete, Conder et al. 2004)

TABLE 16.1.4.6.1
Reported aqueous solubilities of 2,4,6-trinitrotoluene (TNT) at various temperatures

$\ln S = A - B/(T/K)$ (1)

1.

Taylor & Rinkenbach '23		Spanggord et al. 1983		Ro et al. 1996			Phelan & Barnett 2001	
shake flask				shake flask-HPLC/UV			shake flask-HPLC/UV	
t/°C	$S/g\cdot m^{-3}$	t/°C	$S/g\cdot m^{-3}$	t/°C	pH	$S/g\cdot m^{-3}$	t/°C	$S/g\cdot m^{-3}$
	average*							
0.30	110	10	67	6	3.7	52.5	13.9	86
5.9	113	20	104	6	6.9	51.3	23.02	115
20.0	120	30	165	12	6.9	64.0	33.3	191
33.1	203			13	3.7	72.2	42.6	266
44.2	340			13	6.9	64.4	51.8	427
45.0	370			20	4.2	86.2	61.0	641
53.0	534			20	7.3	88.5	33.2	191
57.15	614			20	9.2	96.8	13.6	90
73.25	963			20	9.4	95.7	13.6	92
94.4	1375			20	10.1	91.2		
99.5	1467			21	3.5	74.5		
				21	6.8	82.5		
average of 3 sets of data				21	9.1	88.2		
				25	3.5	101.6		
				25	6.8	100.5		
				25	9	110.5		
				42	4.0	204.9		
				42	6.8	204.5		
				42	9.3	167.6		

$\ln [S/(mg/L)] = 16.12 - 3413/(T/K)$
for pH < 8

2.

Lynch et al. 2001					
shake flask-HPLC/UV					
t/°C	$S/g\cdot m^{-3}$	t/°C	$S/g\cdot m^{-3}$	t/°C	$S/g\cdot m^{-3}$
	pH 4.2		pH 5.7		pH 6.2
2.3	49.5	2.3	54.5	2.4	55.0
2.3	50.5	2.2	54.2	2.4	56.4
2.6	54.9	2.3	47.5	2.4	54.9
2.6	55.7	2.3	47.3	2.4	55.4
4.2	57.6	4.1	47.9	4.7	56.7

TABLE 16.1.4.6.1 (*Continued*)

Lynch et al. 2001					
shake flask-HPLC/UV					
t/°C	S/g·m^{-3}	t/°C	S/g·m^{-3}	t/°C	S/g·m^{-3}
4.2	57.7	4.1	48.2	4.7	57.4
4.2	45.7	4.6	58.1	5.2	56.7
4.2	48.4	4.6	59.1	5.2	56.1
20	100.7	20	96.7	20	99.6
20	99.0	20	98.7	20	100.2
20	99.2	20.1	98.9	20.1	99.5
20	101.7	20.1	100.6	20.1	96.3
20.1	96.3	20.2	98.8	20.1	99.5
20.1	95.9	20.2	99.8	20.1	99.8
20.1	96.0	20.2	97.5	20.2	94.6
20.1	97.8	20.2	100.4	20.2	97.2
36	211.7	35.7	208.5	35.9	216.5
36	213.1	35.7	213.5	35.9	213.9
36	208.5	36	215.2	36	212.2
36	211.6	36	214.3	36	215.3
37.7	219.6	37.7	229.7	37.6	229.4
37.7	219.4	37.7	230.6	37.6	231.4
37.8	218.2	37.7	226.2	38	234.4
37.8	214.8	37.7	228.3	38	235
eq. 1	S/(mg L^{-1})	eq. 1	S/(mg L^{-1})	eq. 1	S/(mg L^{-1})
A	22.741	A	22.399	A	23.244
B	6332	B	6230	B	6506.8

composite correlation eq. : $\ln [S/(\text{mg L}^{-1}) = 16981 - 3607.5/(T/K)$; temp range 2.3–38°C

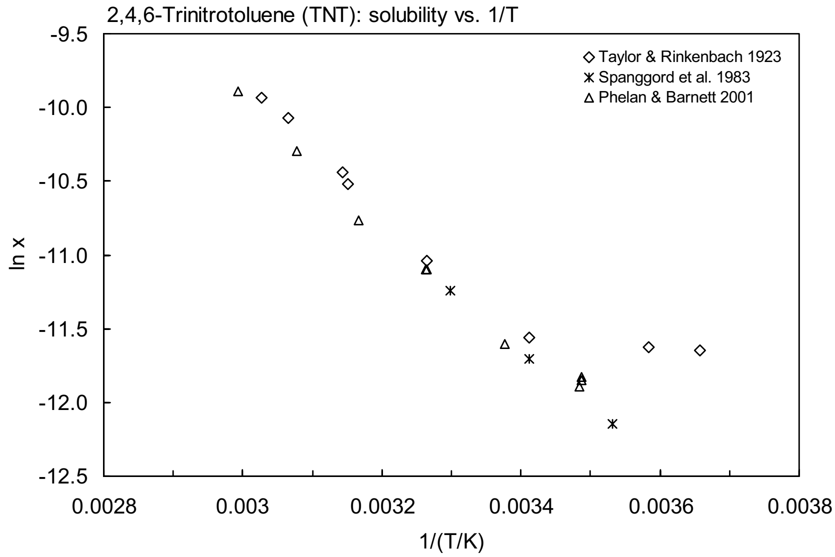


FIGURE 16.1.4.6.1 Logarithm of mole fraction solubility (ln *x*) versus reciprocal temperature for 2,4,6-trinitrotoluene.

TABLE 16.1.4.6.2
Reported vapor pressures of 2,4,6-trinitrotoluene (2,4,6-TNT) at various temperatures and the coefficients for the vapor pressure equations

$\log P = A - B/(T/K)$	(1)	$\ln P = A - B/(T/K)$	(1a)
$\log P = A - B/(C + t/°C)$	(2)	$\ln P = A - B/(C + t/°C)$	(2a)
$\log P = A - B/(C + T/K)$	(3)		
$\log P = A - B/(T/K) - C \cdot \log (T/K)$	(4)		

Edwards 1950		Lenchitz & Velicky 1970		Pella 1977	
Knudsen method		Knudsen effusion		gas saturation-GC	
t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa
53.0	0.0352	54.756	0.0568	14.0	0.000302
60.1	0.0724	59.704	0.0935	19.0	0.000412
60.8	0.0843	64.853	0.1613	25.0	0.00107
61.5	0.0915	70.02	0.3118	25.3	0.00128
61.0	0.0829	72.469	0.3665	26.5	0.00170
72.1	0.4146	72.493	0.3409	35.0	0.00676
72.1	0.4186	75.065	0.5142	40.0	0.00887
78.5	0.8586	65.91	0.1811	45.0	0.0143
78.5	0.7839	68.933	0.2342	50.0	0.0243
78.3	0.8293	73.981	0.4453	55.0	0.0446
79.8	0.8733	76.057	0.5796	56.5	0.05406
80.2	0.9546				
82.4	1.0612	mp/°C	81.1	mp/°C	80.15–81.25
86.9	1.5865				
99.5	5.2529	enthalpy of sublimation:		eq. 2	P/mmHg
99.5	5.4262	ΔH_{subl} = 120.92 kJ mol^{-1}		A	12.31
110.6	11.012		(at 25°C)	B	5175
110.5	10.612				
131.5	46.396	eq. 1	P/mmHg	enthalpy of sublimation:	
141.4	82.793	A	13.0776	ΔH_{subl} = 99.161 kJ mol^{-1}	
142.0	87.728	B	5400.536		
142.5	82.260				
For solid:					
eq. 1	P/cmHg				
A	14.34				
B	6180				
ΔH_{subl} = 118.41 kJ mol^{-1}					
For liquid:					
eq. 1	P/cmHg				
A	10.90				
B	4960				
ΔH_{subl} = 94.98.34 kJ mol^{-1}					

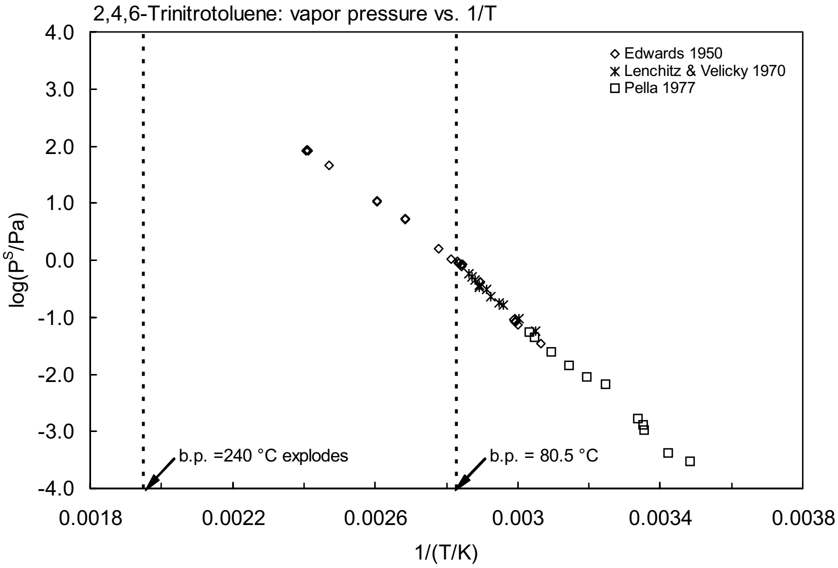
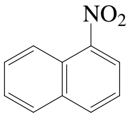


FIGURE 16.1.4.6.2 Logarithm of vapor pressure versus reciprocal temperature for 2,4,6-trinitrotoluene.

16.1.4.7 1-Nitronaphthalene (α-Nitronaphthalene)



Common Name: 1-Nitronaphthalene
Synonym: α-nitronaphthalene
Chemical Name: 1-nitronaphthalene, α-nitronaphthalene
CAS Registry No: 86-57-7
Molecular Formula: $C_{10}H_7NO_2$
Molecular Weight: 173.169
Melting Point (°C):
61 (Lide 2003)
Boiling Point (°C):
304.0 (Weast 1982–83; Dean 1985; Stephenson & Malanowski 1987)
Density (g/cm^3 at 20°C):
1.3320 (Weast 1982–83)
1.2230 (Dean 1985)
Molar Volume (cm^3/mol):
176.1 (calculated-Le Bas method at normal boiling point)
135.8 (calculated-density)
Dissociation Constant pK_a:
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
17.99 (Tsonopoulos & Prausnitz 1971)
Entropy of Fusion, ΔS_{fus} (J/mol K):
54.39 (Tsonopoulos & Prausnitz 1971)
Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F: 0.443 (mp at 61°C)

Water Solubility (g/m^3 or mg/L at 25°C):
50.0 (Aqueous Solubility Database, Yalkowsky et al. 1987)
9.82 (generator column-HPLC/UV, Yu & Xu 1992)
9.83 (calculated-molar concentration, Yu & Xu 1992)
50; 34.6 (quoted exptl.; calculated-group contribution method, Kühne et al. 1995)

Vapor Pressure (Pa at 25°C and reported temperature dependence equations):
0.202 (effusion method-fitted to Antoine eq., Radchenko & Kitiagorodskii 1974)
0.202 (solid, extrapolated-Antoine eq.-I, Stephenson & Malanowski 1987)
0.184 (liquid, extrapolated-Antoine eq.-III, Stephenson & Malanowski 1987)
$\log (P_S/kPa) = 8.31261 - 3579.698/(T/K)$; temp range 309–326 K (solid, Antoine eq.-I, Stephenson & Malanowski 1987)
$\log (P_S/kPa) = 13.223 - 5584/(T/K)$; temp range 325–332 K (solid, Antoine eq.-II, Stephenson & Malanowski 1987)
$\log (P_L/kPa) = 7.8959 - 3468.4/(T/K)$; temp range 332–580 K (liquid, Antoine eq.-III, Stephenson & Malanowski 1987)

Henry's Law Constant (Pa m^3/mol at 25°C):
3.463 (calculated-P/C with selected values)
0.178 (gas stripping-GC, Altschuh et al. 1999)

Octanol/Water Partition Coefficient, log K_{OW}:
3.19 (Hansch & Leo 1979)
3.19 (shake flask, Hansch & Leo 1987)

3.19 (shake flask-UV, Debnath & Hansch 1992)
3.19 (recommended, Sangster 1993)

Octanol/Air Partition Coefficient, log K_{OA}:

Bioconcentration Factor, log BCF:

Sorption Partition Coefficient, log K_{OC}:

Environmental Fate Rate Constants, k, or Half-Lives, $t_{½}$:

Volatilization:

Photolysis: measured photolysis rate constant are: 15.9×10^{-4} s^{-1} in a 6400-L indoor all-Teflon chamber under blacklamp irradiation and 1.37×10^{-4} s^{-1} outdoor in a 1000-L all-Teflon chamber under natural solar irradiation (Atkinson et al. 1989);

photolysis rate $k_{phot} = 1.5 \times 10^{-4}$ s^{-1} with a half-life of 1.7 h (Arey et al. 1990)

Hydrolysis:

Oxidation: rate constant k, for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO3} with NO_3 radical and k_{O3} with O_3 or as indicated, *data at other temperatures see reference:

$k_{OH} = (5.4 \pm 1.8) \times 10^{-12}$ cm^3 $molecule^{-1}$ s^{-1}; $k_{NO3} \leq 7.2 \times 10^{-15}$ cm^3 $molecule^{-1}$ s^{-1}, $k_{O3} < 6.0 \times 10^{-19}$ cm^3 $molecule^{-1}$ s^{-1} and $k_{N2O5} = 1.3 \times 10^{-18}$ cm^3 $molecule^{-1}$ s^{-1} with N_2O_5 and at 298 ± 2 K in the atmosphere (Atkinson et al. 1989)

$k_{OH} = 5.4 \times 10^{-12}$ cm^3 $molecule^{-1}$ s^{-1} with calculated lifetime of 2.9 d; $k_{NO3} \leq 7.2 \times 10^{-15}$ cm^3 $molecule^{-1}$ s^{-1} with calculated lifetime of –13 d, $k_{O3} < 6.0 \times 10^{-19}$ cm^3 $molecule^{-1}$ s^{-1} with a lifetime of > 28 d and $k_{N2O5} = 1.3 \times 10^{-18}$ cm^3 $molecule^{-1}$ s^{-1} with N_2O_5 a calculated lifetime of 2.4 yr at 298 ± 2 K in the atmosphere (Arey et al. 1990)

Biodegradation:

Biotransformation:

Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants:

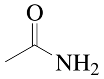
Half-Lives in the Environment:

Air: calculated lifetime of ~2 h based on measured outdoor photolysis rate and rate constants the gas-phase reactions (Atkinson et al. 1989);

photolysis $t_{½} = 1.7$ h using an average 12-h daytime NO_2 photolysis rate $k = 5.2 \times 10^{-3}$ s^{-1} – a dominant atmospheric loss process; calculated lifetimes of 2.9 d, –13 d, > 28 d and 2.4 yr due to reactions with OH radial, NO3 radical, O_3 and N_2O_5 (Arey et al. 1990)

16.1.5 AMIDES AND UREAS

16.1.5.1 Acetamide



Common Name: Acetamide
Synonym: ethanamide
Chemical Name: acetamide, acetic acid amine
CAS Registry No: 60-35-5
Molecular Formula: C_2H_5NO, CH_3CONH_2
Molecular Weight: 59.067
Melting Point (°C):
80.16 (Lide 2003)
Boiling Point (°C):
221 (Lide 2003)
Density (g/cm^3 at 20°C):
0.9986 (78°C, Weast 1982–83)
1.159 (Verschueren, 1983)
Molar Volume (cm^3/mol):
59.2 (calculated-density, Stephenson & Malanowski 1987)
66.9 (calculated-Le Bas method at normal boiling point)
Dissociation Constant pK_a: 7.62
Enthalpy of Vaporization, ΔH_V (kJ/mol):
56.1 (at bp, Riddick et al. 1986)
Enthalpy of Sublimation, ΔH_{subl} (kJ/mol):
78.66 (25°C, Riddick et al. 1986)
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
17.707 (Riddick et al. 1986)
Entropy of Fusion, ΔS_{fus} (J/mol K):
Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F: 0.288 (mp at 80.16°C)

Water Solubility (g/m^3 or mg/L at 25°C or as indicated):
975000 (20°C, Verschueren 1983)
408000 (20°C, Riddick et al. 1986)

Vapor Pressure (Pa at 25°C and reported temperature dependence equations):
8.61 (extrapolated-regression of tabulated data, temp range 65–222°C, Stull 1947)
$\log (P/mmHg) = [-0.2185 \times 14025.3/(T/K)] + 9.088352$; temp range 65.0–222°C (Antoine eq., Weast 1972–73)
100 (Riddick et al. 1986)
$\log (P/kPa) = 8.24516 - 3282.80/(T/K)$; temp range 65–150°C (Antoine eq., Riddick et al. 1986)
$\log (P/kPa) = 7.93409 - 2936.07/(T/K)$; temp range 65–bp (Antoine eq., Riddick et al. 1986)
2.44 (interpolated-Antoine eq.-I, Stephenson & Malanowski 1987)
$\log (P_S/kPa) = 10.9717 - 4050.1/(T/K)$; temp range 298–349 K (solid, Antoine eq.-I, Stephenson & Malanowski 1987)
$\log (P_L/kPa) = 7.97079 - 1998.3/(-89.32 + T/K)$; temp range 381–492 K (liquid, Antoine eq.-II, Stephenson & Malanowski 1987)
$\log (P/mmHg) = -413.1683 + 8.1328 \times 10^3/(T/K) + 172.9\cdot\log (T/K) - 0.16059\cdot(T/K) + 5.3892 \times 10^{-5}\cdot(T/K)^2$; temp range 354–761 K (vapor pressure eq., Yaws 1994)

Henry's Law Constant ($Pa\cdot m^3/mol$ at 25°C):
3.53×10^{-4} (calculated-P/C with selected values)

Octanol/Water Partition Coefficient, $\log K_{OW}$:
–1.09 (shake flask-radiochemical method, Cornford 1982)

–1.26	(shake flask, Log P Database, Hansch & Leo 1987)
–1.26	(shake flask-GC, Sotomatsu et al. 1987)
–1.26	(recommended Sangster 1989, 1993)
–1.23	(calculated-QSAR, Kollig 1993)
–1.26	(recommended, Hansch et al. 1995)

Octanol/Air Partition Coefficient, log K_{OA}:

Bioconcentration Factor, log BCF:

Sorption Partition Coefficient, log K_{OC}:

–1.55	(calculated-K_{OW}, Kollig 1993)

Environmental Fate Rate Constants, k, or Half-Lives, $t_{1/2}$:

Volatilization:

Photolysis:

Oxidation: photooxidation $t_{1/2}$ = 3.2–32 h in air, based on estimated rate constant for the vapor-phase reaction with hydroxyl radical in air (Atkinson 1987; quoted, Howard et al. 1991);
atmospheric transformation lifetime was estimated to be < 1 d (Kelly et al. 1994).

Hydrolysis: overall rate constant $k_h = 5.5 \times 10^{-12}\ s^{-1}$ with $t_{1/2}$ = 3950 yr; acid rate constant $k_A = 8.36 \times 10^{-6}\ s^{-1}$ and base rate constant $k_B = 5.5 \times 10^{-5}\ s^{-1}$ at 25°C and pH 7 (Mabey & Mill 1978)
acid rate constant $k = 0.03\ [M \pm (H^+) \pm h]^{-1}$ at pH 5 and base rate constant $k = 0.17\ [M \pm (OH^-) \pm h]^{-1}$ at pH 9 with first-order hydrolysis $t_{1/2}$ = 3950 yr at pH 7 and 25°C, (Mabey & Mill 1978; quoted, Howard et al. 1991).

Biodegradation: aqueous aerobic biodegradation $t_{1/2}$ = 24–168 h, based on aerobic aqueous screening test data (Malaney & Gerhold 1962, 1969; Urano & Kato 1986; quoted, Howard et al. 1991); aqueous anaerobic biodegradation $t_{1/2}$ = 96–672 h, based on estimated unacclimated aqueous aerobic biodegradation half-life (Howard et al. 1991).

Biotransformation:

Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants:

Half-Lives in the Environment:

Air: photooxidation $t_{1/2}$ = 3.2–32 h, based on estimated rate constant for the vapor-phase reaction with hydroxyl radical in air (Atkinson 1987; quoted, Howard et al. 1991);
atmospheric transformation lifetime was estimated to be < 1 d (Kelly et al. 1994).

Surface water: $t_{1/2}$ = 24–168 h, based on estimated unacclimated aqueous aerobic biodegradation half-life (Howard et al. 1991).

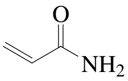
Groundwater: $t_{1/2}$ = 48–336 h, based on estimated unacclimated aqueous aerobic biodegradation half-life (Howard et al. 1991).

Sediment:

Soil: $t_{1/2}$ = 24–168 h, based on estimated unacclimated aqueous aerobic biodegradation half-life (Howard et al. 1991).

Biota:

16.1.5.2 Acrylamide



Common Name: Acrylamide
Synonym: 2-propenamide
Chemical Name: acrylamide
CAS Registry No: 79-06-1
Molecular Formula: C_3H_5NO, $CH_2{=}CHCONH_2$
Molecular Weight: 71.078
Melting Point (°C):
    84.5 (Lie 2003)
Boiling Point (°C):
    192.5 (Lide 2003)
Density (g/cm^3 at 20°C):
    1.122 (30°C, Dean 1985)
Molar Volume (cm^3/mol):
    80.8 (calculated-Le Bas method at normal boiling point)
Dissociation Constant pK_a:
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
Entropy of Fusion, ΔS_{fus} (J/mol K):
Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F: 0.261 (mp at 84.5°C)

Water Solubility (g/m^3 or mg/L at 25°C):
    2050000 (quoted, Verschueren 1983)
    2150000 (30°C, Dean 1985)

Vapor Pressure (Pa at 25°C and reported temperature dependence equations):
    0.616 (average, extrapolated-Antoine eq.-I and II, Stephenson & Malanowski 1987)
    $\log (P_L/kPa) = 7.395 - 3213/(/K)$, temp range 357–413K (Antoine eq.-I, Stephenson & Malanowski 1987)
    $\log (P_L/kPa) = 10.31055 - 3994.667/(T/K)$, temp range 373–413 K (Antoine eq.-II, Stephenson & Malanowski 1987)
    $\log (P/mmHg) = 17.0034 - 4.4434 \times 10^3/(T/K) - 1.7158 \cdot \log (T/K) + 2.0063 \times 10^{-6} \cdot (T/K) - 8.0394 \times 10^{-10} \cdot (T/K)^2$; temp range 358–477 K (vapor pressure eq., Yaws 1994)

Henry's Law Constant (Pam^3/mol at 25°C):

Octanol/Water Partition Coefficient, log K_{OW}:
    –0.90 (shake flask, Fujisawa & Masuhara 1980, 1981)
    –1.24 (calculated-HPLC-RT correlation, Fujisawa & Masuhara 1981)
    –0.67 (shake flask, Log P Database, Hansch & Leo 1987)
    –0.78 (recommended, Sangster 1989)
    –0.67 (recommended, Hansch et al. 1995)

Octanol/Air Partition Coefficient, log K_{OA}:

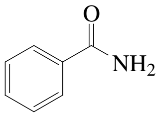
Bioconcentration Factor, log BCF:

Sorption Partition Coefficient, log K_{OC}:
    –0.969 (calculated-K_{OW}, Kollig 1993)

Environmental Fate Rate Constants, k, or Half-Lives, $t_{1/2}$:

Half-Lives in the Environment:
    Surface water: measured rate constant $k = (1.0 \pm 0.1) \times 10^5\ M^{-1}\ s^{-1}$ for direct reaction with ozone in water at pH 5.4–5.8 and 22 ± 1°C, with $t_{1/2}$ = 0.3 s at pH 7 (Yao & Haag 1991).

16.1.5.3 Benzamide



Common Name: Benzamide
Synonym: benzoylamide
Chemical Name: benzamide
CAS Registry No: 55-21-0
Molecular Formula: C_7H_7NO, $C_6H_5CONH_2$
Molecular Weight: 121.137
Melting Point (°C):
  127.3 (Lide 2003)
Boiling Point (°C):
  290 (Lide 2003)
Density (g/cm^3 at 20°C):
Molar Volume (cm^3/mol):
  112.2 (130°C, Stephenson & Malanowski 1987)
  132.4 (calculated-Le Bas method at normal boiling point)
Dissociation Constant pK_a:
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
Entropy of Fusion, ΔS_{fus} (J/mol K):
Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F: 0.0992 (mp at 127.3°C)

Water Solubility (g/m^3 or mg/L at 25°C or as indicated):
  13500 (20–25°C, shake flask-gravimetric method, Dehn 1917)
  13499 (Tsonopoulos & Prausnitz 1971)
  13490 (Windholz 1983)
  13515 (1 g in 74 mL, Budavari 1989)

Vapor Pressure (Pa at 25°C and reported temperature dependence equations):
  0.00522 (extrapolated, Antoine eq., Stephenson & Malanowski 1987)
  $\log (P_S/kPa) = 11.69847 - 5062.899/(T/K)$, temp range 325–342 K (solid, Antoine eq., Stephenson & Malanowski 1987)

Henry's Law Constant (Pam^3/mol at 25°C):
  4.52×10^{-5} (calculated-P/C, this work)

Octanol/Water Partition Coefficient, log K_{OW}:
  0.64 (shake flask-UV, Fujita et al. 1964)
  0.65 (shake flask, Leo et al. 1971; Hansch & Leo 1979; Hansch & Leo 1987)
  0.66 (shake flask-UV, Yaguzhinskii et al.1973)
  0.84 (HPLC-k′ correlation, Hammers et al. 1982)
  0.64 (shake flask-UV, Sotomatsu et al. 1987)
  0.50 (centrifugal partition chromatography CPC, Berthod et al. 1988)
  0.81 (RP-HPLC-RT correlation, ODS column with masking agent, Bechalany et al. 1989)
  0.64 (recommended, Sangster 1989, 1993)
  0.65 (counter-current chromatography, Vallat et al. 1990)
  0.65 (CPC-RV correlation, El Tayar et al. 1991)
  0.64 (shake flask-GC, Alcorn et al. 1993)
  0.64 (recommended, Hansch et al. 1995)

Octanol/Air Partition Coefficient, log K_{OA}:

Bioconcentration Factor, log BCF:

Sorption Partition Coefficient, log K_{OC}:

0.954; 1.301; 1.756 (sediment; Alfisol soil; Podzol soil, von Oepen et al. 1991)
1.46 (soil, quoted exptl., Meylan et al. 1992)
1.71 (soil, calculated-MCI χ and fragment contribution, Meylan et al. 1992)
1.46 (soil, mean value, Kördel et al. 1993)
1.46 (soil, calculated-MCI $^1\chi$, Sabljic et al. 1995)
1.46; 1.71 (HPLC-screening method; calculated-PCKOC fragment method, Müller & Kördel 1996)
1.87, 2.17, 1.12, 1.36, 1.645 (first generation Eurosoils ES-1, ES-2, ES-3, ES-4, ES-5, shake flask/batch equilibrium-HPLC/UV, Gawlik et al. 1998)
1.46, 1.22; 2.18, 1.75, 1.88, 1.83, 1.31 (soil: quoted lit., calculated-K_{OW}; HPLC-screening method using LC-columns of different stationary phases, Szabo et al. 1999)
1.747, 1.358, 1.236 (second generation of European reference soil set, Eurosoils ES-1, ES-3, ES-5, shake flask/batch equilibrium-HPLC/UV and HPLC-k′ correlation, Gawlik et al. 2000)

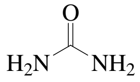
Environmental Fate Rate Constants, k, or Half-Lives, $t_{½}$:

Volatilization:
Photolysis:
Oxidation: aqueous photooxidation $t_{½}$ = 960–7.4 × 10^4 h, based on measured rates for reaction with OH radical in water (Anbar et al. 1966; Dorfman and Adams 1973; selected, Howard et al. 1991);
photooxidation $t_{½}$ = 3.1 – 31 h in air, based on estimated rate constant for the vapor-phase reaction with hydroxyl radicals in air (Atkinson et al. 1987; selected, Howard et al. 1991).
Hydrolysis: not expected to be significant based on estimated half-lives for hydrolysis of acetamide of 261, 3950, and 46 yr at pH 5,7,9, respectively, which were calculated using experimental acid and base hydrolysis rate constants for acetamide (Mabey & Mill 1978; selected, Howard et al. 1991).
Biodegradation: aqueous aerobic biodegradation $t_{½}$ = 48 – 360 h, and aqueous anaerobic biodegradation $t_{½}$ = 192 – 1400 h, both based on grab sample aerobic soil column test data (Fournier & Salle 1974; selected, Howard et al. 1991).
Biotransformation:
Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants:

Half-Lives in the Environment:

Air: photooxidation $t_{½}$ = 3.1 – 31 h, based on estimated rate constant for the vapor-phase reaction with hydroxyl radical in air (Atkinson et al. 1987; selected, Howard et al. 1991).
Surface water: $t_{½}$ = 48 – 360 h, based on grab sample aerobic soil column test data (Fournier & Salle 1974; selected, Howard et al. 1991).
Ground water: $t_{½}$ = 96 – 720 h, based on grab sample aerobic soil column test data (Fournier & Salle 1974; selected, Howard et al. 1991).
Sediment:
Soil: $t_{½}$ = 48 – 360 h, based on grab sample aerobic soil column test data (Fournier & Salle 1974; selected, Howard et al. 1991).
Biota:

16.1.5.4 Urea



Common Name: Urea
Synonym: carbamide, carbonyldiamide, Aquacare, Aqiadrate, Basodexam, Keratinamin, Nutraplus, Onychomal, Pastaron, Ureaphil, Ureophil, Ureapearl
Chemical Name: urea, carbamide, carbonyldiamide
CAS Registry No: 57-13-6
Molecular Formula: CH_4N_2O, H_2NCONH_2
Molecular Weight: 60.055
Melting Point (°C):
133 (Lide 2003)
Boiling Point (°C):
decompose (Weast 1982–83; Lide 2003)
Density (g/cm^3):
1.323 (Weast 1982–83)
Dissociation Constant, pKa:
Molar Volume (cm^3/mol):
58.0 (calculated-Le Bas method at normal boiling point)
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
Entropy of Fusion, ΔS_{fus} (J/mol K):
Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol ± K), F: 0.0872 (mp at 133°C)

Water Solubility (g/m^3 or mg/L at 25°C or as indicated. Additional data at other temperatures designated * are compiled at the end of this section):

975000* (shake flask, measured range 0–69.5°C, Speyers 1902)
790000 (20–25°C, shake flask-gravimetric method, Dehn 1917)
1047000* (20°C, shake flask, measured range 0–70°C, Pinck & Kelly 1925)
53.97 wt %* (23.85°C, synthetic method, measured range 18.72–73.11°C, Shnidman & Sunier 1932)
$\log x = -609.8/(T/K) + 1.468$; temp range 20–70°C (synthetic method, Shnidman & Sunier 1932)
0.4388* (60°C, mole fraction solubility, synthetic method, measured range 60–100°C, Kakinuma 1941)
997400 (W indholz 1983)
1000000 (Dean 1985; Budavari 1989)

Vapor Pressure (Pa at 25°C and reported temperature dependence equations):

1.61×10^{-3} (extrapolated-Antoine eq., Stephenson & Malanowski 1987)
$\log (P_S/kPa) = 9.565 - 4579/(T/K)$; temp range 345–368 K (solid, Antoine eq., Stephenson & Malanowski 1987)

Henry's Law Constant (Pam^3/mol):

Octanol/Water Partition Coefficient, log K_{OW}:

–1.09 (Hansch & Leo 1979)
–3.00 (Kenaga & Goring 1980)
–1.21, –1.79 to –0.62 (shake flask method: mean, range of mean values, OECD 1981)
–1.54 (shake flask-radiochemical method, Cornford 1982)
–1.57 (HPLC-RT correlation, Harnish et al. 1983)
–1.56 (shake flask, OECD 1981 Guidelines, Geyer et al. 1984)
–1.66, –2.11 (shake flask, Log P Database, Hansch & Leo 1987)
–1.60 (shake flask-UV, pH 7.4, Huang 1990)
–2.11 (from Medchem software value, Chessells et al. 1992)
–2.11 (recommended, Sangster 1993)
–1.66 (Hansch et al. 1995)

Octanol/Air Partition Coefficient, log K_{OA}:

Bioconcentration Factor, log BCF:

4.068	(alga *chlorella fusca*, wet wt. basis, Geyer et al. 1984)
–0.10	(alga *chlorella fusca*, calculated-K_{OW}, Geyer et al. 1984)

Sorption Partition Coefficient, log K_{OC}:

0.50, 0.62	(soil, quoted, calculated-MCI χ and fragment contribution, Meylan et al. 1992)
0.90	(soil, calculated-MCI ${}^1\chi$, Sabljic et al. 1995)

Environmental Fate Rate Constants, k, and Half-Lives, $t_{½}$:

Half-Lives in the Environment:

TABLE 16.1.5.4.1
Reported aqueous solubilities of urea at various temperatures

Speyers 1902		Shnidman & Sunier 1932						Kakinuma 1941	
re-calcd by Pinck & Kelly		synthetic method-heating -shake flask						synthetic method	
t/°C	S/g·m^{-3}	t/°C	wt %	*x*	t/°C	wt %	*x*	t/°C	*x*
		urea 1#			urea 2#				
0	674000	18.72	51.10	0.2387	21.59	52.80	0.2513	60	0.4388
11.0	875000	26.80	55.37	0.2712	23.85	53.97	0.2602	65	0.4610
19.8	975000	27.31	55.83	0.2740	30.38	57.51	0.2888	70	0.4903
31.7	1310000	35.42	59.94	0.3099	35.15	59.97	0.3102	75	0.5204
51.4	1930000	37.36	60.87	0.3183	41.11	62.95	0.3377	80	0.6617
69.5	2530000	43.94	64.19	0.3489	43.85	64.31	0.3510	85	0.5843
		46.56	65.39	0.3618	54.97	69.53	0.4065	90	0.6190
		54.77	69.33	0.4041	55.88	70.10	0.4131	95	0.6542
		67.02	70.38	0.4163	69.13	71.49	0.4294	100	0.6910
ΔH_{sol}/(kJ mol^{-1})		61.76	72.59	0.4428	63.79	73.64	0.4561		
25°C		73.11	77.57	0.5093	70.49	76.60	0.4956	log *x* = A –B/(T/K)	
								A	1.5314
		mp/°C	132.7		mp/°C	132.6		B	631.86

mole fraction solubility expressed as:
log *x* = – 609.8/(T/K) + 1.468; temp range 20–70°C

Pinck & Kelly 1925	
shake flask	
t/°C	S/g·m^{-3}
0	670000
10.0	840000
20.0	1047000
30.0	1360000
39.7	1654000
50.0	2050000
50.6	2064000
60.0	2460000
68.5	2950000
70.0	3146000

urea 1# – urea made by synthetic NH_2 + CO_2 process—re-crystallized from water
urea 2# – urea made from calcium-cyanamid — re-crystallized from water and methanol

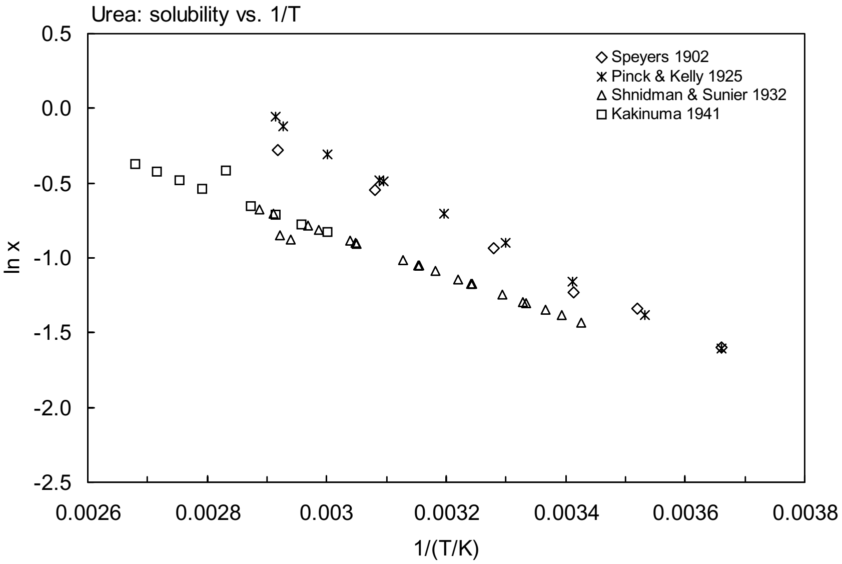
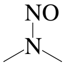


FIGURE 16.1.5.4.1 Logarithm of mole fraction solubility (ln *x*) versus reciprocal temperature for urea.

16.1.6 NITROSAMINES

16.1.6.1 *N*-Nitrosodimethylamine



Common Name: Dimethylnitrosoamine
Synonym: *N*-nitrosodimethylamine, *N*-methyl-*N*-nitrosomethanamine, nitrous dimethylamine
Chemical Name: dimethylnitrosoamine, *N*-nitrosodimethylamine
CAS Registry No: 62-75-9
Molecular Formula: $C_2H_6N_2O$, $CH_3N(NO)CH_3$
Molecular Weight: 74.081
Melting Point (°C):
Boiling Point (°C):
152 (Lide 2003)
Density (g/cm^3 at 20°C):
1.005 (18°C, Verschueren 1983)
Molar Volume (cm^3/mol):
73.7 (10°C, Stephenson & Malanowski 1987)
87.7 (calculated-Le Bas method at normal boiling point)
Dissociation Constant pK_a:
< 1.0 (Kollig 1993)
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
Entropy of Fusion, ΔS_{fus} (J/mol K):
Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F:

Water Solubility (g/m^3 or mg/L at 25°C):
miscible (Mirvish et al. 1976)

Vapor Pressure (Pa at 25°C and the reported temperature dependence equations):
1080 (Mabey et al. 1982)
730 (extrapolated-Antoine eq., Stephenson & Malanowski 1987)
$\log (P_L/kPa) = 7.10632 - 2159.476/(T/K)$, temp range 309–423 K (Antoine eq., Stephenson & Malanowski 1987)

Henry's Law Constant (Pa m^3/mol at 25°C):
3.344 (calculated, Mabey et al. 1982)

Octanol/Water Partition Coefficient, log K_{OW}:
0.06 (Radding et al. 1977)
–0.57 (shake flask-UV, Singer et al. 1977)
–0.68 (calculated-f const., Mabey et al. 1982)
0.46 (30.5°C, shake flask-HPLC, Vera et al. 1992)
0.76 (calculated, Kollig 1993)
–0.57 (recommended, Sangster 1993)
–0.57 (recommended, Hansch et al. 1995)

Octanol/Air Partition Coefficient, log K_{OA}:

Bioconcentration Factor, log BCF:
–0.96 (microorganisms-water, calculated-K_{OW}, Mabey et al. 1982)

Sorption Partition Coefficient, log K_{OC}:
–1.00 (sediment-water, calculated-K_{OW}, Mabey et al. 1982)
0.448 (calculated-K_{OW}, Kollig 1993)

Environmental Fate Rate Constants, k, or Half-Lives, $t_{½}$:

Volatilization:

Photolysis: both aqueous and atmospheric photolysis $t_{½}$ = 0.5–1.0 h, based on measured rate of photolysis in the vapor phase under sunlight (Hanst et al. 1977; quoted, Howard et al. 1991).

Hydrolysis:

Oxidation: rate constant k, for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO3} with NO_3 radical and k_{O3} with O_3 or as indicated, *data at other temperatures see reference:

rate constants k < 3600 M^{-1} h^{-1} for singlet oxygen, and k < 3600 M^{-1} h^{-1} for peroxy radical at 25°C (Mabey et al. 1982);

$k_{OH} = 3.0 \times 10^{-12}$ cm^3 $molecule^{-1}$ s^{-1} and $k_{O3} \leq 1 \times 10^{-20}$ cm^3 $molecule^{-1}$ s^{-1} at 298 K (Tuazon et al. 1984);

photooxidation $t_{½}$ = 25.4–254 h in air, based on measured rate constant for the reaction with OH radical in air (Howard et al. 1991);

$k_{OH} = (2.53 - 3.6) \times 10^{-12}$ cm^3 $molecule^{-1}$ s^{-1} for the gas-phase reactions with OH radical at 296–298 K (Atkinson 1989).

Biodegradation: aqueous aerobic $t_{½}$ = 504–4320 h, based on aerobic soil die-away test data; and aqueous anaerobic $t_{½}$ = 2016–17280 h, based on estimated unacclimated aqueous aerobic biodegradation half-life (derived from results of Tate & Alexander 1975; and Oliver et al. 1979; Howard et al. 1991).

Biotransformation: rate constant for bacterial transformation $k = 3 \times 10^{-12}$ mL ± $cell^{-1}$ ± h^{-1} in water (Mabey et al. 1982).

Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants:

Half-Lives in the Environment:

Air: $t_{½}$ = 0.5–1.0 h, based on measured rate of photolysis in the vapor phase under sunlight (Hanst et al. 1977; quoted, Howard et al. 1991);

estimated photolysis $t_{½}$ ~ 5 min, $t_{½}$ = 3 d for reaction with OH radical and $t_{½}$ > 2 yr for reaction with O_3 (Tuazon et al. 1984);

photooxidation $t_{½}$ = 25.4–254 h, based on measured rate constant for the reaction with OH radical in air (Atkinson 1985; quoted, Howard et al. 1991).

Surface water: $t_{½}$ = 0.5–1.0 h, based on measured rate of photolysis in the vapor phase under sunlight (Hanst et al. 1977; quoted, Howard et al. 1991).

Groundwater: $t_{½}$ = 1008–8640 h, based on estimated unacclimated aqueous aerobic biodegradation half-life (Howard et al. 1991).

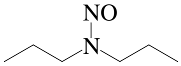
Sediment:

Soil: degradation $t_{½}$ ~ 3 wk in 4 aerobic soils (shake flask-GC, Oliver et al. 1979)

$t_{½}$ = 504–4320 h, based on aerobic soil die-away test data (derived from data of Tate & Alexander 1975 and Oliver et al. 1979, Howard et al. 1991).

Biota:

16.1.6.2 *N*-Nitrosodipropylamine



Common Name: Di-*n*-Propylnitrosoamine
Synonym: N-nitrosodi-*n*-propylamine, N-nitroso-N-propyl-1-propanamine
Chemical Name: di-*n*-propylnitrosoamine, N-nitrosodi-*n*-propylamine
CAS Registry No: 621-64-7
Molecular Formula: $C_6H_{14}N_2O$, $CH_3CH_2CH_2N(NO)CH_2CH_2CH_3$
Molecular Weight: 130.187
Melting Point (°C):
Boiling Point (°C):
206 (Lide 2003)
Density (g/cm^3 at 20°C):
Molar Volume (cm^3/mol):
176.5 (calculated-Le Bas method at normal boiling point)
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
Entropy of Fusion, ΔS_{fus} (J/mol K):
Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F:

Water Solubility (g/m^3 or mg/L at 25°C):
9900 (Mirvish et al. 1976)

Vapor Pressure (Pa at 25°C):
53.33 (37°C, calculated-Troutin's rule, Mabey et al. 1982)

Henry's Law Constant (Pam^3/mol at 25°C):
0.638 (calculated-P/C, Mabey et al. 1982)
0.355 (calculated-P/C, this work)

Octanol/Water Partition Coefficient, log K_{OW}:
1.31 (calculated as per Leo et al. 1971 from Mirvish et al. 1976 data, Callahan et al. 1979)
1.36 (shake flask-UV, Singer et al. 1977)
1.49 (calculated-f const., Mabey et al. 1982)
2.35 (30.5°C, shake flask-HPLC, Vera et al. 1992)
2.45 (recommended, Sangster 1993)
1.35 (Kollig 1993)
1.36 (recommended, Hansch et al. 1995)

Octanol/Air Partition Coefficient, log K_{OA}:

Bioconcentration Factor, log BCF:
0.99 (microorganisms-water, calculated-K_{OW}, Mabey et al. 1982)

Sorption Partition Coefficient, log K_{OC}:
1.18 (sediment-water, calculated-K_{OW}, Mabey et al. 1982)
1.09 (calculated-K_{OW}, Kollig 1993)

Environmental Fate Rate Constants, k, or Half-Lives, $t_{½}$:
Volatilization:
Photolysis: both aqueous and atmospheric photolysis $t_{½}$ = 0.17–1.0 h, based on measured rate of photolysis in the vapor phase under sunlight (Oliver 1981; quoted, Howard et al. 1991).
Hydrolysis:

Oxidation: rate constants in water for singlet oxygen $k < 3600\ M^{-1}\ h^{-1}$ and for peroxy radical $k < 3600\ M^{-1}\ h^{-1}$ at 25°C (Mabey et al. 1982);

photooxidation $t_{½}$ = 2.66–26.6 h in air, based on estimated rate constant for the reaction with hydroxyl radicals in air (Howard et al. 1991).

Biodegradation: aqueous aerobic $t_{½}$ = 504–4320 h, based on aerobic soil die-away test data, and aqueous anaerobic $t_{½}$ = 2016–17280 h, based on estimated unacclimated aqueous aerobic biodegradation half-life (derived rom results of Tate & Alexander 1975 and Oliver et al. 1979, Howard et al. 1991).

Biotransformation: rate constant for bacterial biotransformation $k \sim 3 \times 10^{-12}$ mL ± $cell^{-1}$ ± h^{-1} in water (Mabey et al. 1982).

Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants:

Half-Lives in the Environment:

Air: photooxidation $t_{½}$ = 2.66–26.6 h, based on estimated rate constant for the reaction with hydroxyl radicals in air (Howard et al. 1991).

Surface water: $t_{½}$ = 0.17–1.0 h, based on measured rate of photolysis in the vapor phase under sunlight (Oliver 1981; quoted, Howard et al. 1991).

Groundwater: $t_{½}$ = 1008–8640 h, based on estimated unacclimated aqueous aerobic biodegradation half-life (Howard et al. 1991).

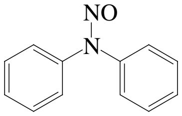
Sediment:

Soil: degradation $t_{½}$ ~ 3 wk in 4 aerobic soils (shake flask-GC, Oliver et al. 1979)

$t_{½}$ = 504 – 4320 h, based on aerobic soil die-away test data (derived from results of Tate & Alexander 1975 and Oliver et al. 1979, Howard et al. 1991).

Biota

16.1.6.3 Diphenylnitrosoamine



Common Name: Diphenylnitrosoamine
Synonym: N-nitrosodiphenylamine, N-nitroso-N-phenylbenzamine
Chemical Name: diphenylnitrosoamine, N-nitrosodiphenylamine
CAS Registry No: 86-30-6
Molecular Formula: $C_{12}H_{10}N_2O$, $C_6H_5N(NO)C_6H_5$
Molecular Weight: 198.219
Melting Point (°C):

66.5	(Weast 1982–83; Lide 2003)

Boiling Point (°C):

151–153	(Windholz 1976; Callahan et al. 1979)

Density (g/cm^3 at 20°C):
Molar Volume (cm^3/mol):

220.5	(calculated-Le Bas method at normal boiling point)

Dissociation Constant pK_a:
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
Entropy of Fusion, ΔS_{fus} (J/mol K):
Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F: 0.392 (mp at 66.5°C)

Water Solubility (g/m^3 or mg/L at 25°C):

35.1	(shake flask-LSC, Banerjee et al. 1980)
40.0	(calculated-S, Mabey et al. 1982)

Vapor Pressure (Pa at 25°C):

13.33	(estimated, Mabey et al. 1982)

Henry's Law Constant (Pam^3/mol at 25°C):

66.87	(calculated-P/C, Mabey et al. 1982)

Octanol/Water Partition Coefficient, log K_{OW}:

3.13	(shake flask-LSC, Banerjee et al. 1980;)
3.13	(recommended, Sangster 1993)
3.13	(recommended, Hansch et al. 1995)

Octanol/Air Partition Coefficient, log K_{OA}:

Bioconcentration Factor, log BCF:

2.63	(microorganisms-water, calculated-K_{OW}, Mabey et al. 1982)
2.34	(quoted, Isnard & Lambert 1988)

Sorption Partition Coefficient, log K_{OC}:

2.81	(sediment-water, calculated-K_{OW}, Mabey et al. 1982)
2.84	(calculated-K_{OW}, Kollig 1993)

Environmental Fate Rate Constants, k, or Half-Lives, $t_{1/2}$:

Volatilization:
Photolysis:
Hydrolysis:

Oxidation: rate constants in water for singlet oxygen $k < 3600\ M^{-1}\ h^{-1}$ and for peroxy radical $k < 3600\ M^{-1} \pm h^{-1}$ at 25°C (Mabey et al. 1982);

photooxidation $t_{1/2} = 0.70 - 7.0$ h in air, based on measured rate constant for the reaction with hydroxyl radicals in air (Howard et al. 1991).

Biodegradation: aqueous aerobic $t_{1/2} = 240 - 816$ h, based on data from one soil-die-away test; a range was bracketed around the reported $t_{1/2} = 22$ d (Mallik & Tesfai 1981; quoted, Howard et al. 1991); aqueous anaerobic $t_{1/2} = 960 - 3264$ h, based on estimated unacclimated aqueous aerobic biodegradation half-life (Howard et al. 1991).

Biotransformation: rate constant for bacterial transformation $k = 1 \times 10^{-10}\ mL \pm cell^{-1} \pm h^{-1}$ in water (Mabey et al. 1982).

Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants:

Half-Lives in the Environment:

Air: photooxidation $t_{1/2} = 0.70 - 7.0$ h, based on estimated rate constant for the reaction with hydroxyl radicals in air (quoted, Howard et al. 1991).

Surface water: $t_{1/2} = 240 - 816$ h, based on estimated unacclimated aqueous aerobic biodegradation half-life (Howard et al. 1991).

Groundwater: $t_{1/2} = 480 - 1632$ h, based on estimated unacclimated aqueous aerobic biodegradation half-life (Howard et al. 1991).

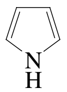
Sediment:

Soil: $t_{1/2} = 240 - 816$ h, based on estimated unacclimated aqueous aerobic biodegradation half-life (Howard et al. 1991).

Biota:

16.1.7 HETEROCYCLIC COMPOUNDS

16.1.7.1 Pyrrole



Common Name: Pyrrole
Synonym: 1H-pyrrole
Chemical Name: pyrrole, 1H-pyrrole
CAS Registry No: 109-97-7
Molecular Formula: C_4H_4NH
Molecular Weight: 67.090
Melting Point (°C):
–23.39 (Lide 2003)
Boiling Point (°C):
129.79 (Lide 2003)
Density (g/cm^3 at 20°C):
0.9691 (Weast 1982–83; Dean 1985)
0.96985, 0.96565 (20°C, 25°C, Riddick et al. 1986)
Molar Volume (cm^3/mol):
69.2 (20°C, calculated-density, Stephenson & Malanowski 1987)
78.2 (calculated-Le Bas method at normal boiling point
Dissociation Constant, pK_a:
–4.40 (Perrin 1972)
–3.80 (Riddick et al. 1986)
–4.10 (Sangster 1989)
Enthalpy of Vaporization, ΔH_V (kJ/mol):
45.15, 38.75 (25°C, bp, Riddick et al. 1986)
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
7.908 (Riddick et al. 1986)
Entropy of Fusion, ΔS_{fus} (J/mol K):
Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F: 1.0

Water Solubility (g/m^3 or mg/L at 25°C):
47000 (Dean 1985)
45000 (Riddick et al. 1986)

Vapor Pressure (Pa at 25°C and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):
358285* (176.67°C, static-Bourdon gauge, measured range 176.67–271.11°C, Kobe et al. 1956)
1102* (ebulliometry, extrapolated-Antoine eq., measured range 65.67–166°C, Scott et al. 1967; Osborn & Douslin 1968)
$\log(P/\text{mmHg}) = 7.30295 - 1507.015/(t/{}^\circ\text{C} + 211.010)$; temp range 65.67–166°C (Antoine eq., ebulliometry, Scott et al. 1967)
$\log[(P/\text{atm}) = [1 - 402.914 \pm (T/\text{K})] \times 10{\wedge}\{0.870073 - 5.43768 \times 10^{-4} \pm (T/\text{K}) + 4.16086 \times 10^{-7} \pm (T/\text{K})^2\}$, temp range: 65.67–166°C (ebulliometric method, Cox eq., Scott et al. 1967)
$\log(P/\text{mmHg}) = 7.30275 - 1506.877/(t/{}^\circ\text{C} + 210.995)$, temp range 65.57–166°C (ebulliometric method, Antoine eq., Scott et al. 1967; Osborn & Douslin 1968)
$\log[(P/\text{atm}) = [1 - 402.915 \pm (T/\text{K})] \times 10{\wedge}\{0.872196 - 5.54923 \times 10^{-4} \pm (T/\text{K}) + 4.30369 \times 10^{-7} \pm (T/\text{K})^2\}$, temp range: 65.57–166°C (ebulliometric method, Cox eq., Osborn & Douslin 1968)
8386* (60.3°C, isoteniscope method, measured range 60.3–100.3°C, Eon et al. 1971)
1136 (calculated-Cox eq., Chao et al. 1983)
$\log(P/\text{atm}) = [1 - 402.916/(T/\text{K})] \times 10{\wedge}\{0.880256 - 6.05913 \times 10^{-4} \pm (T/\text{K}) + 5.02726 \times 10^{-7} \pm (T/\text{K})^2\}$; temp range: 250.0–635.0 K (Cox eq., Chao et al. 1983)

1100 (extrapolated-Antoine eq., Boublik et al. 1984)
log (P/kPa) = 6.42113 – 1502.586/(129.775 + t/°C); temp range 65.67–166°C (Antoine eq. from exptl. data of Scott et al. 1967, Boublik et al. 1984)
1100 (extrapolated-Antoine eq., Dean 1985, 1992)
log (P/mmHg) = 7.29470 – 1501.56/(210.42 + t/°C); temp range 66–166°C (Antoine eq., Dean l985, 1992)
1100 (quoted lit., Riddick et al. 1986)
log (P/kPa) = 6.42765 – 1506.877/(210.995 + t/°C); temp range not specified (Antoine eq., Riddick et al. 1986)
1103 (extrapolated-Antoine eq., Stephenson & Malanowski 1987)
log (P_L/kPa) = 6.42263 – 1504.171/(–62.39 + T/K); temp range 338–440 K (Antoine eq., Stephenson & Malanowski 1987)
log (P/mmHg) = 54.1597 – 4.2745×10^3/(T/K) –15.873·log (T/K) – 4.5171×10^{-10}·(T/K) + 4.2338×10^{-6}·$(T/K)^2$; temp range 250–640 K (vapor pressure eq., Yaws 1994)

Henry's Law Constant (Pa m^3/mol at 25°C):
1.640 (calculated-P/C with selected values)

Octanol/Water Partition Coefficient, log K_{OW} at 25°C or as indicated
0.75 (shake flask-AS, Hansch & Anderson 1967; Leo et al. 1971; Hansch & Leo 1979)
0.62 (HPLC-RV correlation, Garst 1984)
0.82 (23°C, shake flask-HPLC, De Voogt et al. 1988)
0.80 (23°C, TLC-RT correlation, De Voogt et al. 1990)
0.75 (recommended, Sangster 1989, 1993)
0.75 (recommended, Hansch et al. 1995)

Octanol/Air Partition Coefficient, log K_{OA}:

Bioconcentration Factor, log BCF:

Sorption Partition Coefficient, log K_{OC}:

Environmental Fate Rate Constants, k, or Half-Lives, $t_{½}$:
Volatilization:
Photolysis:
Oxidation: rate constant k, for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO3} with NO_3 radical and k_{O3} with O_3 or as indicated, *data at other temperatures and/or the Arrhenius expression see reference:
$k_{OH} = (1.22 \pm 0.04) \times 10^{-10}$ cm^3 $molecule^{-1}$ s^{-1} at 295 K (relative rate method, Atkinson et al. 1984)
$k_{O3} = 1.6 \times 10^{-17}$ cm^3 ± $molecule^{-1}$ s^{-1} with loss rate of 1.0 d^{-1}, $k_{OH} = 1.2 \times 10^{-10}$ cm^3 $molecule^{-1}$ s^{-1} with loss rate of 10 d^{-1} and $k_{NO3} = 4.9 \times 10^{-11}$ cm^3 $molecule^{-1}$ s^{-1} with loss rate of 1000 d^{-1} (review, Atkinson & Carter 1984)
$k_{O3} = 1.6 \times 10^{-17}$ cm^3 ± $molecule^{-1}$ s^{-1} with loss rate of 1.0 d^{-1}, $k_{OH} = 1.2 \times 10^{-10}$ cm^3 $molecule^{-1}$ s^{-1} with loss rate of 5.2 d^{-1} and $k_{NO3} = 4.9 \times 10^{-11}$ cm^3 $molecule^{-1}$ s^{-1} with loss rate k = 1000 d^{-1} (review, Atkinson 1985)
$k_{NO3} = (4.9 \pm 1.1) \times 10^{-11}$ cm^3 $molecule^{-1}$ s^{-1} at 295 ± 1 K (relative rate method, Atkinson et al. 1985)
$k_{O3} = 1.6 \times 10^{-17}$ cm^3 ± $molecule^{-1}$ s^{-1} with calculated tropospheric lifetime τ = 24 h, $k_{OH} = 1.2 \times 10^{-10}$ cm^3 $molecule^{-1}$ s^{-1} with τ(calc) = 2.3 h during daylight hours, $k_{NO3} = 4.9 \times 10^{-11}$ cm^3 $molecule^{-1}$ s^{-1} with τ(calc) = 1.4 min during nighttime hours at room temp. (Atkinson et al. 1985)
$k_{OH} = 1.2 \times 10^{-10}$ cm^3 $molecule^{-1}$ s^{-1} with a loss rate of 5.2 d^{-1} at room temp. (Atkinson 1985)
k_{OH}* = $(1.03 \pm 0.06) \times 10^{-10}$ cm^3 $molecule^{-1}$ s^{-1} at 298 K, measured range 298–442 K (flash photolysis-resonance fluorescence, Wallington et al. 1988)
k_{OH}* = 9.31×10^{-10} cm^3 $molecule^{-1}$ s^{-1} at 298 K, measured range 298–442 K (flash photolysis-resonance fluorescence, Atkinson 1989)
$k_{OH} = 1.10 \times 10^{-12}$ cm^3 $molecule^{-1}$ s^{-1} at 298 K (recommended, Atkinson 1989)
k_{OH}(calc) = 287.45×10^{-12} cm^3 $molecule^{-1}$ s^{-1} (molecular orbital calculations, Klamt 1993)
Hydrolysis:

Biodegradation:
Biotransformation:
Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants:

Half-Lives in the Environment:

Air: calculated lifetimes of 2.3 h, 1.4 min and 24 h due to gas-phase reactions with OH radical (concn of 1×10^6 cm^{-3} during daylight hours), No_3 radical (conc of 2.4×10^6 cm^{-3} during nighttime hours) and O_3 (clean tropospheric conc of 7.2×10^{11} molecule cm^{-3}), respectively, at room temp. (Atkinson et al. 1985)

TABLE 16.1.7.1.1
Reported vapor pressures of pyrrole at various temperatures and the coefficients for the vapor pressure equations

$\log P = A - B/(T/K)$ (1) $\ln P = A - B/(T/K)$ (1a)
$\log P = A - B/(C + t/°C)$ (2) $\ln P = A - B/(C + t/°C)$ (2a)
$\log P = A - B/(C + T/K)$ (3)
$\log P = A - B/(T/K) - C \cdot \log (T/K)$ (4)

Kobe et al. 1956		**Scott et al. 1967**		**Eon et al. 1971**	
static-Bourdon gauge		**ebulliometry**		**isoteniscope/manometry**	
t/°C	**P/Pa**	**t/°C**	**P/Pa**	**t/°C**	**P/Pa**
176.67	358285	65.671	9582	60.3	8386
182.22	399626	68.522	10884	70.3	13025
187.78	454747	71.374	12335	80.3	19732
193.33	509867	77.098	15740	90.3	29198
198.89	571878	79.970	17725	100.3	42263
204.44	647669	82.847	19920		
210.00	730351	88.622	25007	ΔH_V/(kJ mol^{-1}) = 41.84	
215.56	806142	94.422	31160		
221.11	895713	100.244	38547		
226.67	992174	106.096	47359		
232.22	1081746	111.972	57803		
237.78	1185097	117.875	70109		
243.33	1309119	123.806	84525		
248.89	1440031	129.764	101325		
254.44	1564053	135.753	120798		
260.00	1715635	141.768	143268		
265.56	1867217	147.812	169052		
271.11	2032580	153.884	198530		
		159.984	232087		
		166.109	270110		
		eq. 2	P/mmHg		
		A	7.30295		
		B	1507.015		
		C	210.010		
		bp/°C	129.764		
		ΔH_V/(kJ mol^{-1}) = 45.10			

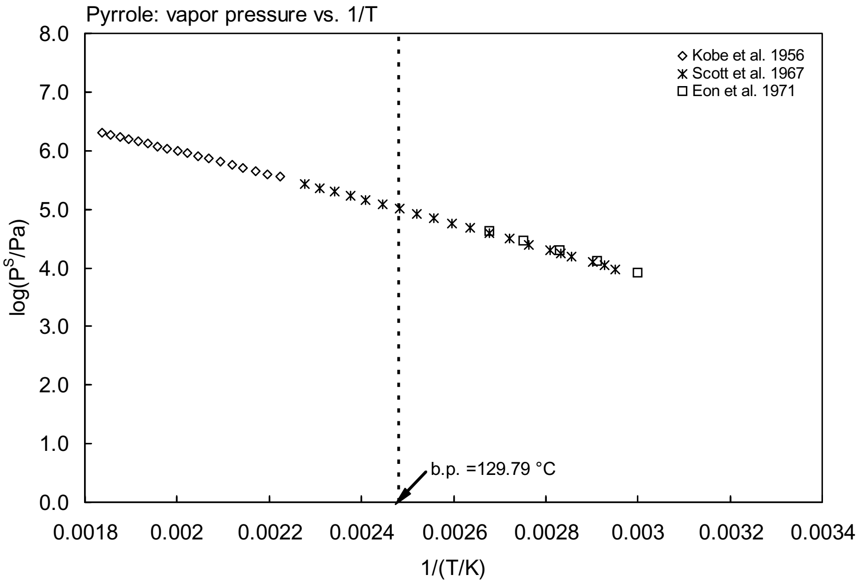
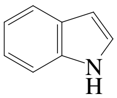


FIGURE 16.1.7.1.1 Logarithm of vapor pressure versus reciprocal temperature for pyrrole.

16.1.7.2 Indole



Common Name: Indole
Synonym: benzo[*b*]pyrrole, 1-benzo[*b*]pyrrole, 1H-indole
Chemical Name: indole
CAS Registry No: 120-72-9
Molecular Formula: C_8H_7N
Molecular Weight: 117.149
Melting Point (°C):
  52.5 (Weast 1982–83; Lide 2003)
Boiling Point (°C):
  254.0 (Weast 1982–83; Stephenson & Malanowski 1987)
  253.6 (Lide 2003)
Density (g/cm^3 at 20°C):
  1.2200 (Weast 1982–83)
  1.0643 (Dean 1985)
Molar Volume (cm^3/mol):
  133.4 (calculated-Le Bas method at boiling point)
Dissociation Constant, pK_a:
  –3.5, –3.62 (Perrin 1972)
  –3.17 (Sangster 1989)
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
Entropy of Fusion, ΔS_{fus} J/mol K:
Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F: 0.537 (mp at 52.5°C)

Water Solubility (g/m^3 or mg/L at 25°C):
  3558 (shake flask-GC, Price 1976)
  1874 (Pearlman et al. 1984)

Vapor Pressure (Pa at 25°C and reported temperature dependence equations):
  2.24 (extrapolated-Antoine eq., Boublik et al. 1984)
  $\log (P/kPa) = 6.369 - 1933.005/(254.707 + t/°C)$; temp range 193.3–254.7°C (Antoine eq., Boublik et al. 1984)
  1.565 (calculated-Antoine eq., Stephenson & Malanowski 1987)
  $\log (P_S/kPa) = 10.3289 - 3916/(T/K)$; temp range 291–319 K, (solid, Antoine eq., Stephenson & Malanowski 1987)
  $\log (P/mmHg) = 94.1625 - 6.9431 \times 10^3/(T/K) - 30.613 \cdot \log (T/K) + 9.928 \times 10^{-3} \cdot (T/K) + 1.7461 \times 10^{-13} \cdot (T/K)^2$; temp range 274–790 K (vapor pressure eq., Yaws 1994)

Henry's Law Constant (Pam^3/mol at 25°C):
  0.14 (calculated-P/C with selected values)

Octanol/Water Partition Coefficient, log K_{OW}:
  1.14 ± 0.01 (shake flask-UV, Iwasa et al. 1965)
  2.14 (shake flask-UV, Hansch & Anderson 1967)
  2.25 (shake flask-UV at pH 7.4, Rogers & Cammarata 1969)
  2.00 (unpublished result, Leo et al. 1971)
  2.00, 2.25, 2.13 (Hansch & Leo 1979)
  1.66 (RP-HPLC-RT correlation, Veith et al. 1979a)
  2.17 (RP-HPLC-RT correlation, Hanai & Hubert 1982)
  2.14 (inter-laboratory studies, shake flask average, Eadsforth & Moser 1983)

1.92	(inter-laboratory studies, HPLC average, Eadsforth & Moser 1983)
2.16 ± 0.03	(HPLC-RV correlation-ALPM, Garst & Wilson 1984)
1.81	(HPLC-k′ correlation, Eadsforth 1986)
2.16	(HPLC-RT correlation, Minick et al. 1988)
2.14	(recommended, Sangster 1989; 1993)
2.27	(23°C, shake flask-HPLC, De Voogt et al. 1988, 1990)
2.07	(HPLC-RT correlation, De Voogt et al. 1990)
2.19	(HPLC-RT correlation, Ritter et al. 1994)
2.14	(recommended, Hansch et al. 1995)

Octanol/Air Partition Coefficient, log K_{OA}:

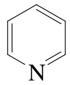
Bioconcentration Factor, log BCF:

Sorption Partition Coefficient, log K_{OC}:

Environmental Fate Rate Constants or Half-Lives:

Half-Lives in the Environment:

16.1.7.3 Pyridine



Common Name: Pyridine
Synonym:
Chemical Name: pyridine
CAS Registry No: 110-86-1
Molecular Formula: C_5H_5N
Molecular Weight: 79.101
Melting Point (°C):
    –41.7 (Lide 2003)
Boiling Point (°C):
    115.23 (Lide 2003)
Density (g/cm^3 at 20°C):
    0.9819 (Weast 1982–83)
Molar Volume (cm^3/mol):
    80.6 (calculated-density, Rohrschneider 1973)
    93.0 (calculated-Le Bas method at normal boiling point)
Dissociation Constant, pK:
    5.23 (pK_a, Leo et al. 1971; Jori et al. 1983; Zachara et al. 1987)
    5.198, 5.21, 5.22, 5.229 (Perrin 1972)
    5.54 (UV, Yeh & Higuchi 1976)
    5.23, 5.16 (quoted, shake flask-TN, Clarke 1984)
    5.17 (pK_{BH^+}, Dean 1985; Riddick et al. 1986)
    5.21 (pK_a, Sangster 1989)
Enthalpy of Vaporization, ΔH_V (kJ/mol):
    40.41, 36.39 (25°C, bp, Riddick et al. 1986)
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
    7.414 (Riddick et al. 1986)
Entropy of Fusion, ΔS_{fus} (J/mol K):
Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F: 1.0

Water Solubility (g/m^3 or mg/L at 25°C):
    miscible (Andon & Cox 1952; Andon et al. 1954; Jori et al. 1983; Riddick et al. 1986)
    miscible (Dean 1985; Zachara et al. 1987; Stephenson 1993a)
    miscible (Yaws et al. 1990)

Vapor Pressure (Pa at 25°C and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):
    2666* (24.8°C, summary of literature data, temp range –18.9 to 115.4°C, Stull 1947)
    2520 (interpolated-regression of tabulated data, Stull 1947)
    620, 2109 (0, 20°C, static method-tensimeter, Brown & Barbaras 1947)
    2775* (ebulliometry, measured range 47.3–115.5°C, extrapolated-Antoine eq., Herington & Martin 1953)
    $\log (P/mmHg) = 7.05811 - 1384.991/(216.296 + t/°C)$; temp range 47.3–115.5°C (Antoine eq., ebulliometric measurements, Herington & Martin 1953)
    2774* (gas saturation, measured range 20–40°C, Andon et al. 1954)
    461637* (176.67°C, static-Bourdon gauge, measured range 176.67–343.33°C, Kobe et al. 1956)
    19920* (67.299°C, comparative ebulliometry, measured range 67.299–152.886°C, McCullough et al. 1957)
    $\log (P/mmHg) = 7.04162 - 1374.103/(215.014 + t/°C)$; temp range 67.3–152.9°C (Antoine eq. ebulliometry, McCullough et al. 1957)
    2763* (ebulliometry, calculated-Antoine eq., Osborn & Douslin 1968)

$\log(P/\text{mmHg}) = 7.04144 - 1373.990/(t/°\text{C} + 215.001)$; temp range 67.3–152.9°C (ebulliometric method, Antoine eq., Osborn & Douslin 1968)

$\log[(P/\text{atm}) = [1 - 399.384 \pm (T/\text{K})] \times 10\hat{}\{0.856586 - 6.60597 \times 10^{-4} \pm (T/\text{K}) + 5.93625 \times 10^{-7} \pm (T/\text{K})^2\}$, temp range: 67.3–152.9°C (ebulliometric method, Cox eq., Osborn & Douslin 1968)

2789 (calculated-Antoine eq., Cabani et al. 1971)

$\log(P/\text{mmHg}) = [-0.2185 \times 9649.4/(T/\text{K})] + 8.347670$; temp range –18.9 to 115.4°C (Antoine eq., Weast 1972–73)

2767 (calculated-Cox eq., Chao et al. 1983)

$\log(P/\text{atm}) = [1 - 388.399/(T/\text{K})] \times 10\hat{}\{0.848882 - 6.09810 \times 10^{-4} \pm (T/\text{K}) + 5.15399 \times 10^{-7} \pm (T/\text{K})^2\}$; temp range: 235.0–620.0 K (Cox eq., Chao et al. 1983)

2775, 2763 (extrapolated-Antoine equations, Boublik et al. 1984)

$\log(P/\text{kPa}) = 6.18358 - 1385.39/(115.256 + t/°\text{C})$; temp range 47.3–115.47°C (Antoine eq. from reported exptl. data of Herington & Martin 1953, Boublik et al. 1984)

$\log(P/\text{kPa}) = 6.16609 - 1373.826/(115.235 + t/°\text{C})$; temp range 67.3–152.9°C (Antoine eq. from reported exptl. data of McCullough et al. 1957, Boublik et al. 1984)

2763 (extrapolated-Antoine eq., Dean 1985, 1992)

$\log(P/\text{mmHg}) = 7.04115 - 1373.80/(214.98 + t/°\text{C})$; temp range 67–153°C (Antoine eq., Dean l985, 1992)

2773 (Howard et al. 1986; quoted, Banerjee et al. 1990)

2700 (selected, Riddick et al. 1986)

$\log(P/\text{kPa}) = 6.18595 - 1386.683/(216.469 + t/°\text{C})$, temp range not specified (Antoine eq., Riddick et al. 1986)

2770 (interpolated-Antoine eq. II, Stephenson & Malanowski 1987)

$\log(P_L/\text{kPa}) = 6.17372 - 1379.953/(-57.436 + T/\text{K})$; temp range 323–426 K (Antoine eq. I, Stephenson & Malanowski 1987)

$\log(P_L/\text{kPa}) = 6.30308 - 1448.781/(-50.948 + T/\text{K})$; temp range 296–353 K (Antoine eq. II, Stephenson & Malanowski 1987)

$\log(P_L/\text{kPa}) = 6.16446 - 1373.263/(-58.18 + T/\text{K})$; temp range 348–434 K (Antoine eq. III, Stephenson & Malanowski 1987)

$\log(P_L/\text{kPa}) = 6.284 - 1455.584/(-48.272 + T/\text{K})$; temp range 431–558 K (Antoine eq. IV, Stephenson & Malanowski 1987)

$\log(P_L/\text{kPa}) = 7.25663 - 2578.625/(115.604 + T/\text{K})$; temp range 552–620 K (Antoine eq. V, Stephenson & Malanowski 1987)

2773, 1653 (measured, calculated-solvatochromic parameters, Banerjee et al. 1990)

2573* (24.82°C, ebulliometry, measured range 23.55–116.23°C, Łencka 1990)

$\ln(P/\text{kPa}) = 14.1480 - 3132.3/[(T/\text{K}) - 59.179]$; temp range 295.7–388.4 K (ebulliometric measurements, Antoine eq., Łencka 1990)

$\log(P/\text{mmHg}) = 33.5541 - 3.1318 \times 10^3/(T/\text{K}) - 8.8646 \cdot \log(T/\text{K}) + 7.1293 \times 10^{-12} \cdot (T/\text{K}) + 2.2813 \times 10^{-6} \cdot (T/\text{K})^2$; temp range 232–620 K (vapor pressure eq., Yaws 1994)

Henry's Law Constant ($\text{Pa} \cdot \text{m}^3/\text{mol}$ at 25°C or as indicated):

0.895 (volatility ratio-transpiration method, Andon et al. 1954)

0.900 (exptl., Hine & Mookerjee 1975)

0.595, 0.766 (calculated-group contribution, calculated-bond contribution, Hine & Mookerjee 1975)

1.114 (modified gas-stripping, Hawthorne et al. 1985)

1.120 (computed, Yaws et al. 1991)

0.305 (calculated-molecular structure, Russell et al. 1992)

27.78 (20°C, selected from literature experimentally measured data, Staudinger & Roberts 2001)

$\log K_{AW} = -1.508 - 128/(T/\text{K})$ (van't Hoff eq. derived from literature data, Staudinger & Roberts 2001)

Octanol/Water Partition Coefficient, $\log K_{OW}$:

0.65 (shake flask-UV, Iwasa et al. 1965)

0.64 (Gehring et al. 1967)

0.65, 0.64 (Leo et al. 1971; Hansch & Leo 1979)

0.66 (HPLC-RT correlation, Mirrlees et al. 1976)

0.63 ± 0.02 (shake flask at pH 7, Unger et al. 1978)

0.63 (shake flask-titration, Clarke 1984; Clarke & Cahoon 1987)

0.63 ± 0.06	(HPLC-RV correlation-ALPM, Garst & Wilson 1984)
0.62	(shake flask-UV at pH 7.4, El Tayar et al. 1984)
0.63	(shake flask-potentiometric titration, Clarke 1984)
0.54	(calculated- activity coeff. γ from UNIFAC, Campbell & Luthy 1985)
1.28	(HPLC-k′ correlation, Eadsforth 1986)
0.79	(calculated-γ from UNIFAC, Banerjee & Howard 1988)
0.70	(shake flask-CPC, Berthod et al. 1988)
0.63	(shake flask-HPLC at pH 7, De Voogt et al. 1988, 1990)
0.65	(recommended, Sangster 1989, 1993)
0.70	(RP-TLC-RT correlation, De Voogt et al. 1990)
0.65	(shake flask-UV, Yamagami et al. 1990)
0.60	(pH 7.2, Hansch et al. 1995)

Octanol/Air Partition Coefficient, log K_{OA}:

Bioconcentration Factor, log BCF:

Sorption Partition Coefficient, log K_{OC}:

–1.805	(estimated of Anvil Points subsurface materials, Zachara et al. 1987)
–2.541	(estimated of Loring subsurface materials, Zachara et al. 1987)
0.340	(calculated-K_{OW}, Kollig 1993)

Environmental Fate Rate Constants, k, Half-Lives, $t_{1/2}$

Volatilization:

Photolysis:

Oxidation: rate constant k; for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO3} with NO_3 radical and k_{O3} with O_3 or as indicated *data at other temperatures see reference:

photooxidation $t_{1/2}$ = 14.7–24.4 yr in water, based on measured rate data for the reaction with hydroxyl radical in aqueous solution (Dorfman & Adams 1973; selected, Howard et al. 1991)

$k_{OH} = (4.9 \pm 0.4) \times 10^{-13}$ cm³ molecule⁻¹ s⁻¹ with atmospheric lifetimes of 46 d in clean troposphere and 23 d in moderately polluted atmosphere; $k_{O3} < 1.1 \times 10^{-20}$ cm³ molecule⁻¹ s⁻¹ with atmospheric lifetimes of > 4 yr in clean troposphere and > 1.3 yr in moderately polluted atmosphere at room temp. (relative rate method, Atkinson et al. 1987)

$k_{OH} = (0.494 - 0.256) \times 10^{-12}$ cm^3 $molecule^{-1}$ s^{-1} at 296–297 K (review, Atkinson 1989)

k_{OH}(calc) = 0.45×10^{-12} cm^3 $molecule^{-1}$ s^{-1} at room temp. (molecular orbital calculations, Klamt 1993)

Hydrolysis:

Biodegradation: aqueous aerobic $t_{1/2}$ = 24–168 h, based on unacclimated grab sample of aerobic soil (Sims & Sommers 1985; quoted, Howard et al. 1991); aqueous anaerobic $t_{1/2}$ = 168–672 h, based on anaerobic acclimated screening test data (Naik et al. 1972; selected, Howard et al. 1991).

Biotransformation:

Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants:

Half-Lives in the Environment:

Air: atmospheric lifetimes of 46 d in clean troposphere and 23 d in moderately polluted atmosphere, based on the gas-phase reaction with hydroxyl radical in air at room temp. and > 4 yr in clean troposphere and > 1.3 yr in moderately polluted atmosphere, based on the gas-phase reaction with O_3 (calculated rate constant) in air at room temp. (Atkinson et al. 1987);

photooxidation $t_{1/2}$ = 128–1284 h, based on measured rate data for the reaction with hydroxyl radical in air (selected, Howard et al. 1991).

Surface water: photooxidation $t_{1/2}$ = 14.7–24.4 yr, based on measured rate data for the reaction with hydroxyl radical in aqueous solution (Dorfman & Adams 1973; selected, Howard et al. 1991);

$t_{1/2}$ = 24–168 h, based on estimated aqueous aerobic biodegradation half-life (Howard et al. 1991).

Groundwater: $t_{1/2}$ = 48–336 h, based on estimated aqueous aerobic biodegradation half-life (Howard et al. 1991).

Sediment:

Soil: disappears in less than 7 d in soil suspensions (Sims & O'Loughlin 1989);

$t_{1/2}$ = 24–168 h, based on unacclimated grab sample of aerobic soil (Sims & Sommers 1985; selected, Howard et al. 1991).

Biota:

TABLE 16.1.7.3.1
Reported vapor pressures of pyridine at various temperatures and the coefficients for the vapor pressure equations

$\log P = A - B/(T/K)$	(1)	$\ln P = A - B/(T/K)$	(1a)
$\log P = A - B/(C + t/°C)$	(2)	$\ln P = A - B/(C + t/°C)$	(2a)
$\log P = A - B/(C + T/K)$	(3)		
$\log P = A - B/(T/K) - C \cdot \log (T/K)$	(4)		
$\log P = A[1 - B/(T/K)]$	(5) where $\log A = a - b(T/K) + c(T/K)^2$		

1.

Stull 1947		**Herington & Martin 1953**		**Andon et al. 1954**		**Kobe et al. 1956**	
summary of literature data		**ebulliometry**		**gas saturation**		**static-Bourdon gauge**	
t/°C	**P/Pa**	**t/°C**	**P/Pa**	**t/°C**	**P/Pa**	**t/°C**	**P/Pa**
–18.9	133.3	47.327	8506	20	2109	176.67	461637
2.50	666.6	52.71	10820	25	2774	182.22	502988
13.2	1333	58.349	13806	40	6013	187.78	564988
24.8	2666	68.403	20805			193.33	633889
38.0	5333	75.77	27592			198.89	702790
46.8	7999	82.43	35246			204.44	778581
57.8	13332	82.728	35597			210.00	868153
75.0	26664	88.459	43472			215.56	950834
95.6	53329	92.749	50279			221.11	1047295
115.4	101325	100.994	65759			226.67	1157537
		105.356	75351			232.22	1267778
mp/°C	–42	107.169	79679			237.78	1378020
		110.028	86860			243.33	1495152
		113.222	95488			248.89	1632954
		113.232	95536			254.44	1763866
		113.374	95905			260.00	1908558
		114.015	97713			265.56	2067030
		114.699	99692			271.11	2232392
		115.112	100914			276.67	2397755
		115.287	101402			282.22	2590678
		115.407	101758			287.78	2790491
		115.473	101977			293.33	2997194
						298.89	3183226
		bp/°C	115.256			304.44	3438160
		ΔH_V/(kJ mol^{-1}) = 36.39				310.00	3672423
		Antoine eq.				315.56	3941137
		eq. 2	P/mmHg			321.11	4216741
		A	7.05811			326.67	4478565
		B	1384.991			332.22	4774839
		C	216.296			337.78	5084894
						343.33	5429399

(*Continued*)

TABLE 16.1.7.3.1 (*Continued*)

2.

McCullough et al. 1957		Osborn & Douslin 1968		Lencka 1990	
comparative ebulliometry		ebulliometry		ebulliometry	
t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa
67.299	19920	67.299	19920	23.55	2394
75.154	25007	73.154	25007	24.82	2573
79.045	31160	79.054	31160	27.0	2902
84.847	38547	84.974	38547	29.26	3290
90.946	47359	90.946	47359	31.63	3720
96.958	57803	96.958	57803	35.86	4626
103.008	70109	103.008	70109	41.0	6035
109.101	84525	109.101	84525	48.51	8525
115.234	101325	115.234	101325	54.17	10999
121.408	120789	121.408	120798	60.65	14321
127.622	143268	127.622	143268	69.25	20650
133.878	169052	133.878	169053	76.97	27794
140.174	198530	140.174	198517	83.45	35213
146.509	232067	146.509	232088	88.70	42359
152.886	270110	152.886	270111	91.76	47951
				96.68	55423
mp/°C	115.23	Antoine eq		100.01	61720
Antoine eq		eq. 2	P/mmHg	102.18	66148
eq. 2	P/mmHg	A	7.04144	106.03	74603
A	7.04162	B	1373.990	112.70	91299
B	1374.103	C	215.001	116.23	101277
C	215.014				
		data also fitted to Cox eq.		eq. 3	cP/kPa
data also fitted to Cox eq.				A	14.1480
eq. 5	P/atm			B	3132.30
A				C	59.719
a	0.858631				
$10^{-4}b$	6.7114				
$10^{-7}c$	6.0722				
B	388.394				

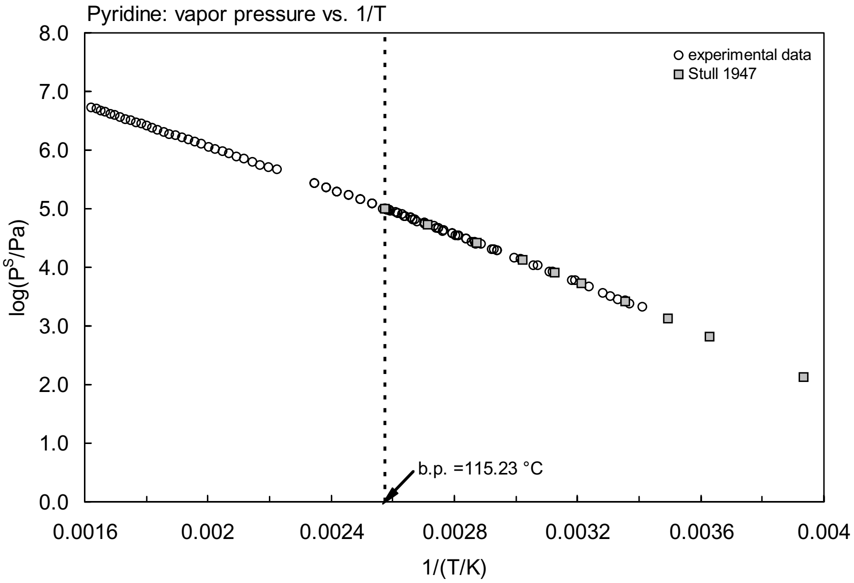
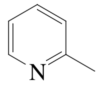


FIGURE 16.1.7.3.1 Logarithm of vapor pressure versus reciprocal temperature for pyridine.

16.1.7.4 2-Methylpyridine



Common Name: 2-Methylpyridine
Synonym: α-picoline, 2-picoline
Chemical Name: 2-methylpyridine, α-picoline
CAS Registry No: 109-06-8
Molecular Formula: $C_5H_4NCH_3$
Molecular Weight: 93.127
Melting Point (°C):
    –66.68 (Lide 2003)
Boiling Point (°C):
    129.38 (Lide 2003)
Density (g/cm^3 at 20°C):
    0.9443 (Weast 1982–83)
    0.9444, 0.93981 (20°C, 25°C, Riddick et al. 1986)
Molar Volume (cm^3/mol):
    98.6 (20°C, calculated-density)
    115.2 (calculated-Le Bas method at normal boiling point)
Dissociation Constant, pK:
    5.957, 6.06 (Perrin 1972)
    5.97 (pK_a, 20°C, Weast 1982–83)
    6.00 (p$K_{BH}{}^+$, Riddick et al. 1986; quoted, Howard 1990)
Enthalpy of Vaporization, ΔH_V (kJ/mol):
    42.919, 36.271 (25°C, bp, Riddick et al. 1986)
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
    9.724 (Riddick et al. 1986)
Entropy of Fusion, ΔS_{fus} (J/mol K):
Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F: 1.0

Water Solubility (g/m^3 or mg/L at 25°C):
    miscible (Andon & Cox 1952)
    miscible (Riddick et al. 1986; Yaws et al. 1990)
    miscible (Stephenson 1993a)

Vapor Pressure (Pa at 25°C and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):
    1370* (interpolated-regression of tabulated data, temp range –11.0 to 128.8°C, Stull 1947)
    308, 1140 (0, 20.3°C, static method-tensimeter, Brown & Barbaras 1947)
    1277 (manometry, calculated-Antoine eq., Hopke & Sears 1951)
    1496* (ebulliometry, extrapolated-Antoine eq., measured range 64.3–130°C, Herington & Martin 1953)
    $\log (P/\text{mmHg}) = 7.03450 - 1417.578/(211.874 + t/°C)$; temp range 64.3–130°C (ebulliometric measurements, Antoine eq., Herington & Martin 1953)
    1496 (calculated-Antoine eq., Andon et al. 1954)
    19920* (79.794°C, comparative ebulliometry, measured range 79.8–168°C. Scott et al. 1963a)
    $\log (P/\text{mmHg}) = 7.03202 - 1415.494/(t/°C + 211.589)$; temp range 79.8–168°C (ebulliometric measurements, Antoine eq., Scott et al. 1963a)
    1493 (ebulliometry, calculated-Antoine eq., Osborn & Douslin 1968)
    $\log (P/\text{mmHg}) = 7.03192 - 1415.424/(t/°C + 211.589)$; temp range 79.8–168°C (ebulliometric measurements, Antoine eq., Osborn & Douslin 1968)
    $\log [(P/\text{atm}) = [1 - 402.536 \pm (T/K)] \times 10\text{\^{}}\{0.866637 - 6.80114 \times 10^{-4} \pm (T/K) + 6.00534 \times 10^{-7} \pm (T/K)^2\}$, temp range: 79.8–168°C (ebulliometric method, Cox eq., Osborn & Douslin 1968)

log (P/mmHg) = [–0.2185 × 9933.2/(T/K)] + 8.290910; temp range –11.0 to 128.8°C (Antoine eq., Weast 1972–73)
1500 (calculated-Cox eq., Chao et al. 1983)
log (P/atm) = [1– 402.320/(T/K)] × 10^{0.887914 – 7.70705 × 10^{-4} ± (T/K) + 6.85261 × 10^{-7} ± $(T/K)^2$}; temp range: 215.0–620.0 K (Cox eq., Chao et al. 1983)
1067 (20°C, Verschueren 1983)
1494, 1498 (extrapolated-Antoine equations, Boublik et al. 1984)
log (P/kPa) = 6.16509 – 1421.237/(212.286 + t/°C); temp range 64.363–130.04°C (Antoine eq. from reported exptl. data of Herington & Martin 1953, Boublik et al. 1984)
log (P/kPa) = 6.15718 – 1415.663/(211.617 + t/°C); temp range 79.79–168.36°C (Antoine eq. from reported exptl. data of Scott et al. 1963, Boublik et al. 1984)
1494 (extrapolated-Antoine eq., Dean 1985, 1992)
log (P/mmHg) = 7.0324 – 1415.73/(211.63 + t/°C), temp range: 80–168°C (Antoine eq., Dean 1985, 1992)
1333 (Riddick et al. 1986)
log (P/kPa) = 6.15940 – 1417.578/(211.874 + t/°C); temp range not specified (Antoine eq., Riddick et al. 1986)
1386 (extrapolated-Antoine eq., Stephenson & Malanowski 1987)
log (P_L/kPa) = 5.2309 – 1164.1/(–71.0 + T/K); temp range 209–245 K (Antoine eq.-I, Stephenson & Malanowski 1987)
log (P_L/kPa) = 6.1558 – 1415.29/(–61.521 + T/K); temp range 352–442 K (Antoine eq.-II, Stephenson & Malanowski 1987)
log (P_L/kPa) = 6.15522 – 1414.906/(–61.566 + T/K); temp range 352–442 K (Antoine eq.-III, Stephenson & Malanowski 1987)
log (P_L/kPa) = 6.32356 – 1546.248/(–44.271 + T/K), temp range: 429–537 K (Antoine eq.-IV, Stephenson & Malanowski 1987)
log (P_L/kPa) = 7.32144 – 2667.496/(107.978 + T/K); temp range 521–621 K (Antoine eq.-V, Stephenson & Malanowski 1987)
1500* (ebulliometry, interpolated-Antoine eq., measured range 295.7–388.4 K, Łencka 1990)
ln (P/kPa) = 14.1560 – 3249.15/[(T/K) – 61.863); temp range 295.7–388.4 K (ebulliometric measurements, Antoine eq., Łencka 1990)
log (P/mmHg) = 34.3728 – 3.2825 × 10^3/(T/K) –9.0927·log (T/K) – 3.6324 × 10^{-10}·(T/K) + 2.1425 × 10^{-6}·$(T/K)^2$; temp range 206–621 K (vapor pressure eq., Yaws 1994)

Henry's Law Constant (Pa·m^3/mol at 25°C or as indicated and reported temperature dependence equations):
1.010 (measured volatility ratio-transpiration method, Andon et al. 1954)
1.010 (exptl., Hine & Mookerjee 1975)
0.821, 0.749 (calculated-group contribution, calculated-bond contribution, Hine & Mookerjee 1975)
2.90 (computed-vapor-liquid equilibrium VLE data, Yaws et al. 1991)
30.22 (20°C, selected from literature experimentally measured data, Staudinger & Roberts 2001)
log K_{AW} = –0.700 – 354/(T/K) (van't Hoff eq. derived from literature data, Staudinger & Roberts 2001)

Octanol/Water Partition Coefficient, log K_{OW}:
0.52 (HPLC-RT correlation, Schultz & Moulton 1985)
1.11 (shake flask, Log P Database, Hansch & Leo 1987)
1.11 (shake flask-UV, Yamagami et al. 1990)
1.11 (recommended, Sangster 1989; 1993)
1.11 (recommended, Hansch et al. 1995)

Octanol/Air Partition Coefficient, log K_{OA}:

Bioconcentration Factor, log BCF:
0.602 (calculated-K_{OW}, Lyman et al. 1982)

Sorption Partition Coefficient, log K_{OC}:

Environmental Fate Rate Constants, k, or Half-Lives, $t_{½}$:

Volatilization: using Henry's law constant, $t_{1/2}$ = 88 h for a model river 1 m deep flowing at 1 m/s with a wind velocity of 3 m/s (estimated, Howard 1990).
Photolysis:
Oxidation: photooxidation $t_{1/2}$ = 11.2 d in air, based on the gas-phase reaction with photochemically produced hydroxyl radicals in air (Atkinson 1987; quoted, Howard 1990).
Hydrolysis:
Biodegradation:
Biotransformation:
Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants:

Half-Lives in the Environment:
Air: $t_{1/2}$ = 11.2 d, based on the gas-phase reaction with photochemically produced hydroxyl radicals in air (Atkinson 1987; quoted, Howard 1990).
Surface water: estimated $t_{1/2}$ = 1.0 d for methylpyridine in Rhine River in case of a first order reduction process (Zoeteman et al. 1980)
Groundwater:
Sediment:
Soil:
Biota:

TABLE 16.1.7.4.1
Reported vapor pressures of 2-methylpryridine at various temperatures and the coefficients for the vapor pressure equations

$\log P = A - B/(T/K)$	(1)	$\ln P = A - B/(T/K)$	(1a)
$\log P = A - B/(C + t/°C)$	(2)	$\ln P = A - B/(C + t/°C)$	(2a)
$\log P = A - B/(C + T/K)$	(3)		
$\log P = A - B/(T/K) - C \cdot \log (T/K)$	(4)		

Stull 1947		Herington & Martin 1953		Scott et al. 1963(a)		Lencka 1990	
summary of literature data		ebulliometry		comparative ebulliometry		ebulliometry	
t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa
–11.1	133.3	64.363	10660	79.794	19920	18.49	1015
12.6	666.6	69.916	13459	85.853	25007	22.09	1264
24.4	1333	76.836	17758	91.942	31160	24.58	1463
37.4	2666	82.362	21954	98.074	38547	26.74	1657
51.2	5333	88.566	27600	104.252	47359	30.60	2062
59.9	7999	93.617	33044	110.472	57803	33.71	2446
71.4	13332	101.283	42906	116.736	70109	40.03	3414
89.0	26664	108.594	54434	123.038	84525	48.69	5258
108.4	53329	114.552	65581	129.387	101325	57.60	7942
128.8	101325	117.647	72020	135.773	120798	71.51	14375
		122.132	82297	142.207	143268	80.35	20380
mp/°C	–70.0	126.992	91140	148.683	169052	87.31	26426
		125.664	94663	155.201	198530	94.31	33920
		127.828	96885	161.761	232087	101.18	42854
		128.591	99021	168.356	270110	104.03	47076
		129.290	100985			109.24	55653
		129.608	101879	bp/°C	129.39	113.01	62604
		130.037	103095	Antoine eq.		115.31	67182

TABLE 16.1.7.4.1 (*Continued*)

Stull 1947		Herington & Martin 1953		Scott et al. 1963(a)		Lencka 1990	
summary of literature data		ebulliometry		comparative ebulliometry		ebulliometry	
t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa
				eq. 2	P/mmHg	119.20	75535
		bp/°C	129.408	A	7.03202	122.93	84296
		ΔH_V/(kJ mol^{-1}) = 37.76		B	1415.494	125.77	92024
		eq. 2	P/mmHg	C	211.598	129.88	102813
		A	7.03450				
		B	1417.578			Antoine eq.	
		C	211.874			eq. 3	P/kPa
						A	14.1560
						B	3249.15
						C	61.383

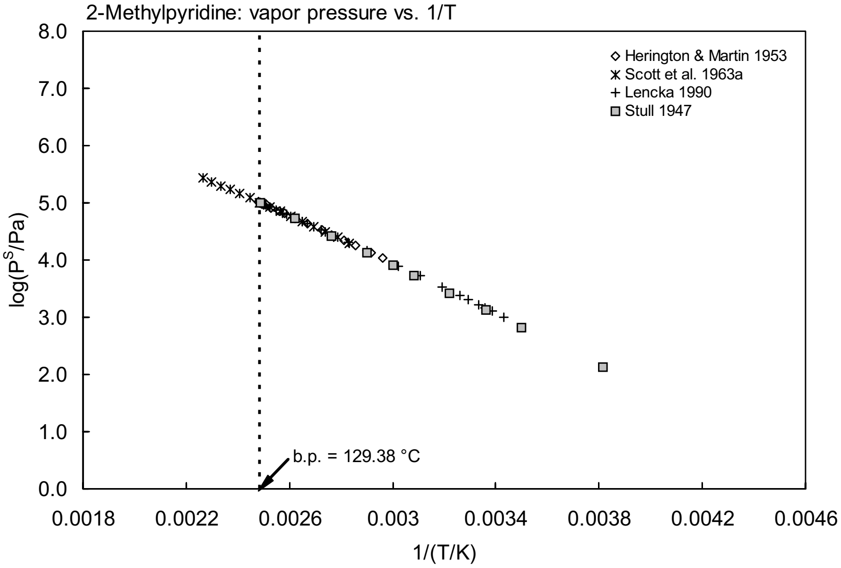
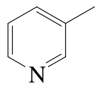


FIGURE 16.1.7.4.1 Logarithm of vapor pressure versus reciprocal temperature for 2-methylpyridine.

16.1.7.5 3-Methylpyridine



Common Name: 3-Methylpyridine
Synonym: β-picoline, 3-picoline
Chemical Name: 3-methylpyridine, β-picoline
CAS Registry No: 108-99-6
Molecular Formula: $C_5H_4NCH_3$
Molecular Weight: 93.127
Melting Point (°C):
–18.14 (Lide 2003)
Boiling Point (°C):
144.14 (Lide 2003)
Density (g/cm^3 at 20°C):
0.9443 (Weast 1982–83)
0.9566 (Riddick et al. 1986)
Molar Volume (cm^3/mol):
97.35 (20°C, calculated-density)
115.2 (calculated-Le Bas method at normal boiling point)
Dissociation Constant, pK:
5.67, 5.703 (Perrin 1972)
5.68 (pK$_a$, 20°C, Weast 1982–83; pK$_a$, protonated cation + 1, Dean 1985)
5.75 (pK$_{BH}{}^+$, Riddick et al. 1986)
5.65 (pK$_a$, Sangster 1989)
Enthalpy of Vaporization, ΔH_V (kJ/mol):
45.233, 37.323 (25°C, bp, Riddick et al. 1986)
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
14.18 (Riddick et al. 1986)
Entropy of Fusion, ΔS_{fus} (J/mol K):
Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F: 1.0

Water Solubility (g/m^3 or mg/L at 25°C):
miscible (Andon & Cox 1952; Andon et al. 1954; Yaws et al. 1990)
miscible (Riddick et al. 1986; Howard 1993)
miscible (Stephenson 1993a)

Vapor Pressure (Pa at 25°C or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):
150.7, 594.6 (0, 20°C, static method-tensimeter, Brown & Barbaras 1947)
794* (ebulliometry, extrapolated-Antoine eq., Herington & Martin 1953)
$\log (P/\text{mmHg}) = 7.03247 - 1469.894/(209.907 + t/°C)$; temp range 81.2–145.1°C (ebulliometric measurements, Antoine eq., Herington & Martin 1953)
794 (calculated-Antoine eq., Andon et al. 1954)
9582* (74.036ºC, comparative ebulliometry, measured range 74.036–184.568ºC, Scott et al. 1963b)
$\log (P/\text{mmHg}) = 7.05375 - 1484.208/(t/°C + 211.532)$, temp range 79.8–168°C (ebulliometric measurements, Antoine eq., Scott et al. 1963b)
811 (ebulliometry, calculated-Antoine eq., Osborn & Douslin 1968)
$\log (P/\text{mmHg}) = 7.30275 - 1506.877/(t/°C + 210.995)$, temp range: 74–185°C, (ebulliometric measurements, Antoine eq., Osborn & Douslin 1968)
$\log\ [(P/\text{atm}) = [1 - 417.287 \pm (T/K)] \times 10\text{^}\{0.854256 - 6.02835 \times 10^{-4} \pm (T/K) + 5.00169 \times 10^{-7} \pm (T/K)^2\}$, temp range: 74–185°C (ebulliometric method, Cox eq., Osborn & Douslin 1968)
806 (calculated-Cox eq., Chao et al. 1983)

log (P/atm) = [1– 417.217/(T/K)] × 10^{0.865977 – 6.48542×10^{-4} ± (T/K) + 5.41256×10^{-7} ± $(T/K)^2$}; temp range: 255.0–645.0 K (Cox eq., Chao et al. 1983)

796, 800 (extrapolated-Antoine equations, Boublik et al. 1984)

log (P/kPa) = 6.16152 – 1472.639/(210.214 + t/°C); temp range 81.3–145.1°C (Antoine eq. from reported exptl. data of Herington & Martin 1953, Boublik et al. 1984)

log (P/kPa) = 6.17577 – 1482.229/(211.305 + t/°C); temp range 74.03–184.6°C (Antoine eq. from reported exptl. data of Scott et al. 1963, Boublik et al. 1984)

800 (extrapolated-Antoine eq., Dean 1985, 1992)

log (P/mmHg) = 7.05021 – 1481.78/(211.25 + t/°C); temp range 74–185°C (Antoine eq., Dean l985, 1992)

1333 (Riddick et al. 1986)

log (P/kPa) = 6.15737 – 1469.894/(209.907 + t/°C); temp range not specified (Antoine eq., Riddick et al. 1986)

802 (extrapolated-Antoine eq., Stephenson & Malanowski 1987)

log (P_S/kPa) = 11.245 – 3246.9/(T/K); temp range 225–255 K (Antoine eq.-I, Stephenson & Malanowski 1987)

log (P_L/kPa) = 6.17593 – 1482.943/(–61.705 + T/K); temp range 347–458 K (Antoine eq.-II, Stephenson & Malanowski 1987)

log (P_L/kPa) = 6.17791 – 1484.285/(–61.554 + T/K); temp range 347–458 K (Antoine eq.-III, Stephenson & Malanowski 1987)

log (P_L/kPa) = 6.18988 – 1491.897/(–60.745 + T/K); temp range 347–381 K (Antoine eq.-IV, Stephenson & Malanowski 1987)

log (P_L/kPa) = 6.16648 – 1476.25/(–62.502 + T/K); temp range 374–458 K (Antoine eq.-V, Stephenson & Malanowski 1987)

log (P_L/kPa) = 6.38586 – 1659.184/(–38.176 + T/K); temp range 450–570 K (Antoine eq.-VI, Stephenson & Malanowski 1987)

log (P_L/kPa) = 7.57549 – 3151.52/(161.352 + T/K); temp range 561–645 K (Antoine eq.-II, Stephenson & Malanowski 1987)

log (P/mmHg) = 35.2679 – 3.4364×10^3/(T/K) – 9.3555·log (T/K) – 1.3286×10^{-10}·(T/K) + 2.0461×10^{-6}·$(T/K)^2$; temp range 255–645 K (vapor pressure eq., Yaws 1994)

Henry's Law Constant (Pa·m^3/mol at 25°C or as indicated):

0.788 (volatility ratio-transpiration method, Andon et al. 1954)

0.784; 0.637; 0.749 (exptl.; calculated-group contribution; calculated-bond contribution, Hine & Mookerjee 1975)

1.836 (computed-vapor-liquid equilibrium VLE data, Yaws et al. 1991)

12.69 (20°C, selected from literature experimentally measured data, Staudinger & Roberts 2001)

log K_{AW} = –0.826 – 348/(T/K) (van't Hoff eq. derived from literature data, Staudinger & Roberts 2001)

Octanol/Water Partition Coefficient, log K_{OW}:

1.20 (HPLC-RT correlation, Mirrlees et al. 1976)

1.20 ± 0.02 (shake flask at pH 7, Unger et al. 1978)

1.19 (HPLC-RT correlation, Lewis et al. 1983)

1.18 ± 0.01 (HPLC-RV correlation-ALPM, Garst 1984; Garst & Wilson 1984)

1.20 (shake flask, Log P Database, Hansch & Leo 1985, 1987)

1.20 (recommended, Sangster 1989, 1993)

1.20 (recommended, Hansch et al. 1995)

Octanol/Air Partition Coefficient, log K_{OA}:

Bioconcentration Factor, log BCF:

0.699 (calculated-K_{OW}, Lyman et al. 1982; quoted, Howard 1993)

Sorption Partition Coefficient, log K_{OC}:

2.029 (soil, calculated-K_{OW}, Lyman et al. 1982; quoted, Howard 1993)

Environmental Fate Rate Constants, k, or Half-Lives, $t_{½}$:

Volatilization:

Photolysis:

Oxidation: estimated photooxidation rate constant k = 1.43×10^{-12} cm^3 molecule^{-1} s^{-1} for the vapor-phase reaction with 5×10^5 hydroxyl radicals/cm^3 in air at 25°C which corresponds to an atmospheric half-life of 11 d (Atkinson 1987; quoted, Howard 1993).

Hydrolysis:
Biodegradation:
Biotransformation:
Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants:

Half-Lives in the Environment:

Air: atmospheric $t_{½}$ = 11 d from estimated photooxidation rate constant $k = 1.43 \times 10^{-12}\ cm^3 \pm molecule^{-1}\ s^{-1}$ for the vapor-phase reaction with 5×10^5 hydroxyl radicals/cm^3 in air at 25°C (Atkinson 1987; quoted, Howard 1993).

Surface water: estimated $t_{½}$ = 1.0 d for methylpyridine in Rhine River in case of a first order reduction process (Zoeteman et al. 1980)

TABLE 16.1.7.5.1
Reported vapor pressures of 3-methylpyridine at various temperatures and the coefficients for the vapor pressure equations

$\log P = A - B/(T/K)$ (1) $\ln P = A - B/(T/K)$ (1a)
$\log P = A - B/(C + t/°C)$ (2) $\ln P = A - B/(C + t/°C)$ (2a)
$\log P = A - B/(C + T/K)$ (3)
$\log P = A - B/(T/K) - C \cdot \log (T/K)$ (4)

Herington & Martin 1953		Scott et al. 1963(b)	
ebulliometry		comparative ebulliometry	
t/°C	P/Pa	t/°C	P/Pa
81.282	12871	74.036	9582
85.275	15061	77.115	10884
92.059	19478	80.202	12335
97.519	23773	85.303	13949
103.922	29747	86.403	15740
109.006	35349	89.524	17725
115.583	43796	92.658	19920
121.932	53445	98.946	25007
129.368	66822	105.270	31160
132.163	72471	111.640	38547
137.714	84938	118.052	47359
140.871	92693	124.508	57803
142.132	95948	131.008	70109
142.639	97265	137.551	84525
143.293	99017	144.135	101325
143.577	99782	150.767	120798
143.993	100927	157.441	143268
144.320	101791	164.156	169052
144.659	102725	170.918	198530
145.101	103988	177.821	232087
		184.568	270110
bp/°C	144.143		
ΔH_V/(kJ mol^{-1}) = 37.76		bp/°C	144.14
eq. 2	P/mmHg		
A	7.03247	Antoine	
B	1469.894	eq. 2	P/mmHg
C	209.907	A	7.05375
		B	1484.208
		C	211.532

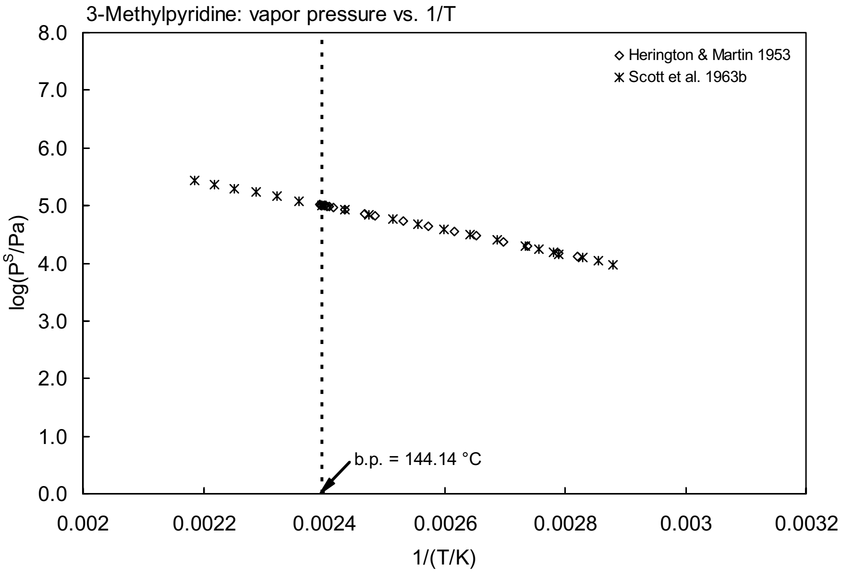
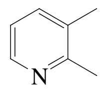


FIGURE 16.1.7.5.1 Logarithm of vapor pressure versus reciprocal temperature for 3-methylpyridine.

16.1.7.6 2,3-Dimethylpyridine



Common Name: 2,3-Dimethylpyridine
Synonym: 2,3-lutidine
Chemical Name: 2,3-dimethylpyridine, 2,3-lutidine
CAS Registry No: 583-61-9
Molecular Formula: C_7H_9N, $C_5H_3N(CH_3)_2$
Molecular Weight: 107.153
Melting Point (°C):
 –15.5 (Stephenson & Malanowski 1987)
Boiling Point (°C):
 161.12 (Lide 2003)
Density (g/cm^3 at 20°C):
 0.9461, 0.9421 (20°C, 25°C, Coulson et al. 1959)
 0.9319 (25°C, Weast 1982–83)
Molar Volume (cm^3/mol):
 115.0 (calculated-density, Stephenson & Malanowski 1987)
 135.9 (calculated-Le Bas method at normal boiling point)
Dissociation Constant, pK:
 6.70 (20°C, Perrin 1972)
 6.57 (pK_a, Weast 1982–83)
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
Entropy of Fusion, ΔS_{fus} (J/mol K):
Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F: 1.0

Water Solubility (g/m^3 or mg/L at 25°C or as indicated. Additional data at other temperatures designated * are compiled at the end of this section):
 104000* (20°C, shake flask-GC, measured range 16–90°C, Stephenson 1993a)

Vapor Pressure (Pa at 25°C and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):
 366.6, 922.6, 7119 (25, 40, 81.2°C, calculated-empirical method with bp and Antoine eq., Andon et al. 1954)
 346.4* (ebulliometry, extrapolated-Antoine eq., measured range 99.5–162.4°C, Coulson et al. 1959)
 $\log (P/mmHg) = 7.05075 - 1528.935/(205.499 + t/°C)$; temp range 99.5–162.4°C (Antoine eq., ebulliometry, Coulson et al. 1959)
 359.0 (calculated-Cox eq., Chao et al. 1983)
 $\log (P/atm) = [1 - 434.216/(T/K)] \times 10\hat{}\{0.881714 - 6.74484 \times 10^{-4} \pm (T/K) + 5.55055 \times 10^{-7} \pm (T/K)^2\}$; temp range: 260.0–655.0 K (Cox eq., Chao et al. 1983)
 425.5 (extrapolated-Antoine eq., Boublik et al. 1984)
 $\log (P/kPa) = 6.45509 - 1739.902/(229.887 + t/°C)$; temp range 155.3–162.4°C (Antoine eq. from reported exptl. data of Coulson et al. 1959, Boublik et al. 1984)
 352.2 (extrapolated-Antoine eq., Stephenson & Malanowski 1987)
 $\log (P_L/kPa) = 6.18881 - 1538.772/(-66.477 + T/K)$; temp range; 372–476 K (Antoine eq., Stephenson & Malanowski 1987)
 457 (extrapolated-Antoine eq., Dean 1992)
 $\log (P/mmHg) = 7.447 - 1832.6/(240.1 + t/°C)$; temp range 155–162°C (Antoine eq., Dean. 1992)
 2000* (54.556°C, comparative ebulliometry, measured range 327.706–475.952 K, data fitted to Wagner eq., Steele et al. 1995)

Henry's Law Constant ($Pa{\cdot}m^3/mol$ at 25°C or as indicated and reported temperature dependence equations):
 0.725 (volatility ratio-transpiration method, Andon et al. 1954)
 0.732 (exptl., Hine & Mookerjee 1975)

0.859, 0.732 (calculated.-group contribution, bond contribution, Hine & Mookerjee 1975)
21.01 (20°C, selected from literature experimentally measured data, Staudinger & Roberts 2001)
log K_{AW} = 0.039 – 617/(T/K), (van't Hoff eq. derived from literature data, Staudinger & Roberts 2001)

Octanol/Water Partition Coefficient, log K_{OW}:

Octanol/Air Partition Coefficient, log K_{OA}:

Bioconcentration Factor, log BCF:

Sorption Partition Coefficient, log K_{OC}:

Environmental Fate Rate Constants, k, or Half-Lives, $t_{½}$:

Half-Lives in the Environment:

Surface water: estimated $t_{½}$ = 13.0 d for dimethylpyridine in Rhine River in case of a first order reduction process (Zoeteman et al. 1980)

TABLE 16.1.7.6.1
Reported aqueous solubilities and vapor pressures of 2,3-dimethylpyridine at various temperatures

Aqueous solubility		Vapor pressure			
Stephenson 1993a		Coulson et al. 1959		Steele et al. 1995	
shake flask-GC/TC		ebulliometry		comparative ebulliometry	
t/°C	S/g·m⁻³	t/°C	P/Pa	T/K	P/Pa
16.0	171500	99.543	14583	327.706	2000
18.0	121500	107.822	19765	333.396	2666
20.0	104000	116.337	26607	341.852	3999.9
25.0	86000	122.909	33113	348.166	5333
30.0	69100	128.606	39759	357.560	7998.9
35.0	59900	133.429	46191	364.611	10666
40.0	53700	137.704	52572	370.315	13332
50.0	48200	141.757	59255	376.239	16665
60.0	43700	145.829	66652	381.163	19933
70.0	43000	148.764	72421	387.649	25023
80.0	43300	152.203	79677	387.646	25023
90.0	43500	155.326	86769	394.176	31177
		157.94	93067	400.749	38565
		158.603	94703	407.364	47375
		159.141	96085	414.025	57817
		160.125	98614	420.729	70120
		160.668	100030	427.477	84533
		161.199	101438	434.270	101325
		161.682	102701	441.106	120790
		162.077	103788	447.989	143250
		162.412	104696	454.913	169020
				461.885	198490
		mp/°C	–15.22	468.897	232020
		bp/°C	161.157	475.982	270020
		ΔH_V = 41.07 kJ/mol			
		Antoine eq.		Data fitted to Wagner eq.	
		log P = A – B/(C + t/°C)			
			P/mmHg		
		A	7.05075		
		B	1528.935		
		C	205.499		

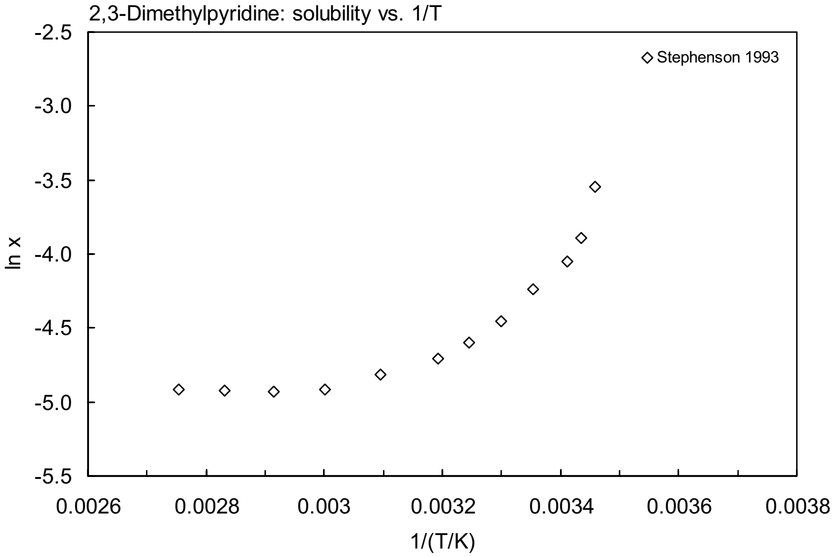


FIGURE 16.1.7.6.1 Logarithm of mole fraction solubility (ln *x*) versus reciprocal temperature for 2,3-dimethylpyridine.

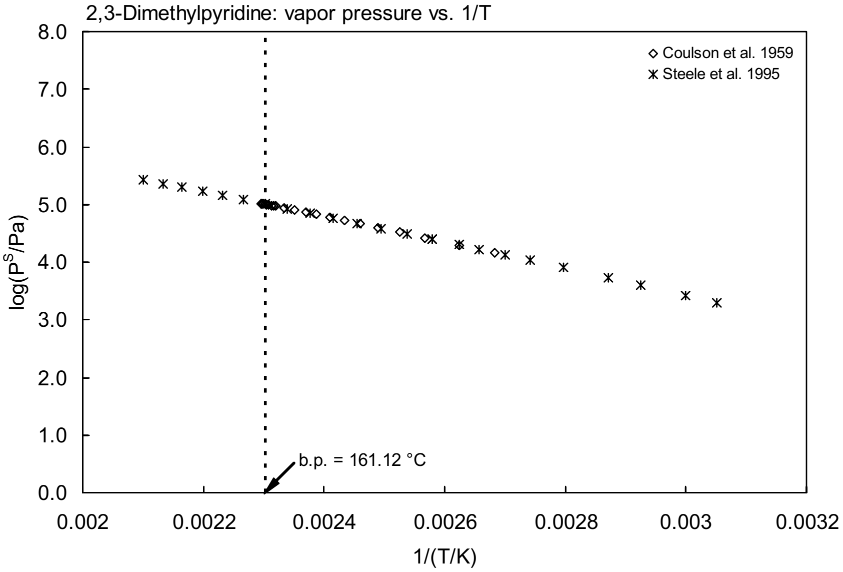
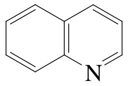


FIGURE 16.1.7.6.2 Logarithm of vapor pressure versus reciprocal temperature for 2,3-dimethylpyridine.

16.1.7.7 Quinoline



Common Name: Quinoline
Synonym: benzo[b]-pyridine, 1-benzazine
Chemical Name: quinoline
CAS Registry No: 91-22-5
Molecular Formula: C_9H_7N
Molecular Weight: 129.159
Melting Point (C):
  –14.78 (Lide 2003)
Boiling Point (°C):
  237.16 (Lide 2003)
Density (g/cm^3 at 20°C):
  1.0929 (Weast 1982–83)
  1.09771, 1.08579 (15, 30°C, Riddick et al. 1986)
Molar Volume (cm^3/mol):
  118.1 (calculated-density, Rohrschneider 1973)
  144.7 (calculated-Le Bas method at normal boiling point)
Dissociation Constant, pK:
  4.90 (pK_a, 20°C, Weast 1982–83; Zachara et al. 1987; Matzner et al. 1991)
  4.80 (pK_a, protonated cation + 1, Dean 1985)
  4.94 (p$K_{BH}{}^+$, Riddick et al. 1986)
  4.87 (pK_a, Sangster 1989)
Enthalpy of Vaporization, ΔH_V (kJ/mol):
  49.71 (at bp, Riddick et al. 1986)
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
  10.79 (Riddick et al. 1986)
Entropy of Fusion, ΔS_{fus} (J/mol K):
Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F: 1.0

Water Solubility (g/m^3 or mg/L at 25°C or as indicated. Additional data at other temperatures designated * are compiled at the end of this section):
  6110 (Albersmeyer 1958)
  6840 (shake flask-HPLC/UV, Fu & Luthy 1985, 1986)
  6386* (20.35°C, equilibrium cell-GC, measured range 20.35–225°C, Leet et al. 1987)
  5426 (centrifuge-HPLC at pH 7 and pH 8, Matzner et al. 1991)
  8400, 6600 (20°C, 30°C, shake flask-GC, Stephenson 1993a)

Vapor Pressure (Pa at 25°C and reported temperature dependence equations. Additional data at other temperatures designated *, are compiled at the end of this section):
  15.51* (extrapolated-regression of tabulated data, temp range 59.7–237.7°C, Stull 1947)
  1.213 (extrapolated, Maczynski & Maczynska 1965)
  11.20* (25.16°C, gas saturation-IR, measured range 12.62–35.9°C, Van De Rostyne & Prausnitz 1980)
  $\ln(P/\text{mmHg}) = 20.96 - 6993.2/(T/K)$; temp range 12.62–35.9°C (gas saturation-IR, Van De Rostyne & Prausnitz 1980)
  11.14 (calculated-bp, Mackay et al. 1982)
  12.83 (calculated-Cox eq., Chao et al. 1983)
  $\log(P/\text{atm}) = [1 - 510.552/(T/K)] \times 10\text{^}\{0.897177 - 6.73559 \times 10^{-4} \pm (T/K) + 4.69070 \times 10^{-7} \pm (T/K)^2\}$; temp range: 290.0–780.0 K (Cox eq., Chao et al. 1983)
  11.04 (extrapolated-Antoine eq., Boublik et al. 1984)

log (P/kPa) = 5.94201 – 1668.355/(186.212 + t/°C), temp range 164.7–237.9°C (Antoine eq. from reported exptl. data, Boublik et al. 1984)
11.05 (extrapolated-Antoine eq., Dean 1985, 1992)
log (P/mmHg) = 6.81759 – 1668.73/(186.26 + t/°C), temp range 164–238°C (Antoine eq., Dean 1985, 1992)
1.216 (recommended, Neely & Blau 1985)
12.8 (Howard et al. 1986)
11.2 (Riddick et al. 1986)
log (P/kPa) = 5.92679 – 1656.30/(184.78 + t/°C); temp range not specified (Antoine eq., Riddick et al. 1986)
42120* (472.85 K, vapor-liquid equilibrium, measured range 472.85–548.05 K, Klara et al. 1987)
log (P/kPa) = 14.4961 – 4390.0/(65.19 + T/K); temp range 472.85–548.05 K (vapor-liquid equilibrium, Klara et al. 1987)
log (P_L/kPa) = 5.92679 – 1656.3/(–88.37 + T/K); temp range 433–511 K (Antoine eq.-I, Stephenson & Malanowski 1987)
log (P_L/kPa) = 7.15102 – 2846.253/(41.795 + T/K); temp range 463–794 K (Antoine eq.-II, Stephenson & Malanowski 1987)
6.145 (calculated-solvatochromic parameters, Banerjee et al. 1990)
log (P/mmHg) = $76.5432 - 5.7748 \times 10^3/(T/K) - 24.619\cdot\log(T/K) + 8.4666 \times 10^{-3}\cdot(T/K) + 3.5586 \times 10^{-13}\cdot(T/K)^2$; temp range 258–782 K (vapor pressure eq., Yaws 1994)

Henry's Law Constant (Pa m^3/mol at 25°C):
0.0253 (calculated-P/C, Smith & Bomberger 1980)
0.026 (calculated-P/C, Mackay 1985)
0.168 (calculated-P/C, Meylan & Howard 1991)
0.0697 (estimated-bond contribution, Meylan & Howard 1991)

Octanol/Water Partition Coefficient, log K_{OW}:
2.03 (shake flask-UV, Iwasa et al. 1965)
2.06 (shake flask-UV at pH 7.4, Rogers & Cammarata 1969)
2.03 (Schultz et al. 1970)
2.04 (HPLC-RT correlation, Mirrlees et al. 1976)
2.04 ± 0.02 (shake flask at pH 7, Unger et al. 1978)
2.02 (Hansch & Leo 1979)
2.01 ± 0.02 (HPLC-RV correlation-ALPM, Garst & Wilson 1984)
1.88 (HPLC-k′ correlation, Haky & Young 1984)
2.20 (calculated-activity coeff. γ from UNIFAC, Banerjee & Howard 1988)
2.10 (shake flask-HPLC, De Voogt et al. 1988, 1990)
2.09 (28°C, shake flask-UV at pH 7.4, Go & Ngiam 1988)
2.03 (recommended, Sangster 1989, 1993)
2.10, 2.15 (HPLC-RT correlation, shake flask-electrometric titration, Slater et al. 1994)
2.03 (recommended, Hansch et al. 1995)
2.17 ± 0.66, 2.33 ± 0.56 (HPLC-k′ correlation: ODS–65 column, Diol–35 column, Helweg et al. 1997)
1.91 (microemulsion electrokinetic chromatography-retention factor correlation, Jia et al. 2003)

Octanol/Air Partition Coefficient, log K_{OA}:

Bioconcentration Factor, log BCF:

Sorption Partition Coefficient, log K_{OC}:
1.04 (Coyote Creek sediment with organic content of 1.9%, Smith et al. 1978)
1.96, 2.10, 1.67, 1.72 (estimated-K_{OW}, Karickhoff 1985)
1.42, 1.62 (estimated-S, Karickhoff 1985)
2.20 (best estimate, Karickhoff 1985)
0.251 (estimated Anvil Points subsurface materials, Zachara et al. 1987)
–1.516 (estimated Loring subsurface materials, Zachara et al. 1987)
2.89; 3.05 (humic acid, HPLC-k′ correlation; quoted lit., Nielsen et al. 1997)

Environmental Fate Rate Constants, k, or Half-Lives, $t_{½}$:

Volatilization: $t_{½}$ = 7000 h in stream, $t_{½}$ = 35000 h in eutrophic pond and $t_{½}$ = 28000 h in eutrophic lake and oligotrophic lake, based on transformation and transport of quinoline predicted by the one-compartment model (Smith et al. 1978).

Photolysis:

k = 7.8 × 10^{-7} s^{-1}, assuming exposed to 12-h sunlight per day in June, photolysis $t_{½}$ = 1200 h in stream, $t_{½}$ = 3000 h in eutrophic lake and pond and $t_{½}$ = 600 h in oligotrophic lake, based on transformation and transport of quinoline predicted by the one-compartment model (Smith et al. 1978)

k(aq.) = 3.6 × 10^{-7} s^{-1} for summer with $t_{½}$ = 535 h and k = 5.0 × 10^{-8} s^{-1} for winter with $t_{½}$ = 3851 h both at pH 6.9 and under sunlight at 40°N (Mill et al. 1981; quoted, Howard et al. 1991)

photolytic $t_{½}$ = 550 h in aquatics (Haque et al. 1980)

$t_{½}$ = 5–12 d for disappearance via direct photolysis in aqueous media (Harris 1982)

Oxidation:

k = 2.8 M^{-1} s^{-1} for the reaction with RO_2 radical with $t_{½}$ > 10^4 h in stream, eutrophic pond and lake and oligotrophic lake, based on RO_2 concentration of 10^{-9} M on transformation and transport of quinoline predicted by the one-compartment model (Smith et al. 1978)

k(aq.) = 3.5 × 10^{-7} s^{-1} with $t_{½}$ = 548 h under natural sunlight conditions for midday, midsummer at a latitude of 40°N; k(aq.) = 2.8 M^{-1} s^{-1} with $t_{½}$ = 8 yr for free-radical oxidation in air-saturated water (NRCC 1983)

photooxidation $t_{½}$ = 10–99 h in air, based on an estimated rate constant for vapor phase reaction with hydroxyl radicals in air (Atkinson 1987; quoted, Howard et al. 1991)

first-order photodegradation k = 8.0 × 10^{-6} s^{-1} at 313 nm of in organic-free water with $t_{½}$ = 24.0 h and k = 8.4 × 10^{-6} s^{-1} in lake water with $t_{½}$ = 23 h both saturated with air (Kochany & Maguire 1994)

Hydrolysis: no hydrolyzable groups (Howard et al. 1991).

Biodegradation:

$t_{½}$ = 0.5 h in stream, eutrophic lake and pond and $t_{½}$ = 10000 h in oligotrophic lake, based on transformation and transport of quinoline predicted by the one-compartment model (Smith et al. 1978);

Biodegradation k = 7.4 × 10^{-5} mL $cell^{-1}$ d^{-1} in enrichment culture (Klečka1985);

$t_{½}$(aq. aerobic) = 72–240 h, based on an acclimated fresh water grab sample data (Rogers et al. 1984; quoted, Howard et al. 1991);

$t_{½}$(aq. anaerobic) = 288–960 h, based on estimated aqueous aerobic biodegradation half-life (Howard et al. 1991)

Biotransformation:

Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants:

Half-Lives in the Environment:

Air: $t_{½}$ = 10 – 99 h, based on an estimated rate constant for vapor phase reaction with hydroxyl radicals in air (Atkinson 1987; selected, Howard et al. 1991);

atmospheric transformation lifetime was estimated to be 1 to 5 d (Kelly et al. 1994).

Surface water: half-life for all processes, except for dilution: $t_{½}$ = 0.5 h in stream, eutrophic lake and pond and $t_{½}$ = 600 h in oligotrophic lake, based on transformation and transport of quinoline predicted by the one-compartment model (Smith et al. 1978);

half-life for all processes, including for dilution: $t_{½}$ = 0.28 h in stream, $t_{½}$ = 0.5 h in eutrophic lake and pond and $t_{½}$ = 600 h in oligotrophic lake, based on transformation and transport of quinoline predicted by the one-compartment model (Smith et al. 1978);

$t_{½}$ = 5 – 12 d for direct photolysis in aqueous media (Harris 1982);

$t_{½}$ = 72 – 240 h, based on an acclimated fresh water grab sample data (Rogers et al. 1984; quoted, Howard et al. 1991);

degrade readily in sunlight in near surface lake water at 40°N latitude in summer with a $t_{½}$ ~ 14 calendar-d while its $t_{½}$(calc) ~ 123 calendar-d in winter (Kochany & Maguire 1994).

Groundwater: $t_{½}$ = 144 – 480 h, based on estimated aqueous aerobic biodegradation half-life (Howard et al. 1991).

Sediment:

Soil: $t_{½}$ = 72 – 240 h, based on estimated aqueous aerobic biodegradation half-life (Howard et al. 1991)

Complete mineralization within 7 – 10 d in batch experiments independent of pH (5.8 and 7.2) (Thomsen et al. 1999)

Biota:

TABLE 16.1.7.7.1
Reported aqueous solubilities and vapor pressures of quinoline at various temperatures and the coefficients for the vapor pressure equations:

Vapor pressure				Aqueous solubility			
Stull 1947		Van De Rostyne & Prausnitz		Klara et al. 1987		Leet et al. 1987	
summary of literate data		gas saturation-IR (1980)		vapor-liquid equilibrium		equilibrium cell-GC	
t/°C	P/Pa	t/°C	P/Pa	T/K	P/Pa	t/°C	S/g·m^{-3}
59.7	133.3	12.62	3.853	472.85	42120	20.35	6386
89.6	666.6	16.71	5.963	504.95	90990	40.05	6458
103.8	1333	21.35	8.159	514.35	112400	64.85	8252
119.8	2666	22.42	9.56	534.35	170300	80.25	10620
136.7	5333	25.16	11.20	548.05	222600	100.05	13920
148.1	7999	28.25	14.80			120.65	20163
163.2	13332	29.10	14.93	eq. 3	P/kPa	145.85	31285
186.2	26664	35.90	24.26	log P = A – B/(C + T/K)		159.65	43555
212.3	53329			A	14.4961	179.85	69602
237.7	101325	eq. 1a	P/mmHg	B	4390.0	199.25	126288
		ln P = A – B/(T/K)		C	65.19	209.05	171494
mp/°C	–15.0	A	20.96			220.25	324333
		B	6993.2			225.05	498697

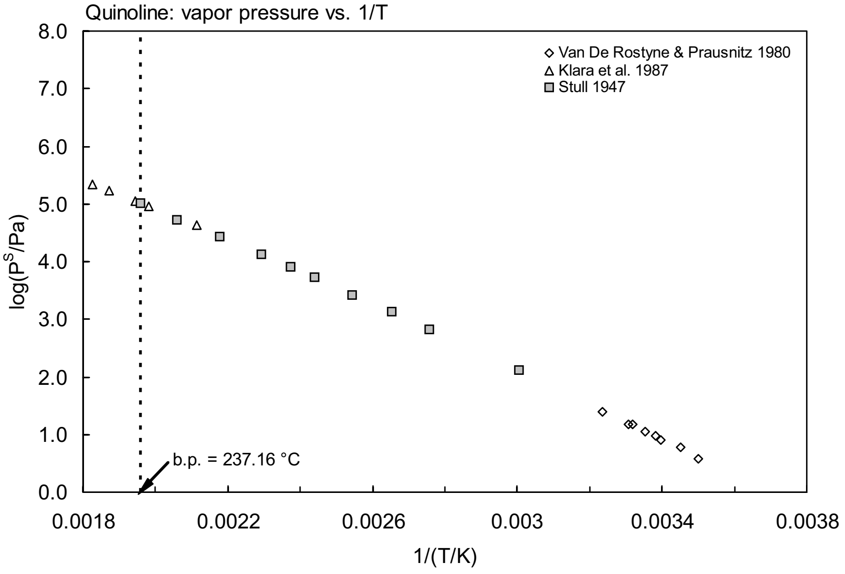
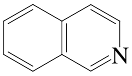


FIGURE 16.1.7.7.1 Logarithm of vapor pressure versus reciprocal temperature for quinoline.

16.1.7.8 Isoquinoline



Common Name: Isoquinoline
Synonym: leucoline
Chemical Name: isoquinoline
CAS Registry No: 119-65-3
Molecular Formula: C_9H_7N
Molecular Weight: 129.159
Melting Point (°C):
    26.47 (Lide 2003)
Boiling Point (°C):
    243.22 (Lide 2003)
Density (g/cm^3 at 20°C):
    1.0986 (Weast 1982–83)
    1.0910 (Dean 1985)
Molar Volume (cm^3/mol):
    118.4 (30°C, Stephenson & Malanowski 1987)
    144.7 (calculated-Le Bas method at normal boiling point)
Dissociation Constant, pK:
    5.40 (pK_a, Perrin 1972)
    5.42 (pK_a, 20°C, Weast 1982–83)
    5.40 (pK_a, protonated cation + 1, Dean 1985)
    5.38 (p$K_{BH}{}^+$, Riddick et al. 1986)
    5.39 (pK_a, Sangster 1989)
Enthalpy of Vaporization, ΔH_V (kJ/mol):
    48.96 (bp, Riddick et al. 1986)
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
    7.448 (Riddick et al. 1986)
Entropy of Fusion, ΔS_{fus} (J/mol K):
Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F: 0.967 (mp at 26.47°C)

Water Solubility (g/m^3 or mg/L at 25°C):
    4520 (Pearlman et al. 1984)

Vapor Pressure (Pa at 25°C and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):
    11.8* (extrapolated-regression of tabulated data, temp range 63.5–240.5°C, Stull 1947)
    7.80 (extrapolated-Cox eq., Chao et al. 1983)
    $\log(P/\text{atm}) = [1 - 516.182/(T/K)] \times 10\text{^}\{0.91210 - 6.33889 \times 10^{-4} \pm (T/K) + 4.267359 \times 10^{-7} \pm (T/K)^2\}$; temp range: 300.0–800.0 K (Cox eq., Chao et al. 1983)
    6.33 (extrapolated-Antoine eq., Boublik et al. 1984)
    $\log(P/\text{kPa}) = 6.03709 - 1723.459/(184.268 + t/°C)$; temp range 166–244°C (Antoine eq. from reported exptl. data, Boublik et al. 1984)
    6.35 (extrapolated-Antoine eq., Dean 1985, 1992)
    $\log(P/\text{mmHg}) = 6.9122 - 1723.4/(184.3 + t/°C)$; temp range 167–244°C (Antoine eq., Dean 1992)
    6.70 (Riddick et al. 1986)
    $\log(P_L/\text{kPa}) = 6.03203 - 1719.5/(-89.12 + T/K)$; temp range 439–517 K (Antoine eq., Stephenson & Malanowski 1987)
    $\log(P/\text{mmHg}) = 45.5737 - 4.4715 \times 10^3/(T/K) - 13.308 \cdot \log(T/K) + 4.0186 \times 10^{-3} \cdot (T/K) - 6.4589 \times 10^{-14} \cdot (T/K)^2$; temp range 299–803 K (vapor pressure eq., Yaws 1994)

Henry's Law Constant (Pa·m^3/mol at 25°C):

19.14 (calculated-P/C with selected values)

Octanol/Water Partition Coefficient, log K_{OW}:

2.08 (shake flask-UV, Hansch & Anderson 1967)
2.09 (HPLC-RT correlation, Mirrlees et al. 1976)
2.08 (recommended, Sangster 1989, 1993)
2.30 ± 0.15, 2.17 ± 0.53 (solvent generated liquid-liquid chromatography SGLLC-correlation, RP-HPLC-k′ correlation, Cichna et al. 1995)
2.08 (recommended, Hansch et al. 1995)
2.21 ± 0.66, 2.2 6 ± 0.56 (HPLC-k′ correlation: ODS-65 column, Diol-35 column, Helweg et al. 1997)

Octanol/Air Partition Coefficient, log K_{OA}:

Bioconcentration Factor, log BCF:

Sorption Partition Coefficient, log K_{OC}:

3.09 (humic acid, HPLC-k′ correlation, Nielsen et al. 1997)

Environmental Fate Rate Constants, k, or Half-Lives, $t_{½}$:

Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants:

k_1 = 82.0 h^{-1}, k_2 = 34.2 h^{-1} (*daphnia pulex*, 21°C, Southworth et al. 1978)

Half-Lives in the Environment:

Biota: elimination $t_{½}$ = 1 min (*daphnia pulex*, Southworth et al. 1978).

TABLE 16.1.7.8.1
Reported vapor pressures of isoquinoline at various temperatures

Stull 1947	
summary of literature data	
t/°C	P/Pa
63.5	133.3
92.7	666.6
107.8	1333
123.7	2666
141.6	5333
152.0	7999
167.6	13332
190.0	26664
214.5	53329
240.5	101325
mp/°C	24.5

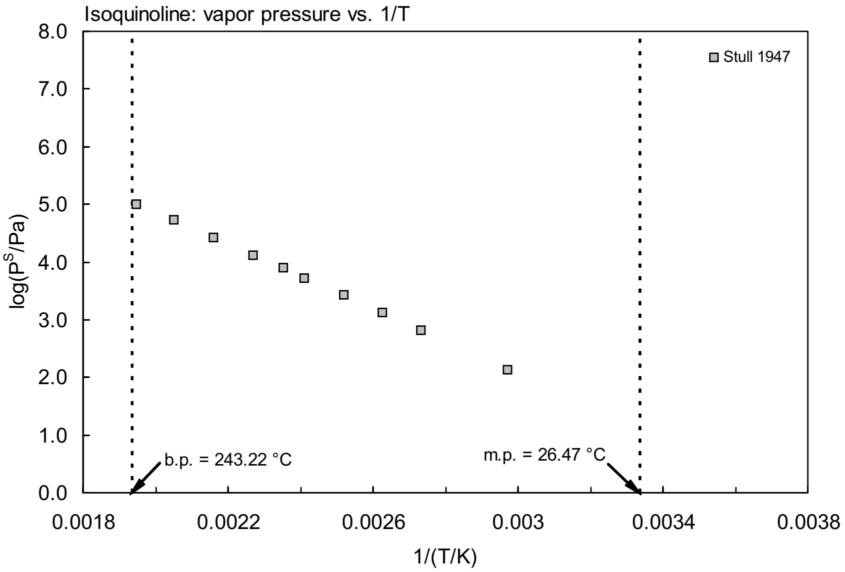
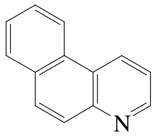


FIGURE 16.1.7.8.1 Logarithm of vapor pressure versus reciprocal temperature for isoquinoline.

16.1.7.9 Benzo[*f*]quinoline



Common Name: Benzo[*f*]quinoline
Synonym: 5,6-benzoquinoline, naphthopyridine
Chemical Name: 5,6-benzoquinoline, benzo(f)quinoline
CAS Registry No: 85-02-9
Molecular Formula: $C_{13}H_9N$
Molecular Weight: 179.217
Melting Point (°C):
94 (Lide 2003)
Boiling Point (°C):
352 (Lide 2003)
Density (g/cm^3 at 20°C):
Molar Volume (cm^3/mol):
196.3 (calculated-Le Bas method at normal boiling point)
Dissociation Constant, pK:
5.15 (Sangster 1993)
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
Entropy of Fusion, ΔS_{fus} (J/mol K):
Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F: 0.210 (mp at 94°C)

Water Solubility (g/m^3 or mg/L at 25°C):
76.1 (shake flask-GC, Smith et al. 1978)
77.1 (Mill et al. 1981)
176.0 (Steen & Karickhoff 1981)
78.7 (average literature value, Pearlman et al. 1984)

Vapor Pressure (Pa at 25°C or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):
0.00747* (25.05°C, gas saturation, measured range 288.26–323.15 K, McEachern et al. 1975)
$\log (P/mmHg) = 4339.977/(T/K) + 10.2555$; temp range 288.26–323.15 K (Antoine eq., gas saturation, McEachern et al. 1975
0.00670 (interpolated-Antoine eq., Stephenson & Malanowski 1987)
$\log (P_L/kPa) = 9.37682 - 4338.411/(T/K)$; temp range 288–323 K (Antoine eq., Stephenson & Malanowski 1987)

Henry's Law Constant (Pa·m^3/mol at 25°C):
0.0096 (calculated-P/C, Smith & Bomberger 1980)

Octanol/Water Partition Coefficient, log K_{OW}:
3.20 (Steen & Karickhoff 1981)
3.40 (TLC-RT correlation, De Voogt et al. 1988)
3.25 (23°C, shake flask-HPLC, pH 7, De Voogt et al. 1990)
3.25, 3.40 (lit. values; Sangster 1993)
3.46 ± 0.64, 3.51 ± 0.53 (HPLC-k′ correlation: ODS-65 column, Diol-35 column, Helweg et al. 1997)

Octanol/Air Partition Coefficient, log K_{OA}:

Bioconcentration Factor, log BCF:
2.18 (mixed microbial populations, Steen & Karickhoff 1981)

Sorption Partition Coefficient, log K_{OC}:

3.11	(Coyote Creek sediment, Smith et al. 1978)
4.64, 4.32	(soil, quoted, calculated-MCI χ and fragment contribution, Meylan et al. 1992)
4.07	(humic acid, HPLC-k′ correlation, Nielsen et al. 1997)

Environmental Fate Rate Constants, k, or Half-Lives, $t_{½}$:

Volatilization: estimated $t_{½} > 10000$ h in river, $t_{½} > 100000$ h in eutrophic pond, eutrophic lake and oligotrophic lake by the one compartment model (Smith et al. 1978).

Photolysis:

$k = (1.4 \pm 0.7) \times 10^{-4}\ s^{-1}$ for transformation and transport when exposed to 12 h sunlight in mid-June with estimated $t_{½} = 2.8$ h in river, $t_{½} = 7.0$ h in eutrophic pond and eutrophic lake and $t_{½} = 1.4$ h in oligotrophic lake from average photolysis rates on a summer day at 40°N latitude by the one compartment model (Smith et al. 1978)

photolytic $t_{½} = 0.52$ h in aquatics (Haque et al. 1980)

$t_{½} = 1$ h for disappearance via direct photolysis in aqueous media (Harris 1982)

Oxidation:

laboratory studied $k < 2.8\ M^{-1}\ s^{-1}$ for the reaction with the RO_2 radicals and estimated $t_{½} > 10^5$ h in river, eutrophic pond, eutrophic lake and oligotrophic lake by the one compartment model (Smith et al. 1978)

$k(aq.) = 3.7 \times 10^{-4}\ s^{-1}$ with $t_{½} = 0.5$ h under natural sunlight conditions for midday, midsummer at a latitude of 40°N; $k(aq.) < 2.8\ M^{-1}\ s^{-1}$ with $t_{½} > 8$ yr for free-radical oxidation in air-saturated water (NRCC 1983)

Hydrolysis:

Biodegradation: estimated $t_{½} = 190$ h in river, eutrophic pond, eutrophic lake and $t_{½} > 10^6$ h in oligotrophic lake by the one compartment model (Smith et al. 1978).

Biotransformation:

Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants:

Half-Lives in the Environment:

Surface water: $t_{½} = 0.5$ h in river water, $t_{½} = 6.9$ h in pond water, $t_{½} = 7.0$ h in eutrophic lake and $t_{½} = 1.4$ h in oligotrophic lake predicted by one-compartment for all processes including dilution (Smith et al. 1978) $t_{½} = 1$ h for disappearance via direct photolysis in aqueous media (Harris 1982).

TABLE 16.1.7.9.1
Reported vapor pressures of benzo[*f*]quinoline at various temperatures

McEachern et al. 1975	
gas saturation	
T/K	P/Pa
288.26	0.00213
293.10	0.00333
298.20	0.00747
303.13	0.0116
308.23	0.0199
313.17	0.0324
318.24	0.0560
323.15	0.0901
	P/mmHg
log P = A – B/(T/K)	
A	10.2555
B	4399.977
$\Delta H_{subl}/(kJ\ mol^{-1}) = 83.094$	
$\Delta S_{subl}/(J\ mol^{-1}\ K^{-1}) = 196.36$	

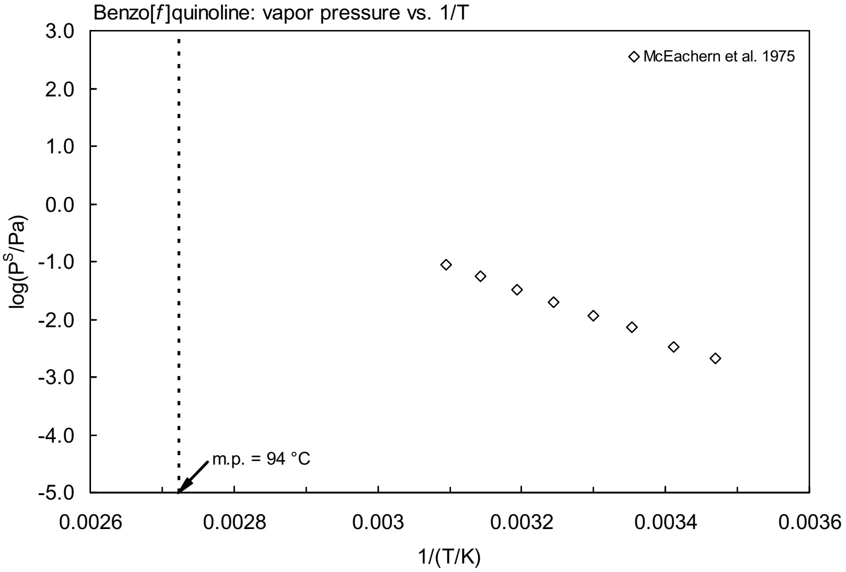
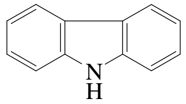


FIGURE 16.1.7.9.1 Logarithm of vapor pressure versus reciprocal temperature for benzo[*f*]quinoline.

16.1.7.10 Carbazole



Common Name: Carbazole
Synonym: 9H-carbazole, dibenzopyrrole
Chemical Name: carbazole
CAS Registry No: 86-74-8
Molecular Formula: $C_{12}H_9N$, $C_6H_4NHC_6H_4$
Molecular Weight: 167.206
Melting Point (°C):
 246.3 (Lide 2003)
Boiling Point (°C):
 354.69 (Lide 2003)
Density (g/cm^3 at 20°C):
 1.260 (25°C, Jiménez et al. 1990)
Molar Volume (cm^3/mol):
 192.9 (calculated-Le Bas method at normal boiling point)
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
Entropy of Fusion, ΔS_{fus} (J/mol K):
Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F: 0.00674 (mp at 246.3°C)

Water Solubility (g/m^3 or mg/L at 25°C):
 1.03 ± 0.05 (20°C, shake flask-GC, Smith et al. 1978)
 1.037 (Mill et al. 1981)
 0.428 (20°C, shake flask-fluorophotometry, Hashimoto et al. 1982)
 1.67, 1.03, 0.908; 1.204 (quoted values; lit. average, Pearlman et al. 1984)

Vapor Pressure (Pa at 25°C and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):
 7999* (248.2°C, summary of literature data, temp range: 248.2–354.8°C, Stull 1947)
 $\log(P/\text{mmHg}) = [-0.2185 \times 15421.6/(T/K)] + 8.251923$; temp range: 248.2–354.8°C (Antoine eq., Weast 1972–73)
 0.0933 (20°C, Smith et al. 1978)
 $\log(P/\text{atm}) = [1 - 627.897/(T/K)] \times 10\text{\^{}}\{0.924810 - 5.18974 \times 10^{-4} \pm (T/K) + 2.68415 \times 10^{-7} \pm (T/K)^2\}$; temp range: 518.0–631.0 K (Cox eq., Chao et al. 1983)
 0.00424 (extrapolated-Antoine eq., Boublik et al. 1984)
 $\log(P/\text{kPa}) = 6.20101 - 2169.73/(162.465 + t/°C)$; temp range 252.6–357.3°C (Antoine eq. from reported exptl. data, Boublik et al. 1984)
 $\log(P/\text{mmHg}) = 7.0863 - 2179.4/(163.5 + t/°C)$; temp range 253–368°C (Antoine eq., Dean 1985, 1992)
 0.0012 (Antoine eq.-I, Stephenson & Malanowski 1987)
 0.0045 (liquid, extrapolated-Antoine eq.-II, Stephenson & Malanowski 1987)
 $\log(P_S/\text{kPa}) = 10.1069 - 4780/(T/K)$; temp range not specified (solid, Antoine eq.-I, Stephenson & Malanowski 1987)
 $\log(P_L/\text{kPa}) = 6.21123 - 2179.424/(-109.636 + T/K)$; temp range 525–631 K (liquid, Antoine eq-II., Stephenson & Malanowski 1987)
 0.0002* (extrapolated-Antoine eq., Knudsen effusion, measured range 73.43–90.80°C, Jiménez et al. 1990)
 $\log(P/\text{Pa}) = 14.64 - 5288.4/(T/K)$; temp range 73.43–90.80°C (Knudsen effusion, Jiménez et al. 1990)
 $\log(P/\text{mmHg}) = -119.857 - 3.2537 \times 10^3/(T/K) + 52.568\cdot\log(T/K) - 4.6797 \times 10^{-2}\cdot(T/K) + 1.4113 \times 10^{-5}\cdot(T/K)^2$; temp range 518–899 K (vapor pressure eq., Yaws 1994)

Henry's Law Constant (Pa·m^3/mol at 25°C):

16.0	(calculated-P/C, Smith & Bomberger 1980)

Octanol/Water Partition Coefficient, log K_{OW}:

3.29	(shake flask-UV at pH 7.4, Rogers 1969)
3.01	(HPLC-k′ correlation, Eadsforth 1986)
3.50	(calculated, Eadsforth 1986)
3.72	(recommended, Sangster 1989, 1993)
3.59	(HPLC-RT correlation, Jenke et al. 1990)
3.84	(shake flask-HPLC at pH 7, De Voogt et al. 1988)
3.47 ± 0.63, 3.22 ± 0.53	(HPLC-k′ correlation: ODS-65 column, Diol-35 column, Helweg et al. 1997)
3.72	(recommended, Hansch et al. 1995)

Octanol/Air Partition Coefficient, log K_{OA}:

Bioconcentration Factor, log BCF:

Sorption Partition Coefficient, log K_{OC}:

2.24	(Coyote Creek sediment, Smith et al. 1978)
4.74	(humic acid, HPLC-k′ correlation, Nielsen et al. 1997)
3.80	(soil-pore water partition coeff., Askov soil - a Danish agricultural soil, Sverdrup et al. 2002)

Environmental Fate Rate Constants, k, or Half-Lives, $t_{½}$:

Volatilization: estimated $t_{½} > 10^5$ h in river, eutrophic pond, eutrophic lake and oligotrophic lake by the one compartment model (Smith et al. 1978).

Photolysis:

$k = 6.6 \times 10^{-5}$ s^{-1} for transformation and transport when exposed to midday sunlight in late January with estimated $t_{½} = 6.0$ h in river, $t_{½} = 15.0$ h in eutrophic pond and eutrophic lake and $t_{½} = 3.0$ h in oligotrophic lake from average photolysis rates on a summer day at 40°N latitude by the one compartment model (Smith et al. 1978)

photolytic $t_{½} = 1.0$ h in aquatics (Haque et al. 1980)

$t_{½} = 3$ h for disappearance via direct photolysis in aquatic media (Harris 1982).

Oxidation:

laboratory investigated $k = 29$ M^{-1} s^{-1} for the reaction with RO_2 radicals and estimated $t_{½} > 240$ h in river, eutrophic pond, eutrophic lake and oligotrophic lake by the one compartment model (Smith et al. 1978)

k(aq.) = 1.9×10^{-4} s^{-1} with $t_{½} = 1.0$ h under natural sunlight conditions for midday, midsummer at a latitude of 40°N; k(aq.) = 29 M^{-1} s^{-1} with $t_{½} = 280$ yr for free-radical oxidation in air-saturated water (NRCC 1983)

Hydrolysis:

Biodegradation: estimated half-lives of 14 h in river, eutrophic pond, eutrophic lake and > 10^3 h in oligotrophic lake by the one compartment model (Smith et al. 1978).

Biotransformation:

Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants:

Half-Lives in the Environment:

Surface water: estimated $t_{½} = 6.0$ h in river, $t_{½} = 15.0$ h in eutrophic pond and eutrophic lake and $t_{½} = 3.0$ h in oligotrophic lake from average photolysis rates on a summer day at 40°N latitude by the one compartment model (Smith et al. 1978);

photolytic $t_{½} = 1.0$ h in aquatics (Haque et al. 1980); $t_{½} = 3$ h for disappearance via direct photolysis in aquatic media (Harris 1982).

TABLE 16.1.7.10.1
Reported vapor pressures of carbazole at various temperatures and the coefficients for the vapor pressure equations

$\log P = A - B/(T/K)$ (1)
$\log P = A - B/(C + t/°C)$ (2)
$\log P = A - B/(C + T/K)$ (3)
$\log P = A - B/(T/K) - C\cdot\log (T/K)$ (4)
$\ln P = A - B/(T/K)$ (1a)
$\ln P = A - B/(C + t/°C)$ (2a)

Stull 1947		**Jiménez et al. 1990**	
summary of literature data		**Knudsen effusion**	
t/°C	**P/Pa**	**t/°C**	**P/Pa**
248.2	7999	73.43	0.0610
265.0	13332	78.72	0.101
292.5	26664	81.0	0.129
323.0	53329	83.59	0.167
354.8	101325	86.67	0.219
		87.13	0.227
mp/°C	244.8	90.80	0.329
		ρ (at 25°C)	1.26 g/cm^3
		eq. 1	P/Pa
		A	14.04
		B	5288.4
		enthalpy of sublimation:	
		$\Delta H_{sub}/(kJ\ mol^{-1})$ = 103.3	
			at 25°C

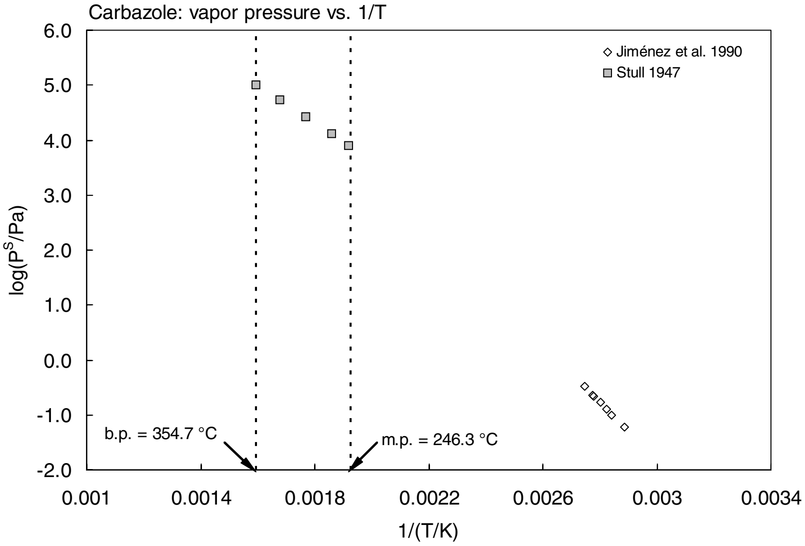
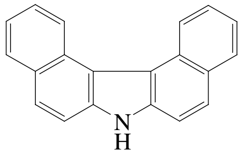


FIGURE 16.1.7.10.1 Logarithm of vapor pressure versus reciprocal temperature for carbazole.

16.1.7.11 Benzo[*c,g*]carbazole



Common Name: Benzo[*c,g*]carbazole
Synonym: 7H-dibenzo[*c,g*]carbazole
Chemical Name: 7H-dibenzo[*c,g*]carbazole
CAS Registry No: 194-59-2
Molecular Formula: $C_{20}H_{13}N$, $C_{10}H_6NHC_{10}H_6$
Molecular Weight: 267.324
Melting Point (°C):
158 (Lide 2003)
Boiling Point (°C)
Density (g/cm^3 at 20°C):
Molar Volume (cm^3/mol):
296.1 (calculated-Le Bas method at normal boiling point)
Dissociation Constant, pK_a:
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
Entropy of Fusion, ΔS_{fus} (J/mol K):
Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F: 0.0496 (mp at 158°C)

Water Solubility (g/m^3 or mg/L at 25°C):
0.063 ± 0.003 (shake flask-GC, Smith et al. 1978)
0.064 (Mill et al. 1981)
0.064 (Pearlman et al. 1984)

Vapor Pressure (Pa at 25°C):
1.33×10^{-7} (estimated by comparison with benzo[*a*]pyrene, Smith et al. 1978)

Henry's Law Constant (Pa·m^3/mol at 25°C):
0.00048 (calculated-P/C, Smith & Bomberger 1980)

Octanol/Water Partition Coefficient, log K_{OW}:
5.75 (calculated-S, Steen & Karickhoff 1981)

Octanol/Air Partition Coefficient, log K_{OA}:

Bioconcentration Factor, log BCF:
4.93 (mixed microbial populations, Steen & Karickhoff 1981)

Sorption Partition Coefficient, log K_{OC}:
4.31 (Coyote Creek sediment, Smith et al. 1978)
6.03, 6.16 (soil, quoted, calculated-MCI χ and fragment contribution, Meylan et al. 1992)

Environmental Fate Rate Constants, k, or Half-Lives, $t_{1/2}$:
Volatilization: estimated $t_{1/2}$ = 15000 h in river, $t_{1/2}$ = 37000 h in eutrophic pond, $t_{1/2}$ = 73000 h in eutrophic lake and oligotrophic lake by the one compartment model (Smith et al. 1978).
Photolysis: rate constant
k = 5.2×10^{-4} s^{-1} for transformation and transport when exposed to midday sunlight in mid-January with estimated $t_{1/2}$ = 1.0 h in river, $t_{1/2}$ = 1.5 h in eutrophic pond and eutrophic lake and $t_{1/2}$ = 0.5 h in oligotrophic lake assuming winter insulation by the one compartment model (Smith et al. 1978)
photolytic $t_{1/2}$ = 0.35 h in aquatics (Haque et al. 1980).

Oxidation:

laboratory studied k = 830 M^{-1} s^{-1} for the reaction with the RO_2 radicals and estimated $t_{½}$ > 700 h in river, eutrophic pond, eutrophic lake and oligotrophic lake by the one compartment model (Smith et al. 1978)

k = 5.5 × 10^{-4} s^{-1} with $t_{½}$ = 0.4 d under natural sunlight conditions for midday, midsummer at a latitude of 40°N; k = 830 M^{-1} s^{-1} with $t_{½}$ = 10 d for free-radical oxidation in air-saturated water (NRCC 1983)

Hydrolysis:

Biodegradation: estimated half-life to be very long in river, eutrophic pond, eutrophic lake and oligotrophic lake by the one compartment model with no acclimated cultures obtained during the screening studies (Smith et al. 1978).

Biotransformation:

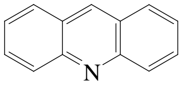
Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants:

Half-Lives in the Environment:

Surface water: $t_{½}$ = 0.36 h in river water, $t_{½}$ = 1.5 h in pond water, $t_{½}$ = 1.5 h in eutrophic lake and $t_{½}$ = 0.5 h in oligotrophic lake for all processes predicted by one-compartment model (Smith et al. 1981);

$t_{½}$ = 10 d for free-radical oxidation in air-saturation water (NRCC 1983).

16.1.7.12 Acridine



Common Name: Acridine
Synonym: 2,3,5,6-dibenzopyridine
Chemical Name: acridine, 2,3,5,6-dibenzopyridine
CAS Registry No: 260-94-6
Molecular Formula: $C_{13}H_9N$
Molecular Weight: 179.217
Melting Point (°C):
  110 (Lide 2003)
Boiling Point (°C):
  344.86 (Lide 2003)
Density (g/cm^3 at 20°C):
  1.005 (Weast 1982–83)
Molar Volume (cm^3/mol):
  196.3 (calculated-Le Bas method at normal boiling point)
Dissociation Constant, pK_a:
  5.60 (Albert 1966; Matzner et al. 1991; Matzner & Bales 1994)
  5.58 (20°C, Weast 1982–83)
  5.60 (protonated cation + 1, Dean 1985)
  10.65 (Sangster 1989)
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
  18.58 ± 0.38 (McEachern et al. 1975)
Entropy of Fusion, ΔS_{fus} (J/mol K):
Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F: 0.147 (mp at 110°C)

Water Solubility (g/m^3 or mg/L at 25°C or as indicated):
  57.4 (Albert 1966)
  38.4 (24°C, shake flask-LSC, Means et al. 1980)
  46.6 (literature average, Pearlman et al. 1984)
  54.8 (centrifuge-HPLC at pH 8, Matzner et al. 1991)

Vapor Pressure (Pa at 25°C and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):
  133.3* (129.4°C, summary of literature data, temp range 129.4–346°C, Stull 1947)
  $\log (P/\text{mmHg}) = [-0.2185 \times 15174.6/(T/K)] + 8.251980$; temp range 129.4–346°C (Antoine eq., Weast 1972–73)
  0.0065* (Langmuir free evaporation, measured range 7.96–50°C, McEachern et al. 1975)
  $\log (P/\text{mmHg}) = 27.076 - 11021.64/(T/K)$; measured range 281.2–323.3 K (Langmuir free evaporation, McEachern et al. 1975)
  0.0075 (extrapolated-Cox eq., Chao et al. 1983)
  $\log (P/\text{atm}) = [1 - 618.827/(T/K)] \times 10\verb|^|\{0.839996 - 4.19344 \times 10^{-4} \pm (T/K) + 3.63487 \times 10^{-7} \pm (T/K)^2\}$; temp range: 402.6–619.2 K (Cox eq., Chao et al. 1983)
  0.2066 (static apparatus-extrapolated from Chebyshev polynomials, Sivaraman & Kobayashi 1983)
  0.0065 (Interpolated-Antoine eq.-I, Stephenson & Malanowski 1987; quoted, Ma et al. 1990)

$\log (P_S/\text{kPa}) = 8.30838 - 3365.943/(-48.723 + T/\text{K})$; temp range 293–367 K (solid, Antoine eq.-I, Stephenson & Malanowski 1987)

$\log (P_L/\text{kPa}) = 6.73664 - 2699.39/(-48.611 + T/\text{K})$; temp range 402–619 K (liquid, Antoine eq.-II, Stephenson & Malanowski 1987)

Henry's Law Constant (Pa·m^3/mol at 25°C):

0.030	(calculated-P/C, Ma et al. 1990)

Octanol/Water Partition Coefficient, log K_{OW}:

3.40	(shake flask-UV, Hansch & Fujita 1964)
3.39	(HPLC-RT correlation, Mirrlees et al. 1976)
3.39	(shake flask at pH 7.4, Unger et al. 1978)
3.62	(shake flask-LSC, Means et al. 1980)
3.29	(shake flask-AS at pH 7.4, Unger & Chiang 1981)
3.31 ± 0.03	(HPLC-RV correlation-ALPM, Garst 1984)
3.35 ± 0.02	(HPLC-RV correlation-ALPM, Garst & Wilson 1984)
3.32	(shake flask-GC at pH 7.0, Haky & Leja 1986)
3.40	(recommended, Sangster 1989, 1993)
3.40	(recommended, Hansch et al. 1995)
3.18 ± 0.64, 3.27 ± 0.53	(HPLC-k′ correlation: ODS-65 column, Diol-35 column, Helweg et al. 1997)

Octanol/Air Partition Coefficient, log K_{OA}:

Bioconcentration Factor, log BCF:

2.40	(selected, Ma et al. 1990)

Sorption Partition Coefficient, log K_{OC}:

4.69	(average of sediments and soil samples, equilibrium sorption isotherm, Means et al. 1980)
3.32	(calculated, Means et al. 1980)
–0.157	(estimated of Loring subsurface material, Zachara et al. 1987)
0.610	(estimated of Anvil Points subsurface material, Zachara et al. 1987)
3.09–3.41	(soil, calculated-K_{OW}, model of Karickhoff et al. 1979, Sabljic 1987)
3.16–3.33	(soil, calculated-K_{OW}, model of Kenaga & Goring 1980, Sabljic 1987)
2.36–2.52	(soil, calculated-K_{OW}, model of Briggs 1981, Sabljic 1987)
2.98–3.30	(soil, calculated-K_{OW}, model of Means et al. 1982, Sabljic 1987)
2.19–2.48	(soil, calculated-K_{OW}, model of Chiou et al. 1983, Sabljic 1987)
4.22, 4.26	(soil, quoted, calculated-MCI χ, Sabljic 1987)
4.11, 3.32	(quoted, calculated-MCI χ, Gerstl & Helling 1987)
4.11, 4.31	(soil, quoted, calculated-MCI χ and fragment contribution, Meylan et al. 1992)
4.00	(HPLC-k′ correlation, Nielsen et al. 1997)
4.79	(soil-pore water partition coeff., Askov soil - a Danish agricultural soil, Sverdrup et al. 2002)

Environmental Fate Rate Constants, k, or Half-Lives, $t_{½}$:

Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants:

$k_1 = 109\ \text{h}^{-1}$, $k_2 = 3.68\ \text{h}^{-1}$ (*daphnia pulex*, 21°C, Southworth et al. 1978)

Half-Lives in the Environment:

Biota: elimination $t_{½}$ = 11.3 min (*daphnia pulex*, Southworth et al. 1978).

TABLE 16.1.7.12.1

Reported vapor pressures of acridine at various temperatures and the coefficients for the vapor pressure equations

$\log P = A - B/(T/K)$ (1) $\ln P = A - B/(T/K)$ (1a)

$\log P = A - B/(C + t/°C)$ (2) $\ln P = A - B/(C + t/°C)$ (2a)

$\log P = A - B/(C + T/K)$ (3)

$\log P = A - B/(T/K) - C\cdot\log(T/K)$ (4)

Stull 1947		McEachern et al. 1975			
summary of literature data		Langmuir free evaporation			
t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa
129.4	133.3	7.96	0.000653	eq. 1a	P/mmHg
165.8	666.6	12.02	0.001027	A	27.076
184.0	1333	16.08	0.002413	B	11021.64
203.5	2666	19.95	0.00329	temp range: 281.2–323.2 K	
224.2	5333	25.05	0.00652	enthalpy of fusion:	
238.7	7999	25.05	0.00656	$\Delta H_{fus}/(kJ\ mol^{-1}) = 18.58$	
256.0	13332	29.98	0.01145	enthalpy of sublimation:	
284.0	26664	35.08	0.0213	$\Delta H_{sub}/(kJ\ mol^{-1}) = 121.75$	
314.3	53329	40.02	0.0380	temp range: 281.2–323.3 K	
345.0	101325	45.09	0.0640	enthalpy of vaporization:	
		50.0	0.1074	$\Delta H_V/(kJ\ mol^{-1}) = 72.59$	
mp/°C	110.5				

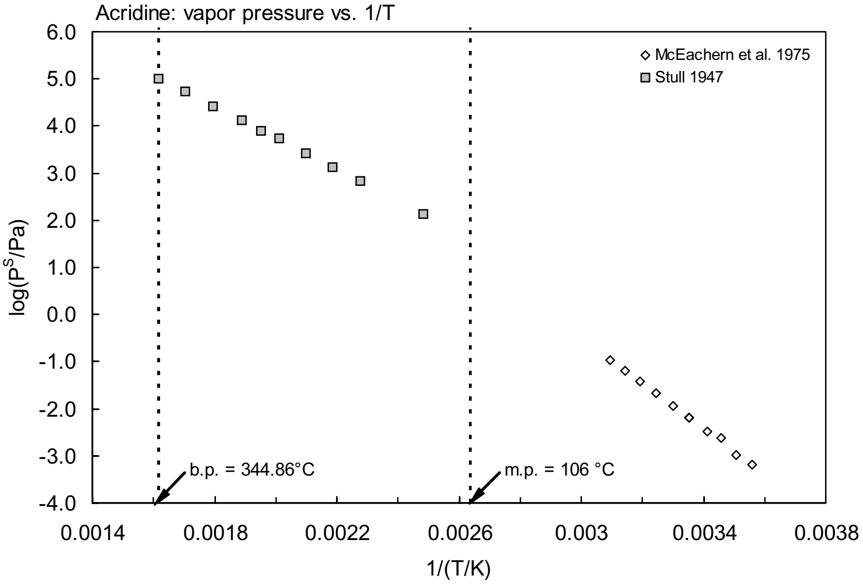


FIGURE 16.1.7.12.1 Logarithm of vapor pressure versus reciprocal temperature for acridine.

16.1.8 SULFUR COMPOUNDS

16.1.8.1 Carbon disulfide

$S{=}C{=}S$

Common Name: Carbon disulfide
Synonym: carbon disulphide
Chemical Name: carbon disulfide
CAS Registry No: 75-15-0
Molecular Formula: CS_2
Molecular Weight: 76.141
Melting Point (°C):
–112.1 (Lide 2003)
Boiling Point (°C):
46 (Lide 2003)
Density (g/cm^3):
1.2632 (20°C, Weast 19820–83)
1.26311, 1.2555 (20°C, 25°C, Riddick et al. 1986)
Molar Volume (cm^3/mol):
66.0 (calculated-Le Bas method at normal boiling point)
Enthalpy of Vaporization, ΔH_V (kJ/mol):
27.522, 26.736 (25°C, bp, Riddick et al. 1986)
Enthalpy of Sublimation, ΔH_{subl} (kJ/mol):
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
4.389 (Riddick et al. 1986)
Entropy of Fusion, ΔS_{fus} (J/mol K):
Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F: 1.0

Water Solubility (g/m^3 or mg/L at 25°C):
2100 (20°C, selected, Riddick et al. 1986)

Vapor Pressure (Pa at 25°C or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):
53329* (28°C, summary of literature data, temp range –73.8 to 46.5°C, Stull 1947)
47359* (24.582°C, comparative ebulliometry, measured range 3.6–80°C, Waddington et al. 1962)
log (P/mmHg) = 6.94194 – 1168.623/(241.534 + t/°C); temp range 3.6–80°C (Antoine eq., comparative ebulliometry, Waddington et al. 1962)
49704* (25.931°C, temp range –17.76 to 45.142°C, Boublik & Aim 1972; quoted, Boublik et al 1984)
log (P/kPa) = 6.86752 – 1169.022/(241.582 + t/°C), temp range 3.6–80°C (Antoine eq. derived from exptl. data of Waddington et al. 1949, Boublik et al. 1984)
log (P/kPa) = 6.03385 – 1151.908/(239.748 + t/°C), temp range –17.76 to 45.14°C (Antoine eq. derived from exptl. data, Boublik et al. 1984)
48210 (selected, Riddick et al. 1986)
log (P/kPa) = 6.06694 – 1168.623/(t/°C + 241.534) temp range not specified (Antoine eq., Riddick et al. 1986)
log (P_L/kPa) = 6.03694 – 1153.5/(–33.22 + T/K); temp range 256–319 K (Antoine eq.-I, Stephenson & Malanowski 1987)
log (P_L/kPa) = 6.07588 – 1174.112/(–30.896 + T/K); temp range 260–353 K (Antoine eq.-II, Stephenson & Malanowski 1987)
log (P_L/kPa) = 6 19814– 1231.307/(–26.024 + T/K); temp range 338–408 K (Antoine eq.-III, Stephenson & Malanowski 1987)
log (P_L/kPa) = 6 80466– 1278.903/(43.404 + T/K); temp range 388–497 K (Antoine eq.-IV, Stephenson & Malanowski 1987)
log (P_L/kPa) = 7.58592 – 2639.181/(165.312 + T/K); temp range 490–533 K (Antoine eq.-V, Stephenson & Malanowski 1987)

39597 (20°C, Howard 1990)

$\log (P/mmHg) = 25.1475 - 2.0349 \times 10^3/(T/K) - 6.7794 \cdot \log (T/K) + 3.4828 \times 10^{-3} \cdot (T/K) - 1.0105 \times 10^{-14} \cdot (T/K)^2$; temp range 162–552 K (vapor pressure eq., Yaws 1994)

Henry's Law Constant (Pa m^3/mol at 25°C or as indicated):

142	(calculated-P/C, Howard 1990)
1946	(calculated-vapor-liquid equilibrium VLE data, Yaws et al. 1991)
1577	(20°C, selected from literature experimentally measured data, Staudinger & Roberts 2001)

$\log K_{AW} = 3.485 - 1077/(T/K)$ (van't Hoff eq. derived from literature data, Staudinger & Roberts 2001)

Octanol/Water Partition Coefficient, log K_{OW}:

1.70–4.60	(Hansch & Leo 1985)
2.14	(recommended, Sangster 1993)
1.94	(recommended, Hansch et al. 1995)

Octanol/Air Partition Coefficient, log K_{OA}:

Bioconcentration Factor, log BCF or log K_B:

0.90	(calculated-solubility, Howard 1990)

Sorption Partition Coefficient, log K_{OC}:

1.80	(calculated-solubility, Howard 1990)

Environmental Fate Rate Constants, k, and Half-Lives, $t_{½}$:

Volatilization: $t_{½}$ = 2.6 h in a model river (Howard 1990)

Photolysis:

Oxidation:

Hydrolysis: $t_{½}$ = 1.1 yr at pH 9 in alkaline solution (Howard 1990)

Biodegradation:

Biotransformation:

Bioconcentration and Uptake and Elimination Rate Constants (k_1 and k_2):

Half-Lives in the Environment:

Air: $t_{½}$: = 9 d degraded by reacting with atomic oxygen and photochemically produced OH radicals (Howard 1990)

TABLE 16.1.8.1.1

Reported vapor pressures of carbon disulfide at various temperatures and the coefficients for the vapor pressure equations

$\log P = A - B/(T/K)$	(1)	$\ln P = A - B/(T/K)$	(1a)
$\log P = A - B/(C + t/°C)$	(2)	$\ln P = A - B/(C + t/°C)$	(2a)
$\log P = A - B/(C + T/K)$	(3)		
$\log P = A - B/(T/K) - C \cdot \log (T/K)$	(4)		

Stull 1947		**Waddington et al. 1962**		**Boublik & Aim 1972**	
summary of literature data		**comparative ebulliometry**		**in Boublik et a. 1984**	
t/°C	**P/Pa**	**t/°C**	**P/Pa**	**t/°C**	**P/Pa**
–73.8	133.3	3.588	19920	–17.76	6967
–54.3	666.6	8.772	25007	~12.358	9306
–44.7	1333	13.999	31168	~7.204	12046
–34.3	2666	19.269	38547	~3.286	14549
–22.5	5333	24.582	47359	1.223	17921
–15.3	7999	29.927	57803	5.076	21314

TABLE 16.1.8.1.1 (*Continued*)

Stull 1947		Waddington et al. 1962		Boublik & Aim 1972	
summary of literature data		comparative ebulliometry		in Boublik et a. 1984	
t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa
–5.1	13332	35.318	70109	9.448	25780
10.4	26664	40.751	84525	12.981	29923
28.0	53329	46.225	101325	17.168	35493
46.5	101325	51.744	120798	21.087	41470
		57.295	143268	25.931	49704
mp/°C	–110.8	62.885	169052	31.522	61295
		68.531	198530	38.041	77125
		74.218	232087	45.142	97853
		79.927	270110		
				bp/°C	46.217
		bp/°C	46.22		
		Antoine eq.		eq. 2	P/kPa
		eq. 2	P/mmHg	A	6.03385
		A	6.94194	B	1151.908
		B	1168.623	C	239.748
		C	241.534		
		data also fitted to Cox eq.			
			see ref.		

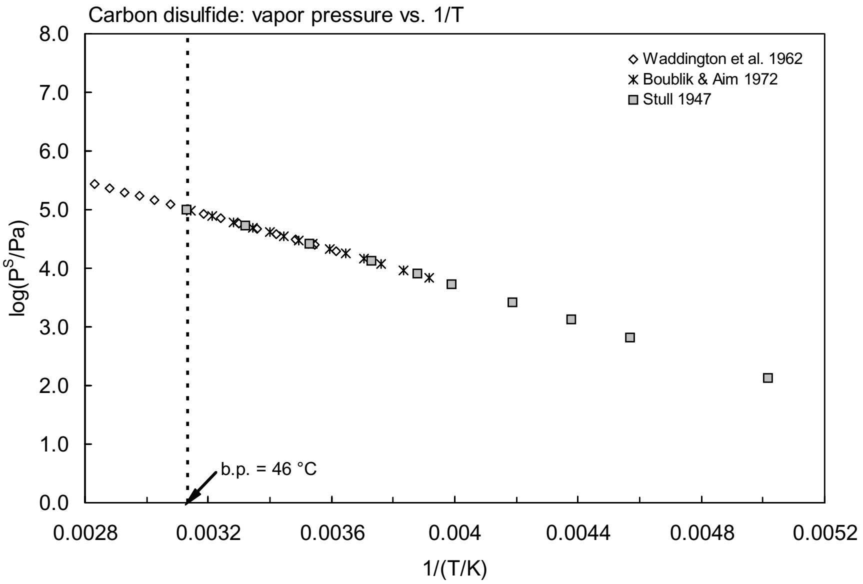
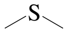


FIGURE 16.1.8.1.1 Logarithm of vapor pressure versus reciprocal temperature for carbon disulfide.

16.1.8.2 Dimethyl sulfide



Common Name: Dimethyl sulfide
Synonym: DMS, methyl sulfide, thiobismethane, 2-thiapropane
Chemical Name: dimethyl sulfide
CAS Registry No: 75-18-3
Molecular Formula: C_2H_6S, $(CH_3)_2S$
Molecular Weight: 62.134
Melting Point (°C):
–98.24 (Lide 2003)
Boiling Point (C):
37.33 (Riddick et al. 1986; Lide 2003)
Density (g/cm^3 at 25°C):
0.84825, 0.84230 (20°C, 25°C, Dreisbach 1961)
0.8423 (Riddick et al. 1986)
Molar Volume (cm^3/mol):
73.2 (Kamlet et al. 1986)
73.8 (20°C, calculated-density)
77.4 (calculated-Le Bas method at normal boiling point)
Dissociation Constant pK_{BH+}:
–6.99 (Riddick et al. 1986)
Enthalpy of Vaporization, ΔH_V (kJ/mol):
27.49, 26.82 (25°C, bp, Dreisbach 1961)
27.65, 27.0 (25°C, bp, Riddick et al. 1986)
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
7.99 (Riddick et al. 1986)
Entropy of Fusion, ΔS_{fus} (J/mol K):
Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F: 1.0

Water Solubility (g/m^3 or mg/L at 25°C):
15606 (Hine & Mookerjee 1975)
6300 (Verschueren 1983)
22000 (estimated-activity coefficient by headspace-GC, Przyjazny et al. 1983)
20000 (Riddick et al. 1986)
19600 (selected, Yaws et al. 1990)

Vapor Pressure (Pa at 25°C and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):
53174* (20.087°C, static method, measured range –22.547 to 20.087°C, Osborn et al. 1942)
log (P/mmHg) = 16.51798 – 1876.370/(T/K) – 3.04727 ± log (T/K); temp range –22.547 to 20.087°C (static method, Osborn et al. 1942)
53329* (18.7°C, summary of literature data, temp range –75.6 to 36°C, Stull 1947)
64650 (calculated from determined data, Dreisbach 1961)
log (P/mmHg) = 6.93138 – 1081.587/(229.746 + t/°C), temp range –50 to 130°C (Antoine eq. for liquid state, Dreisbach 1961)
64501* (interpolated-Antoine eq., temp range –47.4 to 58.319°C, Zwolinski & Wilhoit 1971)
log (P/mmHg) = 6.94879 – 1090.755/(230.799 + t/°C); temp range –47.4 to 58.319°C (liquid, Antoine eq., Zwolinski & Wilhoit 1971)
70300 (Hine & Mookerjee 1975)
log (P/mmHg) =[–0.2185 × 6742.3/(T/K)] + 7.589204; temp range –75 to 224.5°C (Antoine eq., Weast 1972–73)
56000 (20°C, Verschueren 1983)
64443 (calculated-Antoine eq. of Boublik et al. 1973, Przyjazny et al. 1983)
64460 (extrapolated-Antoine eq., Boublik et al. 1984)

log (P/kPa) = 6.27843 – 1196.875/(242.81 + t/°C), temp range –22.55 to 20.09°C (Antoine eq. from reported exptl. data, Boublik et al. 1984)
64470 (extrapolated-Antoine eq., Dean 1985, 1992)
log (P/mmHg) = 7.1509 – 1195.58/(242.68 + t/°C); temp range –22 to 20°C (Antoine eq., Dean 1985, 1992)
64650 (quoted, Riddick et al. 1986)
log (P/kPa) = 6.07369 – 1090.755/(230.799 + t/°C); temp range not specified (Antoine eq., Riddick et al. 1986)
64520 (interpolated, Antoine eq., Stephenson & Malanowski 1987)
log (P_L/kPa) = 6.07043 – 1088.851/(–42.594 + T/K); temp range 268–319 K (Antoine eq.-I, Stephenson & Malanowski 1987)
log (P_L/kPa) = 6.13042 – 1124.998/(–37.961 + T/K); temp range 307–379 K (Antoine eq.-II, Stephenson & Malanowski 1987)
log (P_L/kPa) = 6.42655 – 1344.329/(–7.456 + T/K); temp range 372–453 K (Antoine eq.-III, Stephenson & Malanowski 1987)
log (P_L/kPa) = 7.36327 – 2293.043/(130.243 + T/K); temp range 447–503 K (Antoine eq.-IV, Stephenson & Malanowski 1987)
log (P/mmHg) = 37.2604 – 2.4251 × 10^3/(T/K) –11.384·log (T/K) + 5.8122 × 10^{-3}·(T/K) + 8.5893 × 10^{-14}·$(T/K)^2$; temp range 175–503 K (vapor pressure eq., Yaws 1994)

Henry's Law Constant (Pa·m^3/mol at 25°C or as indicated and reported temperature dependence. Additional data at other temperatures designated * are compiled at the end of this section):
278.1 (1/K_{AW}, exptl., Hine & Mookerjee 1975)
298, 366.6 (calculated-group contribution, calculated-bond contribution, Hine & Mookerjee 1975)
165 (20°C, headspace-GC, Vitenberg et al. 1975)
180.4, 184.7, 173.5 (headspace-GC, concn. of 10, 1.0, 0.1 ppm by weight, Przyjazny et al. 1983)
180.4, 184.7, 173.5 (headspace-GC, concn. of 10, 1.0 and 0.1 ppm by weight, measured range 25–70°C, data presented in graph, Przyjazny et al. 1983)
log (1/K_{AW}) = 1637.3/(T/K) – 4.354; temp range 25–70°C (headspace-GC, concn of 10 ppm by weight, Przyjazny et al. 1983)
log (1/K_{AW}) = 1635.6/(T/K) – 4.358; temp range 25–70°C (headspace-GC, concn of 1.0 ppm by weight, Przyjazny et al. 1983)
log (1/K_{AW}) = 1598.2/(T/K) – 4.205; temp range 25–70°C (headspace-GC, concn of 0.1 ppm by weight, Przyjazny et al. 1983)
163.4 (quoted, Gaffney et al. 1987)
184, 1271 (quoted, calculated-molecular structure, Russell et al. 1992)
138 (20°C, selected from literature experimentally measured data, Staudinger & Roberts 1996)
233.0* (equilibrium headspace-GC, in seawater, measured range 18–44°C, Wong & Wang 1997)
61.97 (equilibrium headspace-GC, Marin et al. 1999)
155 (20°C, selected from literature experimentally measured data, Staudinger & Roberts 2001)
log K_{AW} = 3.556 – 1394/(T/K), (van't Hoff eq. derived from literature data, Staudinger & Roberts 2001)

Octanol/Water Partition Coefficient, log K_{OW}:

Octanol/Air Partition Coefficient, log K_{OA}:

Bioconcentration Factor, log BCF:

Sorption Partition Coefficient, log K_{OC}:

Environmental Fate Rate Constants, k, or Half-Lives, $t_{½}$:
Volatilization:
Photolysis:
Oxidation: rate constant k, for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO3} with NO_3 radical and k_{O3} with O_3 or as indicated, *data at other temperatures and/or the Arrhenius expression see reference:

k_{OH}* = $(9.80 \pm 1.2) \times 10^{-12}$ cm^3 $molecule^{-1}$ s^{-1} at 299.9 K, measured range 299.9–426.5 K (flash photolysis-resonance fluorescence, Atkinson et al. 1978)

k_{OH}* = $(8.28 \pm 0.87) \times 10^{-12}$ cm^3 $molecule^{-1}$ s^{-1} at 297 K, measured range 273–400 K by flash photolysis-resonance fluorescence, Kurylo 1978)

$k_{O(3P)}$* = 57×10^{-12} cm^3 $molecule^{-1}$ s^{-1} for gas-phase reaction with $O(^3P)$ atom at 296 K, measured range 252–493 K (Slagle et al. 1978)

k_{OH}* = $(4.26 \pm 0.56) \times 10^{-11}$ cm^3 $molecule^{-1}$ s^{-1} at 298 K, measured range 248–363 K (flash photolysis-resonance fluorescence, Wine et al. 1981)

k_{OH} = $(1.0 \pm 0.1) \times 10^{-11}$ cm^3 $molecule^{-1}$ s^{-1} with an estimated lifetime $\tau \sim 30$ h in the daytime, k_{NO3} = $(5.4 \pm 0.7) \times 10^{-13}$ cm^3 $molecule^{-1}$ s^{-1} with an estimated $\tau \sim 3$ h in the nighttime hours at 296 ± 2 K (Atkinson et al 1984)

$k_{O3} < 8 \times 10^{-19}$ cm^3 $molecule^{-1}$ s^{-1} with a loss rate of < 0.05 d^{-1}, $k_{OH} = 9.80 \times 10^{-12}$ cm^3 ± $molecule^{-1}$ s^{-1} with a loss rate of 0.8 d^{-1}, and $k_{NO3} = 9.7 \times 10^{-13}$ cm^3 $molecule^{-1}$ s^{-1} with a loss rate of 20 d^{-1} at room temp. (review, Atkinson & Carter 1984)

$k_{O3} < 8 \times 10^{-20}$ cm^3 $molecule^{-1}$ s^{-1} with a loss rate of < 0.004 d^{-1}, $k_{OH} = 6.3 \times 10^{-12}$ cm^3 $molecule^{-1}$ s^{-1} with a loss rate of 0.27 d^{-1}, and $k_{NO3} = 9.7 \times 10^{-13}$ cm^3 $molecule^{-1}$ s^{-1} with a loss rate of 20 d^{-1} at room temp. (review, Atkinson 1985)

k_{OH}* = $(4.09, 4.44) \times 10^{-12}$ cm^3 $molecule^{-1}$ s^{-1} at 298 K, measured range 267–397 K (flash photolysis-resonance fluorescence, Hynes et al. 1986)

k_{OH}* = $(3.60 \pm 0.2) \times 10^{-12}$ cm^3 $molecule^{-1}$ s^{-1} at 297 K, measured range 297–440 K by flash photolysis-resonance fluorescence; $k_{OH} = 9.36 \times 10^{-12}$ cm^3 $molecule^{-1}$ s^{-1} relative rate to *n*-hexane, $k_{OH} = 5.36 \times 10^{-12}$ cm^3 $molecule^{-1}$ s^{-1} relative rate to cyclohexane at 296 K (Wallington et al. 1986a)

k_{NO3}* = $(8.1 \pm 1.3) \times 10^{-13}$ cm^3 $molecule^{-1}$ s^{-1} at 298 K, measured range 280–350 K (flash photolysis-visible absorption, Wallington et al. 1986b)

k_{OH}* = $(5.50 \pm 1.0) \times 10^{-12}$ cm^3 $molecule^{-1}$ s^{-1} at 298 K, measured range 260–393 K (discharge flow-resonance fluorescence, Hsu et al. 1987)

$k_{OH} = (8.0 \pm 0.5) \times 10^{-12}$ cm^3 $molecule^{-1}$ s^{-1} at 298 K (Relative rate method, Barnes et al. 1989)

$k_{OH} = 3.60 \times 10^{-12}$ cm^3 $molecule^{-1}$ s^{-1}; k(soln) = 3.2×10^{-11} cm^3 $molecule^{-1}$ s^{-1} for reaction with OH radical in aqueous solution (Wallington et al. 1988)

k_{NO3}* = $(10.6 \pm 1.3) \times 10^{-13}$ cm^3 $molecule^{-1}$ s^{-1} at room temp., measured range 256–376 K (flow tube-laser induced fluorescence, Dlugokencky & Howard 1988)

k_{OH}* = 4.56×10^{-12} cm^3 $molecule^{-1}$ s^{-1} at 298 K (recommended, Atkinson 1989)

$k_{OH} = 4.57 \times 10^{-12}$ cm^3 $molecule^{-1}$ s^{-1}, $k_{NO3} = 9.77 \times 10^{-13}$ cm^3 $molecule^{-1}$ s^{-1} (Sabljic & Güsten 1990; Müller & Klein 1991)

k_{NO3}* = 1.07×10^{-12} cm^3 $molecule^{-1}$ s^{-1} at 298 K (recommended, Atkinson 1991)

Hydrolysis:

Biodegradation:

Biotransformation:

Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants:

Half-Lives in the Environment:

Air: atmospheric lifetime $\tau \sim 30$ h due to reaction with OH radical in the daytime and $\tau \sim 3$ h due to reaction at night with NO_3 radical (Atkinson et al. 1984);

calculated lifetimes, $\tau > 20$ d due to reaction with O_3 in 24-h, $\tau = 28$ h with OH radical during daytime and $\tau = 120$ min with NO_3 radical during nighttime in "clean" atmosphere; $\tau > 3$ d due to reaction with O_3 in 24-h, $\tau = 420$ min with OH radical in daytime and $\tau = 13$ min with NO_3 in nighttime in "moderately polluted" atmosphere (Winer et al. 1984)

estimated tropospheric chemical lifetimes, $\tau = 2$ d, 2 d and > 15 d for reactions with OH, NO_3 and O_3, respectively, under typical remote tropospheric conditions (Falbe-Hansen et al. 2000)

TABLE 16.1.8.2.1
Reported vapor pressures and Henry's law constants of dimethyl sulfide at various temperatures

Vapor pressure						Henry's law constant	
Osborn et al. 1942		Stull 1947		Zwolinski & Wilhoit 1971		Wong & Wang 1997	
static method-manometer		summary of literature data		selected values		equilibrium headspace-GC	
t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa	t/°C	H/(Pa m^3/mol)
							in seawater
–22.547	6994	–75.6	–133.3	47.4	1333	18	164.6
–10.028	13699	–58.0	666.6	–37.7	2666	25	233.0
0.096	22437	–49.2	1333	–31.5	4000	35	381.7
4.943	28042	–39.4	2666	–26.9	5333	44	556.4
15.138	43512	–28.4	5333	–23.03	6666		
20.087	53174	–21.4	7999	–19.85	7999	log K_{AW} = A – B/(T/K)	
		–12.0	13332	–14.62	10666		K_{AW}
mp/K	174.855	2.60	26664	–10.39	13332	A	4.806
bp/K	310.49	18.7	53329	–2.258	19998	B	1735
		36.0	101325	3.885	26664		
log P = A – B/(T/K) – C·log (T/K)				8.883	33331		
	P/mmHg	mp/°C	–83.2	13.127	39997		
A	16.51798			20.138	53329		
B	1876.370			25.860	66661		
C	3.04727			30.733	79993		
				35.000	93326		
ΔH_{fus}/(kJ mol^{-1}) = 7.985				35.794	95992		
ΔH_V/(kJ mol^{-1}) = 27.98				36.572	98659		
	at 291.06 K			37.333	101325		
				25	64501		
				Antoine eq.			
				log P = A – B/(C + t/°C)			
					P/mmHg		
				A	6.94879		
				B	1090.755		
				C	230.799		
				bp/°C	37.333		
				ΔH_V/(kJ mol^{-1}) =			
				at 25°C	27.65		
				at bp	26.92		

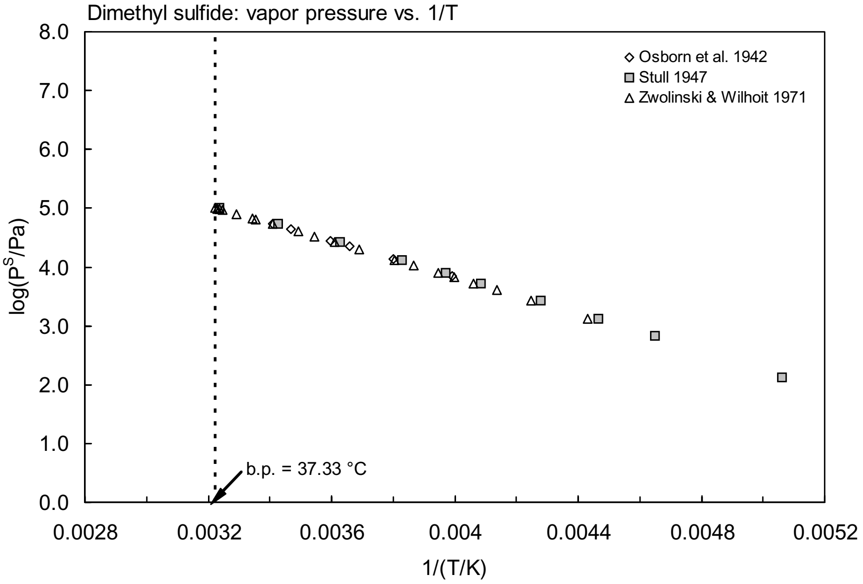


FIGURE 16.1.8.2.1 Logarithm of vapor pressure versus reciprocal temperature for dimethyl sulfide.

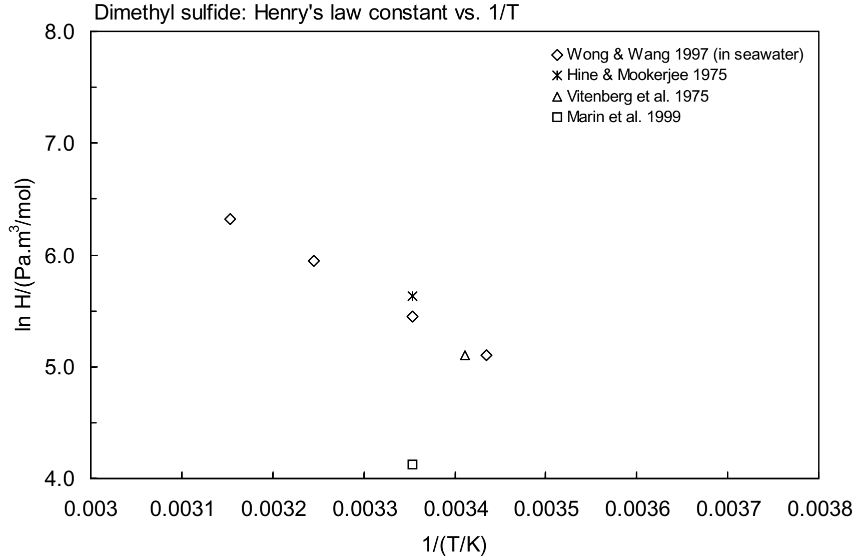
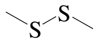


FIGURE 16.1.8.2.2 Logarithm of Henry's law constant versus reciprocal temperature for dimethyl sulfide.

16.1.8.3 Dimethyl disulfide



Common Name: Dimethyl disulfide
Synonym: 2,3-dithiabutane
Chemical Name: dimethyl didisulfide
CAS Registry No: 624-92-0
Molecular Formula: $C_2H_6S_2$, CH_3SSCH_3
Molecular Weight: 94.199
Melting Point (°C):
 –84.67 (Lide 2003)
Boiling Point (°C):
 109.74 (Lide 2003)
Density (g/cm^3):
 1.6025 (20°C, Weast 1982–83)
Dissociation Constant, pK_a:
Molar Volume (cm^3/mol):
 103.0 (calculated-Le Bas method at normal boiling point)
Enthalpy of Vaporization, ΔH_V (kJ/mol):
 38.37, 33.68 (25, bp, Zwolinski & Wilhoit 1971)
Enthalpy of Sublimation, ΔH_{subl} (kJ/mol):
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
Entropy of Fusion, ΔS_{fus} (J/mol K):
Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F: 1.0

Water Solubility (g/m^3 or mg/L at 25°C):
 3400 (estimated-activity coefficient by headspace-GC, Przyjazny et al. 1983)

Vapor Pressure (Pa at 25°C or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):
 3825* (static method, measured range 0–60°C, Scott et al. 1950)
 3813* (interpolated-Antoine eq., temp range 5.356–109.745°C, Zwolinski & Wilhoit 1971)
 $\log (P/mmHg) = 6.97792 - 1396.342/(218.863 + t/°C)$; temp range 5.356 –109.745°C (Antoine eq., Zwolinski & Wilhoit 1971)
 3850 (calculated-Antoine eq. of Boublik et al. 1973, Przyjazny et al. 1983)
 $\log (P/kPa) = 6.18000 - 1389.151/(223.184 + t/°C)$, temp range 0–60°C (Antoine eq. derived from Scott et al. 1950 data, Boublik et al. 1984)
 $\log (P/kPa) = 6.08703 - 1336.665/(217.767 + t/°C)$, temp range 61.4–128,6°C (Antoine eq. derived from Scott et al. 1950 data, Boublik et al. 1984)
 $\log (P_L/kPa) = 6.10018 - 1349.006/(-54.389 + T/K)$, temp range 297–402 K, (Antoine eq., Stephenson & Malanowski 1987)
 $\log (P/mmHg) = 36.232 - 3.1241 \times 10^3/(T/K) - 9.9328 \cdot \log (T/K) + 2.2831 \times 10^{-11} \cdot (T/K) + 3.1730 \times 10^{-6} \cdot (T/K)^2$; temp range 125–499 K (vapor pressure eq., Yaws 1994)

Henry's Law Constant (Pa m^3/mol at 25°C or as indicated):
 121 (20°C, headspace-GC, Vitenberg et al. 1975)
 112, 101 (headspace-GC, concn. of 10 and 1.0 ppm by weight, measured range 25–70°C, data presented in graph, Przyjazny et al. 1983)
 $\log (1/K_{AW}) = 1657.1/(T/K) - 4.211$; temp range 25–70°C (headspace-GC, concn of 10 ppm by weight, Przyjazny et al. 1983)
 $\log (1/K_{AW}) = 1854.4/(T/K) - 4.828$; temp range 25–70°C (headspace-GC, concn of 1.0 ppm by weight, Przyjazny et al. 1983)
 77.5 (20°C, selected from literature experimentally measured data, Staudinger & Roberts 1996, 2001)

$\log K_{AW} = 4.828 - 1384/(T/K)$, (van't Hoff eq. derived from literature data, Staudinger & Roberts 2001)

Octanol/Water Partition Coefficient, $\log K_{OW}$:

1.77	(shake flask, Log P Database, Hansch & Leo 1987)
1.77	(recommended, Sangster 1993)
1.77	(recommended, Hansch et al. 1995)

Octanol/Air Partition Coefficient, $\log K_{OA}$:

Bioconcentration Factor, log BCF or $\log K_B$:

Sorption Partition Coefficient, $\log K_{OC}$:

Environmental Fate Rate Constants, k, and Half-Lives, $t_{½}$, or Lifetimes, τ:

Volatilization:

Photolysis:

Oxidation: rate constant k, for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO3} with NO_3 radical and k_{O3} with O_3 or as indicated, *data at other temperatures see reference:

$k_{OH} = 2.40 \times 10^{-10}$ cm^3 molecule^{-1} s^{-1}, at 297 K (relative rate method, Cox & Sheppard 1980)

$k_{OH}* = (1.84 - 19.8) \times 10^{-10}$ cm^3 molecule^{-1} s^{-1}, at 298 K, measured range 255–377 K (flask photolysis-resonance fluorescence, Wine et al. 1984)

$k_{OH}* = 2.05 \times 10^{-10}$ cm^3 molecule^{-1} s^{-1}, at 298 K (tentative recommended, Atkinson 1985)

$k_{NO3}* = 4.9 \times 10^{-13}$ cm^3 molecule^{-1} s^{-1} at 298 K, measured range 280–350 K (flash photolysis-optical absorption, Wallington et al. 1986)

$k_{NO3}* = (7.3 \pm 1.5) \times 10^{-13}$ cm^3 molecule^{-1} s^{-1} at room temp., measured range 334–382 K (flow tube-laser induced fluorescence, Dlugokencky & Howard 1988)

$k_{NO3} = 7.0 \times 10^{-13}$ cm^3 molecule^{-1} s^{-1}, independent of temperature over the range ~300–380 K (recommended, Atkinson 1991)

Hydrolysis:

Biodegradation:

Biotransformation:

Bioconcentration and Uptake and Elimination Rate Constants (k_1 and k_2):

Half-Lives in the Environment:

TABLE 16.1.8.3.1
Reported vapor pressures of dimethyl disulfide at various temperatures and the coefficients for the vapor pressure equations

$\log P = A - B/(T/K)$ (1) $\ln P = A - B/(T/K)$ (1a)
$\log P = A - B/(C + t/°C)$ (2) $\ln P = A - B/(C + t/°C)$ (2a)
$\log P = A - B/(C + T/K)$ (3)
$\log P = A - B/(T/K) - C \cdot \log(T/K)$ (4)

Scott et al. 1950				Zwolinski & Wilhoit 1971			
static method-manometer		ebulliometric method		selected values			
t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa
0	904	61.411	19920	5.356	1333	106.905	93326
15	2230	67.301	25007	18.299	2666	107.872	95992
20	2936	73.234	31160	25.891	4000	108.819	98659
25	3825	79.201	38547	31.579	5333	109.745	101325
30	4930	85.218	47359	36.177	6666	25.0	3813
35	6301	91.283	57803	40.060	7999	Antoine eq.	
40	7975	97.393	70109	46.435	10666	eq. 2	P/mmHg
45	10007	103.54	84525	51.600	13332	A	6.97792
50	12448	109.738	101325	61.518	19998	B	1396.342
55	15359	115.984	120798	69.008	26664	C	218.863
60	18813	122.273	143268	75.099	33331	bp/°C	109.745
		128.611	169052	80.271	39997	$\Delta H_V/(kJ\ mol^{-1})$ =	
				88.812	53329	at 25°C	38.37
				95.780	66661	at bp	33.68
				101.712	79993		

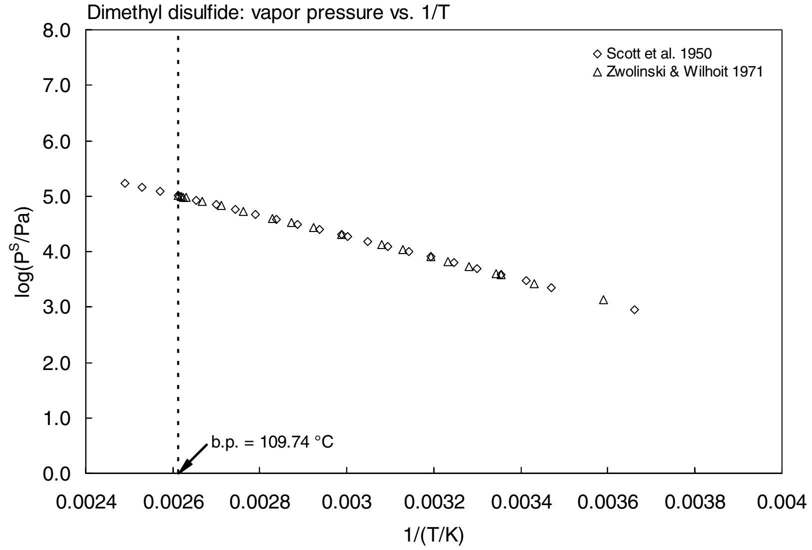
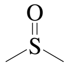


FIGURE 16.1.8.3.1 Logarithm of vapor pressure versus reciprocal temperature for dimethyl disulfide.

16.1.8.4 Dimethyl sulfoxide (DMSO)



Common Name: Dimethyl sulfoxide
Synonym: DMSO, sulfinylbismethane, methyl sulfoxide, methylsulfinylmethane, SQ 9453, DMS-70, DMS-90, Deltan, Demasorb, Demavet, Demeso, Dermasorb, Dolicur, Domoso, Dromisol, Gamasol 90, Hyadur, Rimso-50, Sclerosol, Somipront, Somtexan, Topsym
Chemical Name: dimethyl sulfoxide
CAS Registry No: 67-68-5
Molecular Formula: C_2H_6OS, $(CH_3)_2SO$
Molecular Weight: 78.133
Melting Point (°C):
17.89 (Lide 2003)
Boiling Point (°C):
189.0 (Stephenson & Malanowski 1987; Lide 2003)
Density (g/cm^3 at 25°C):
1.1014 (Weast 1982–83)
Molar Volume (cm^3/mol):
85.7 (calculated-Le Bas method at normal boiling point)
Dissociation Constant pK_a:
1.4 (Riddick et al. 1986)
Enthalpy of Vaporization, ΔH_V (kJ/mol):
52.88, 43.14 (25°C, bp, Riddick et al. 1986)
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
14.368 (Riddick et al. 1986)
Entropy of Fusion, ΔS_{fus} (J/mol K):
Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F: 1.0

Water Solubility (g/m^3 or mg/L at 25°C):
253000 (Riddick et a. 1986)

Vapor Pressure (Pa at 25°C or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):
80.0* (gas saturation, measured range 20–50°C, Douglas 1948)
$\log (P/mmHg) = 26.49588 - 3539.32/(T/K) - 6.000 \pm \ln (T/K)$; temp range 20–50°C (gas saturation, Douglas 1948)
460* (52.35°C, Hg manometer, measured range 325.5–442.1 K, Jakli & van Hook 1972)
$\ln (P/mmHg) = 17.4922 - 4517.79/(T/K - 47.2583)$; temp range 291.7–463 K (Hg manometer, Antoine eq. with literature data, Jakli & van Hook 1972)
56.0 (20°C, Verschueren 1983)
80.9 (extrapolated-Antoine eq., Boublik et al. 1984)
$\log (P/kPa) = 6.64816 - 1922.32/(223.353 + t/°C)$; temp range 52.4–168.95°C (Antoine eq. from reported exptl. data of Jakli & von Hook 1972, Boublik et al. 1984)
80.0 (selected, Riddick et al. 1986)
$\log (P/kPa) = 6.72161 - 1962.06/(225.892 + t/°C)$; temp range not specified (Antoine eq., Riddick et al. 1986)
79.5 (extrapolated-Antoine eq., Stephenson & Malanowski 1987)
$\log (P_L/kPa) = 6.72167 - 1962.05/(-47.258 + T/K)$; temp range 305–464 K (Antoine eq., Stephenson & Malanowski 1987)
$\log (P/mmHg) = 45.4653 - 4.0439 \times 10^3/(T/K) - 13.21 \cdot \log (T/K) + 1.0981 \times 10^{-7} \cdot (T/K) + 6.4155 \times 10^{-6} \cdot (T/K)^2$; temp range 292–465 K (vapor pressure eq., Yaws et al. 1994)

Henry's Law Constant (Pa·m^3/mol):

Octanol/Water Partition Coefficient, log K_{OW}:

–1.35	(shake flask, Hansch & Leo 1979, 1987)
–0.85	(calculated-UNIFAC activity coefficients, Banerjee & Howard 1988)
–1.35	(recommended, Sangster 1989)
–1.35	(recommended, Hansch et al. 1995)

Octanol/Air Partition Coefficient, log K_{OA}:

4.96	(head-space GC, Abraham et al. 2001)

Bioconcentration Factor, log BCF:

Sorption Partition Coefficient, log K_{OC}:

Environmental Fate Rate Constants, k, or Half-Lives, $t_{½}$:

Volatilization:

Photolysis:

Oxidation: rate constant k, for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO3} with NO_3 radical and k_{O3} with O_3 or as indicated, *data at other temperatures see reference:

$k_{OH} = (6.2 \pm 2.2) \times 10^{-11}$ cm^3 molecule^{-1} s^{-1}; $k_{NO3} = (1.7 \pm 0.3) \times 10^{-13}$ cm^3 molecule^{-1} s^{-1}; $k_{O3} < 5.0 \times 10^{-19}$ cm^3 ± molecule^{-1} s^{-1} at room temp (Barnes et al. 1989)

$k_{OH} = (62 \pm 25) \times 10^{-12}$ cm^3 molecule^{-1} s^{-1} at 300 K (Atkinson 1989)

$k_{OH} = (1.0 \pm 0.3) \times 10^{-12}$ cm^3 molecule^{-1} s^{-1} at room temp (Hynes & Wine 1996)

$k_{OH} = (8.7 \pm 1.6) \times 10^{-11}$ cm^3 molecule^{-1} s^{-1} at room temp. (Urbanski et al. 1998)

$k_{OH} = (5.9 \pm 1.5) \times 10^{-11}$ cm^3 ± molecule^{-1} s^{-1} with tropospheric lifetime τ = 5 h, $k_{NO3} = (5.0 \pm 3.8) \times 10^{-13}$ cm^3 molecule^{-1} s^{-1} with tropospheric lifetime τ = 3 d; $k_{O3} < 1.0 \times 10^{-19}$ cm^3 ± molecule^{-1} s^{-1} with tropospheric lifetime τ > 150 d and kCl = $(7.4 \pm 1.0) \times 10^{-11}$ cm^3 molecule^{-1} s^{-1} for reaction wit Cl atoms with tropospheric lifetime τ = 62 d at room temp and 740 torr (Relative rate method, Falbe-Hansen et al. 2000)

Hydrolysis: k = 6.60×10^9 M^{-1} s^{-1} (Buxton et al. 1986)

Biodegradation:

Biotransformation:

Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants:

Half-Lives in the Environment:

Air: estimated tropospheric chemical lifetimes, τ = 5 h, 3 d and > 150 d for reactions with OH, NO_3 and O_3, respectively, under typical remote tropospheric conditions (Falbe-Hansen et al. 2000)

TABLE 16.1.8.4.1
Reported vapor pressures of dimethyl sulfoxide at various temperatures and the coefficients for the vapor pressure equations

log P = A − B/(T/K)	(1)	ln P = A − B/(T/K)	(1a)
log P = A − B/(C + t/°C)	(2)	ln P = A − B/(C + t/°C)	(2a)
log P = A − B/(C + T/K)	(3)	log P = A − B/(C + T/K)	(3a)
log P = A − B/(T/K) − C·log (T/K)	(4)	ln P = A − B/(T/K) − C·ln(T/K)	(4a)

Douglas 1948		Jakli & van Hook 1972			
gas saturation		mercury manometer			
t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa
20	55.6	52.35	460	140.15	22905
25	80.0	56.25	573	148.05	29471
30	113.7	61.45	767	162.15	47036
35	159.3	66.15	993	168.95	56342
40	220.8	74.85	1560	eq. 3	P/mmHg
45	302.6	79.95	2000	A	17.4922
50	409.3	85.65	2653	B	4517.79
		90.26	3293	C	47.2583
eq. 4	P/mmHg	96.05	4226		
A	29.49558	100.45	5106		
B	3539.32	100.55	5133		
C	6.0000	104.95	6246		
		111.95	8359		
bp/°C	192	117.95	10452		
ΔH_V = 52.89 kJ/mol		127.45	14745		

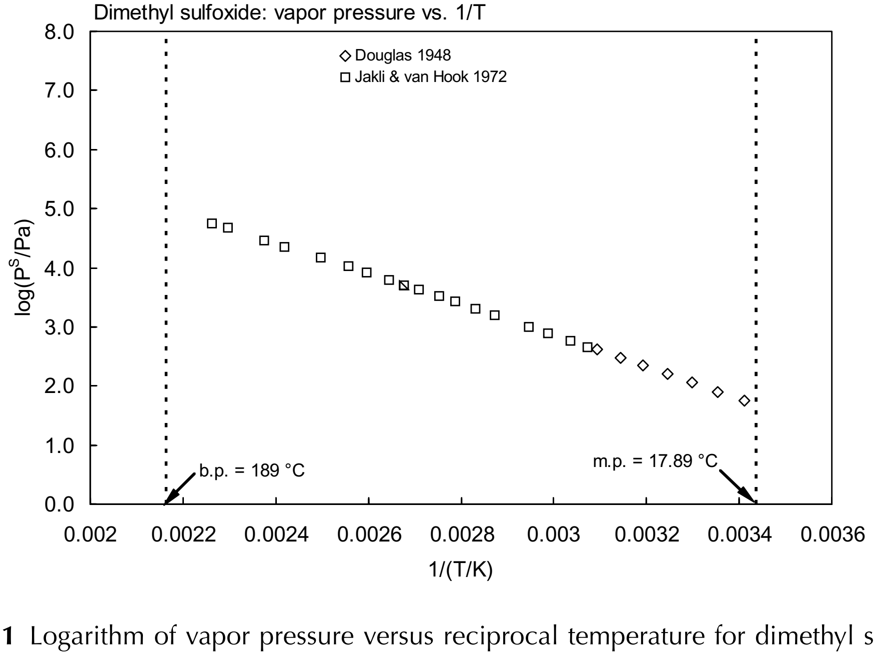
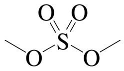


FIGURE 16.1.8.4.1 Logarithm of vapor pressure versus reciprocal temperature for dimethyl sulfoxide.

16.1.8.5 Dimethyl sulfate



Common Name: Dimethyl sulfate
Synonym: sulfuric acid dimethyl ester, DMS
Chemical Name: dimethyl sulfate
CAS Registry No: 77-78-1
Molecular Formula: $C_2H_6O_4S$, $CH_3O\text{-}SO_2\text{-}OCH_3$
Molecular Weight: 126.132
Melting Point (°C):

–27	(Lide 2003)

Boiling Point (°C):

188	(decomposes, Lide 2003)

Density (g/cm^3 at 20°C):

1.3322	(Dean 1985)

Molar Volume (cm^3/mol):

95.0	(20°C, Stephenson & Malanowski 1987)
109.7	(calculated-Le Bas method at normal boiling point)

Dissociation Constant pK_a:
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
Entropy of Fusion, ΔS_{fus} (J/mol K):
Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F: 1.0

Water Solubility (g/m^3 or mg/L at 25°C):

28000	(hydrolyzes, Verschueren 1983; Dean 1985)
28000	(18°C, Budavari 1989)

Vapor Pressure (Pa at 25°C and reported temperature dependence equations):

< 133	(20°C, Verschueren 1983)
128	(extrapolated, Antoine eq., Stephenson & Malanowski 1987)

$\log (P_L/\text{kPa}) = 7.28235 - 2437.54/(T/K)$, temp range 340–470 K, (Antoine eq., Stephenson & Malanowski 1987)
$\log (P/\text{mmHg}) = 33.9406 - 3.853 \times 10^3/(T/K) - 8.5921\cdot\log (T/K) - 1.1705 \times 10^{-10}\cdot(T/K) + 8.226 \times 10^{-7}\cdot(T/K)^2$; temp range 241–758 K (vapor pressure eq., Yaws 1994)

Henry's Law Constant (Pa·m^3/mol):

Octanol/Water Partition Coefficient, log K_{OW}:

Octanol/Air Partition Coefficient, log K_{OA}:

Bioconcentration Factor, log BCF:

Sorption Partition Coefficient, log K_{OC}:

Environmental Fate Rate Constants, k, or Half-Lives, $t_{1/2}$:
Volatilization:
Photolysis:
Oxidation: atmospheric photooxidation $t_{1/2}$ = of 36.5–365 h, based on estimated rate constant for the vapor-phase reaction with OH radical in air (Atkinson 1987; quoted, Howard et al. 1991).
Hydrolysis: first order hydrolysis rate constant $k = 1.6 \times 10^{-4}\ s^{-1}$ at pH 7 and 25°C with $t_{1/2}$ = 1.2 h (Mabey & Mill 1978; quoted, Howard et al. 1991).

Biodegradation: aqueous aerobic biodegradation $t_{1/2}$ ~ 168–672 h and aqueous anaerobic biodegradation $t_{1/2}$ ~ 672–2688 h (Howard et al. 1991).

Biotransformation:

Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants:

Half-Lives in the Environment:

Air: $t_{1/2}$ = 36.5–365 h, based on photooxidation half-life in air from estimated rate constant for the vapor phase reaction with hydroxyl radical in air (Atkinson 1987; quoted, Howard et al. 1991);

atmospheric transformation lifetime (reaction with liquid water) estimated to be < 1 d (Kelly et al. 1994).

Surface water: $t_{1/2}$ = 1.2–12 h, based on overall hydrolysis rate constant for pH 7 at 25°C (Mabey & Mill 1978; quoted, Howard et al. 1991) and for complete hydrolysis in neutral, slightly basic, and acidic aqueous solutions (Lee et al. 1980; quoted, Howard et al. 1991).

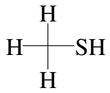
Groundwater: $t_{1/2}$ = 1.2–12 h, based on overall hydrolysis rate constant for pH 7 at 25°C (Mabey & Mill 1978; quoted, Howard et al. 1991) and for complete hydrolysis in neutral, slightly basic, and acidic aqueous solutions (Lee et al. 1980; quoted, Howard et al. 1991).

Sediment:

Soil: $t_{1/2}$ = 1.2–12 h, based on overall hydrolysis rate constant for pH 7 at 25°C and for complete hydrolysis in neutral, slightly basic, and acidic aqueous solutions (Howard et al. 1991).

Biota:

16.1.8.6 Methanethiol



$$\begin{array}{c} H \\ H-\!\!\!\!-\!\!\!\!\!\!\!\!\;\;\;SH \\ H \end{array}$$

Common Name: Methanethiol
Synonym: methyl mercaptan
Chemical Name: methanethiol
CAS Registry No: 74-93-1
Molecular Formula: CH_4S, CH_3SH
Molecular Weight: 48.108
Melting Point (°C):
–123 (Weast 1982–83; Lide 2003)
Boiling Point (°C):
5.9 (Lide 2003)
Density (g/cm^3):
0.8665 (20°C, Weast 1982–83)
Dissociation Constant, pK_a:
Molar Volume (cm^3/mol):
55.3 (20°C, Stephenson & Malanowski 1987)
55.2 (calculated-Le Bas method at normal boiling point)
Enthalpy of Vaporization, ΔH_V (kJ/mol):
23.8, 24.57 (25, bp, Zwolinski & Wilhoit 1971)
Enthalpy of Sublimation, ΔH_{subl} (kJ/mol):
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
Entropy of Fusion, ΔS_{fus} (J/mol K):
Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F: 1.0

Water Solubility (g/m^3 or mg/L at 25°C):
39000 (estimated-activity coefficient by headspace-GC/FID, Przyjazny et al. 1983)

Vapor Pressure (Pa at 25°C or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):
101410* (5.977°C, static method-Hg manometer, measured range –51.3 to 5.977°C, Russell et al. 1942)
$\log (P/mmHg) = 18.27429 - 1769.05/(T/K) - 3.70248 \pm \log (T/K)$; temp range 221.88–279.137 K (static method, Russell, et al. 1942)
101325* (8.7°C, summary of literature data, temp range –90.7 to 7.8°C, Stull 1947)
202117* (extrapolated, summary of literature data, temp range –70.3 to 5.956°C, Zwolinski & Wilhoit 1971)
$\log (P/mmHg) = 7.03163 - 1015.547/(238.706 + t/°C)$; temp range –70.3 to 24.694°C (Antoine eq., Zwolinski & Wilhoit 1971)
202346 (calculated-Antoine eq. of Boublik et al. 1973, Przyjazny et al. 1983)
$\log (P/kPa) = 6.18991 - 1030.496/(248.330 + t/°C)$, temp range –51.28 to 5.977°C, (Antoine eq. derived from Russell et al. 1942 data, Boublik et al. 1984)
$\log (P_L/kPa) = 6.19283 - 1031.216/(-32.916 + T/K)$, temp range 221–283 K, (Antoine eq.-I, Stephenson & Malanowski 1987)
$\log (P_L/kPa) = 6.19219 - 1030.918/(-32.845 + T/K)$, temp range 222–279 K, (Antoine eq.-II, Stephenson & Malanowski 1987)
$\log (P_L/kPa) = 6.13699 - 1006.199/(-35.529 + T/K)$, temp range 267–359 K, (Antoine eq.-III, Stephenson & Malanowski 1987)
$\log (P_L/kPa) = 6.53487 - 1278.361/(5.318 + T/K)$, temp range 345–424 K, (Antoine eq.-IV, Stephenson & Malanowski 1987)

Henry's Law Constant (Pa m^3/mol at 25°C or as indicated):

247 (distilled water, headspace-GC/FID, measured range 25–70°C, data in graph, Przyjazny et al. 1983)
Log (1/K_{AW}) = 1347.1/(T/K) – 3.537; temp range 25–70°C (headspace-GC, Przyjazny et al. 1983)
187 (20°C, selected from literature experimentally measured data, Staudinger & Roberts 1996)
300 (20°C, selected from literature experimentally measured data, Staudinger & Roberts 2001)
log K_{AW} = 3.249 – 1219/(T/K), (van't Hoff eq. derived from literature data, Staudinger & Roberts 2001)

Octanol/Water Partition Coefficient, log K_{OW}:

Octanol/Air Partition Coefficient, log K_{OA}:

Bioconcentration Factor, log BCF or log K_B:

Sorption Partition Coefficient, log K_{OC}:

Environmental Fate Rate Constants, k, and Half-Lives, $t_{½}$:

Volatilization:
Photolysis:
Oxidation: rate constant k, for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO3} with NO_3 radical and k_{O3} with O_3 or as indicated, *data at other temperatures see reference:

k_{OH}* = 3.39 × 10^{-11} cm^3 molecule^{-1} s^{-1} at 299.8 K, measured range 300–423 K (flash photolysis-resonance fluorescence, Atkinson et al. 1977)
k_{OH}* = 3.37 × 10^{-11} cm^3 molecule^{-1} s^{-1} at 298 K, measured range 244–366 K (flash photolysis-resonance fluorescence, Wine et al. 1981)
k_{OH} = 9.7 × 10^{-11} cm^3 molecule^{-1} s^{-1} at 297 K (relative rate method, Cox & Sheppard 1980)
k_{OH} = 2.01 × 10^{-11} cm^3 molecule^{-1} s^{-1} at 293 K (discharge flow-EPR, Mac Leod et al. 1983)
k_{OH} = 2.56 × 10^{-11} cm^3 molecule^{-1} s^{-1} at 296 K (discharge flow-RF, Lee & Tang 1983)
k_{OH}* = (3.04 – 32.5) × 10^{-11} cm^3 molecule^{-1} s^{-1} at 298 K, measured range 254–430 K ((flash photolysis-resonance fluorescence, Wine et al. 1984)
k_{OH}* = 3.31 × 10^{-11} cm^3 molecule^{-1} s^{-1} at 298 K (recommended, Atkinson 1985)
k_{NO3} = 9.2 × 10^{-13} cm^3 ± molecule^{-1} s^{-1}, independent of temperature over the range 250–370 K (IUPAC recommended, Atkinson et al. 1989)
k_{NO3} = 9.3 × 10^{-13} cm^3 ± molecule^{-1} s^{-1}, independent of temperature over the range 254–367 K (Atkinson 1991)

Hydrolysis:
Biodegradation:
Biotransformation:
Bioconcentration and Uptake and Elimination Rate Constants (k_1 and k_2):

Half-Lives in the Environment:

TABLE 16.1.8.6.1
Reported vapor pressures of methanethiol at various temperatures and the coefficients for the vapor pressure equations

$\log P = A - B/(T/K)$	(1)	$\ln P = A - B/(T/K)$	(1a)
$\log P = A - B/(C + t/°C)$	(2)	$\ln P = A - B/(C + t/°C)$	(2a)
$\log P = A - B/(C + T/K)$	(3)		
$\log P = A - B/(T/K) - C \cdot \log (T/K)$	(4)		

Russell et al. 1942		**Stull 1947**		**Zwolinski & Wilhoit 1971**			
static-Hg manometer		**summary of literature data**		**selected values**			
t/°C	**P/Pa**	**t/°C**	**P/Pa**	**t/°C**	**P/Pa**	**t/°C**	**P/Pa**
–53.28	5484	–90.7	133.3	–70.3	1333	3.869	93326
–23.872	26859	–75.3	666.6	–61.5	2666	4.580	95992
–9.474	53235	–67.5	1333	–55.9	4000	5.275	98659
0.029	79913	–58.8	2666	–51.7	5333	5.956	101325
5.977	101410	–49.2	5333	–48.3	6666	25.0	202117
		–43.1	7999	–45.4	7999	eq. 2	P/mmHg
bp/K	279.12	–34.8	13332	–40.7	10666	A	7.03163
		–22.1	26664	–36.87	13332	B	1015.547
eq. 4	P/mmHg	–7.80	53329	–29.55	19998	C	238.706
A	18.27429	8.70	101325	–24.03	26664	bp/°C	5.956
B	1769.05			–19.54	33331	ΔH_V/(kJ mol^{-1}) =	
C	3.70248	mp/°C	–	–15.73	39997	at 25°C	23.8
				–9.44	53329	at bp	24.57
				–4.31	66661		
				0.051	79993		

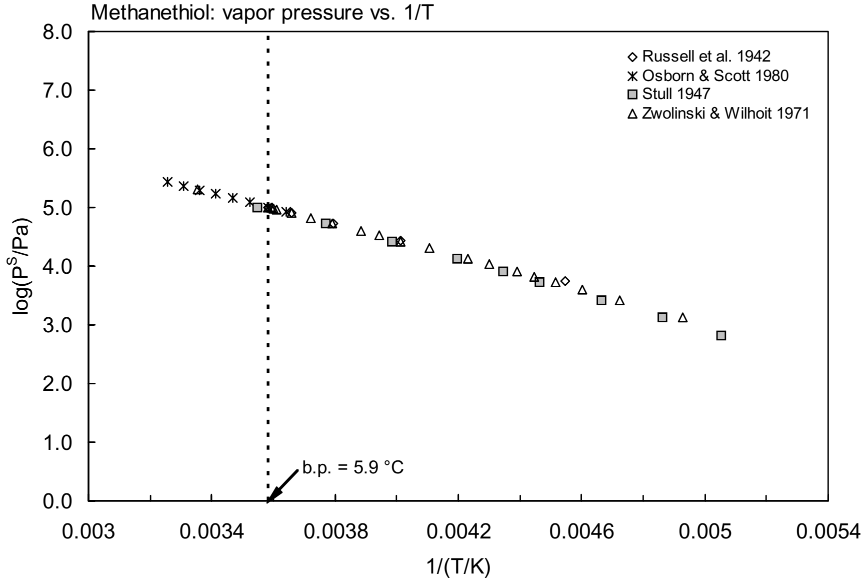
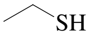


FIGURE 16.1.8.6.1 Logarithm of vapor pressure versus reciprocal temperature for methanethiol.

16.1.8.7 Ethanethiol



Common Name: Ethanethiol
Synonym: ethyl mercaptan, thioethyl alcohol, ethylhydrosulfide
Chemical Name: ethanethiol
CAS Registry No: 75-08-1
Molecular Formula: C_2H_6S, C_2H_5SH
Molecular Weight: 62.134
Melting Point (C):
–147.88 (Lide 2003)
Boiling Point (°C):
35.0 (Stull 1947; Dreisbach 1961; Weast 1982–83; Boublik et al. 1984; Dean 1985; Lide 2003)
Density (g/cm^3 at 20°C):
0.83914, 0.83316 (20°C, 25°C, Dreisbach 1961)
0.8391 (Weast 1982–83)
0.8315 (25°C, Dean 1985)
Molar Volume (cm^3/mol):
74.0 (20°C, calculated-density)
77.4 (calculated-Le Bas method at normal boiling point)
Dissociation Constant pK_a:
Enthalpy of Vaporization, ΔH_V (kJ/mol):
27.30, 26.78 (25°C, bp, Dreisbach 1961)
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
Entropy of Fusion, ΔS_{fus} (J/mol K):
Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F: 1.0

Water Solubility (g/m^3 or mg/L at 25°C):
15600 (Hine & Mookerjee 1975)
12000 (estimated-activity coefficient by headspace-GC/FID, Przyjazny et al. 1983)
15000 (Verschueren 1983)
6800 (Dean 1985)
6760 (20°C, Budavari 1989)
14800 (selected, Yaws et al. 1990)

Vapor Pressure (Pa at 25°C or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):
74630* (interpolated-regression of tabulated data, temp range –76.7 to 35°C, Stull 1947)
70110* (24.933°C, ebulliometric method, measured range 0.405–66.14°C, McCullough et al. 1952)
log (P/mmHg) = 6.95206 – 1084.531/(231.385 + t/°C); temp range 0.405–66.14°C (Antoine eq., ebulliometric method, McCullough et al. 1952)
70300 (calculated from determined data, Dreisbach 1961)
log (P/mmHg) = 6.95206 – 1084.531/(231.385 + t/°C); temp range –40 to 100°C (Antoine eq. for liquid state, Dreisbach 1961)
log (P/mmHg) = 6.95205 – 1084.531/(T/K + 231.385) (Antoine eq., Osborn & Douslin 1966)
66660*, 70290 (23.613°C, interpolated-Antoine eq., Zwolinski & Wilhoit 1971)
log (P/mmHg) = 6.95026 – 1084.531/(231.385 + t/°C); temp range –49.2 to 55.83°C (liquid, Antoine eq., Zwolinski & Wilhoit 1971)
70320 (calculated-Antoine eq. of Boublik et al. 1973, Przyjazny et al. 1983)
58660 (20°C, Verschueren 1983)
70290 (interpolated-Antoine eq., Boublik et al. 1984)
log (P/kPa) = 6.0768 – 1084.455/(231.374 + t/°C), temp range 0.405–66.115°C (Antoine eq. from reported exptl. data of McCullough et al. 1952, Boublik et al. 1984)
70300 (calculated-Antoine eq., Dean 1985, 1992)

log (P/mmHg) = 6.95206 – 1084.531/(231.39 + t/°C); temp range –49 to 56°C (Antoine eq., Dean 1985, 1992)
log (P_L/kPa) = 6.07243 – 1081.984/(–42.085 + T/K), temp range 273–340 K (Antoine eq.-I, Stephenson & Malanowski 1987)
log (P_L/kPa) = 6.08253 – 1086.982/(–41.517 + T/K), temp range 273–313 K (Antoine eq.-II, Stephenson & Malanowski 1987)
log (P_L/kPa) = 6.10279 – 1099.374/(–39.807 + T/K), temp range 303–375 K (Antoine eq.-III, Stephenson & Malanowski 1987)
log (P_L/kPa) = 6.42565 – 1328.598/(–6.231 + T/K), temp range 365–448 K (Antoine eq.-IV, Stephenson & Malanowski 1987)
log (P_L/kPa) = 7.84948 – 2874.377/(200.657 + T/K), temp range 442–499 K (Antoine eq.-V, Stephenson & Malanowski 1987)
log (P/mmHg) = 29.2763 – 2.2725 × 10^3/(T/K) – 7.7769·log (T/K) – 3.8954 × 10^{-11}·(T/K) + 3.517 × 10^{-6}·$(T/K)^2$; temp range 125–499 K (vapor pressure eq., Yaws 1994)

Henry's Law Constant (Pa·m^3/mol at 25°C or as indicated and reported temperature dependence equations):
278.1 (exptl., Hine & Mookerjee 1975)
298, 366.6 (calculated-group contribution, calculated-bond contribution, Hine & Mookerjee 1975)
451 (20°C, headspace-GC, Vitenberg et al. 1975)
360.3 (distilled water, headspace-GC/FID, measured range 25–70°C, data in graph, Przyjazny et al. 1983)
log ($1/K_{AW}$) = 1486.1/(T/K) – 4.147; temp range 25–70°C (headspace-GC, Przyjazny et al. 1983)
292.4 (computed-vapor-liquid equilibrium VLE data, Yaws et al. 1991)
278, 96.44 (quoted, calculated-molecular structure, Russell et al. 1992)
292.5 (20°C, selected from literature experimentally measured data, Staudinger & Roberts 1996, 2001)
log K_{AW} = 4.147 – 1486/(T/K) (van't Hoff eq. derived from literature data, Staudinger & Roberts 2001)

Octanol/Water Partition Coefficient, log K_{OW}:

Octanol/Air Partition Coefficient, log K_{OA}:

Bioconcentration Factor, log BCF:

Sorption Partition Coefficient, log K_{OC}:

Environmental Fate Rate Constants, k, or Half-Lives, $t_{½}$:
Volatilization:
Photolysis:
Oxidation: rate constant k, for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO3} with NO_3 radical and k_{O3} with O_3 or as indicated, *data at other temperatures and the Arrhenius expression see reference:
$k_{O(3P)}$* = 3.0 × 10^{-12} cm^3 ± $molecule^{-1}$ s^{-1} for gas-phase reaction with O(^{3}P) atom at 298 K, measured range 257–495 K (Slagle et al. 1978)
k_{OH} = 3.67 × 10^{-11} cm^3 $molecule^{-1}$ s^{-1} at 296 K (discharge flow-RF, Lee & Tang 1983)
k_{OH} = 2.70 × 10^{-11} cm^3 $molecule^{-1}$ s^{-1} at 293 K (discharge flow-EPR, Mac Leod et al. 1984)
k_{OH}* = 4.26 × 10^{-11} cm^3 $molecule^{-1}$ s^{-1} at 298 K, measured range 252–425 K (flash photolysis-resonance fluorescence, Wine et al. 1984)
k_{OH}* = 4.65 × 10^{-11} cm^3 $molecule^{-1}$ s^{-1} at 298 K (recommended, Atkinson 1985)
k_{OH} = 4.65 × 10^{-11} cm^3 $molecule^{-1}$ s^{-1} at 300 K (relative rate method, Barnes et al. 1986)
k_{OH}* = 4.68 × 10^{-11} cm^3 $molecule^{-1}$ s^{-1} at 298 K (recommended, Atkinson 1989)
k_{NO3} = (1.21 ± 0.28) × 10^{-12} cm^3 $molecule^{-1}$ s^{-1} at 298K (relative rate method, Mac Leod et al. 1986; quoted, Atkinson 1991)
Hydrolysis:
Biodegradation:
Biotransformation:
Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants:

Half-Lives in the Environment:

TABLE 16.1.8.7.1
Reported vapor pressures of ethanethiol at various temperatures and the coefficients for the vapor pressure equations

$\log P = A - B/(T/K)$ (1) $\ln P = A - B/(T/K)$ (1a)
$\log P = A - B/(C + t/°C)$ (2) $\ln P = A - B/(C + t/°C)$ (2a)
$\log P = A - B/(C + T/K)$ (3)
$\log P = A - B/(T/K) - C \cdot \log (T/K)$ (4)

Stull 1947		McCullough et al. 1952		Zwolinski & Wilhoit 1971			
summary of literature data		ebulliometry		selected values			
t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa
–76.7	133.3	0.405	25007	–49.2	1333	eq. 2	P/mmHg
–59.1	666.6	5.236	31160	–39.5	2666	A	6.95206
–50.2	1333	10.111	38547	–33.3	4000	B	1084.531
–40.7	2666	15.017	47359	–28.7	5333	C	231.385
–29.8	5333	19.954	57803	–24.9	6666	bp/°C	35.003
–22.4	7999	24.933	70109	–21.77	7999	ΔH_V/(kJ mol^{-1}) =	
–13.0	13332	29.944	84525	–16.58	10666	at 25°C	27.30
1.50	26664	35.000	101325	–12.38	13332	at bp	26.78
17.7	53329	40.092	120798	–4.304	19998		
35.0	101325	45.221	142368	1.796	26664		
		50.390	169052	6.758	33331		
mp/°C	–121	55.604	198530	10.972	39997		
		60.838	232087	17.932	53329		
		66.115	270110	23.613	66661		
				28.451	79993		
		Antoine eq.		32.686	93326		
		eq. 2	P/mmHg	33.475	95992		
		A	6.95206	34.247	98659		
		B	1084.531	35.003	101325		
		C	231.385	25.0	70288		

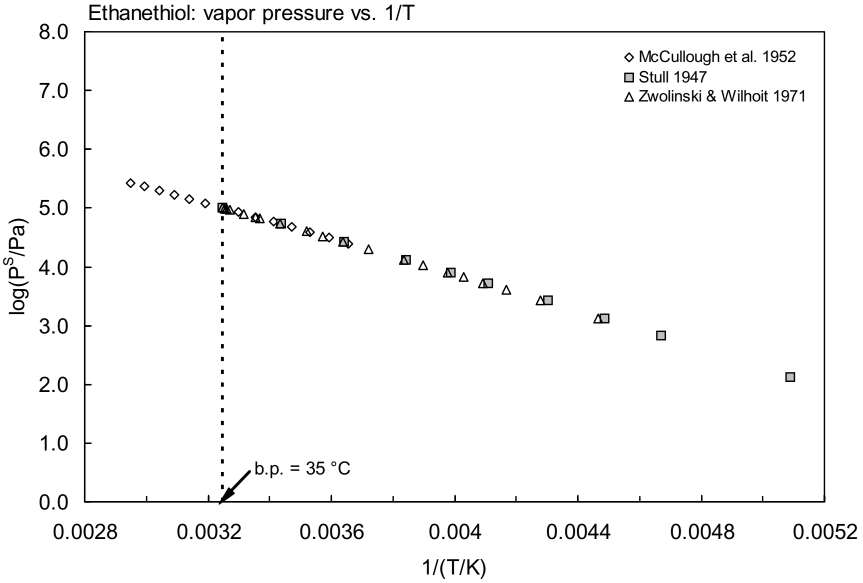
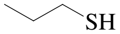


FIGURE 16.1.8.7.1 Logarithm of vapor pressure versus reciprocal temperature for ethanethiol.

16.1.8.8 1-Propanethiol



Common Name: 1-Propanethiol
Synonym: *n*-propyl mercaptan, 1-mercaptopropane
Chemical Name: 1-propanethiol
CAS Registry No: 107-03-9
Molecular Formula: C_3H_8S, $CH_3CH_2CH_2SH$
Molecular Weight: 76.171
Melting Point (°C):
  –113.13 (Lide 2003)
Boiling Point (°C):
  67.8 (Lide 2003)
Density (g/cm^3):
  0.8411 (20°C, Weast 1982–83)
Dissociation Constant, pK_a:
Molar Volume (cm^3/mol):
  99.6 (calculated-density, Stephenson & Malanowski 1987)
Enthalpy of Vaporization, ΔH_V (kJ/mol):
  31.88, 29.53 (25°C, bp, Zwolinski & Wilhoit 1971)
Enthalpy of Sublimation, ΔH_{subl} (kJ/mol):
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
Entropy of Fusion, ΔS_{fus} (J/mol K):
Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F: 1.0

Water Solubility (g/m^3 or mg/L at 25°C):
  3800 (estimated-activity coefficient by headspace-GC/FID, Przyjazny et al. 1983)

Vapor Pressure (Pa at 25°C or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):
  13332* (15.3°C, summary of literature data, temp range –56.0 to 67.4°C, Stull 1947)
  19920* (24.275°C, ebulliometry, measured range 24.3–102.088°C, Pennington et al. 1956)
  log (P/mmHg) = 6.92846 – 1183.307/(T/K + 224.624); temp range 24.3–102.088°C (Antoine eq., ebulliometry, Pennington et al. 1956; Osborn & Douslin 1966)
  20558* (interpolated-Antoine eq., temp range –25 to 90.73°C, Zwolinski & Wilhoit 1971)
  log (P/mmHg) = 6.92846 – 1183.307/(224.624 + t/°C); temp range –25 to 90.73°C (Antoine eq., Zwolinski & Wilhoit 1971)
  20569 (calculated-Antoine eq. of Boublik et al. 1973, Przyjazny et al. 1983)
  log (P/kPa) = 6.05331 – 1183.265/(224.618 + t/°C), temp range 24.27–102.088°C (Antoine eq. derived from Pennington et al. 1956 data, Boublik et al. 1984)
  log (P_L/kPa) = 6.05019 – 1181.703/(–48.687 + T/K), temp range 296–376 K, (Antoine eq., Stephenson & Malanowski 1987)
  log (P/mmHg) = 6.92846 – 1183.307/(224.62 + t/°C), temp range –25 to 91°C (Antoine eq., Dean 1992)

Henry's Law Constant (Pa m^3/mol at 25°C or as indicated):
  414 (distilled water, headspace-GC/FID, measured range 25–70°C, data in graph, Przyjazny et al. 1983)
  log (1/K_{AW}) = 1552.2/(T/K) – 4.428; temp range 25–70°C (headspace-GC, Przyjazny et al. 1983)
  331 (20°C, selected from literature experimentally measured data, Staudinger & Roberts 2001)
  log K_{AW} = 4.428 – 1552/(T/K), (van't Hoff eq. derived from literature data, Staudinger & Roberts 2001)

Octanol/Water Partition Coefficient, log K_{OW}:
  1.81 (shake flask, Log P Database, Hansch & Leo 1987)
  1.81 (recommended, Sangster 1993)
  1.81 (recommended, Hansch et al. 1995)

Octanol/Air Partition Coefficient, log K_{OA}:

Bioconcentration Factor, log BCF or log K_B:

Sorption Partition Coefficient, log K_{OC}:

Environmental Fate Rate Constants, k, and Half-Lives, $t_{½}$:

Volatilization:
Photolysis:
Oxidation: rate constant k, for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO3} with NO_3 radical and k_{O3} with O_3 or as indicated, *data at other temperatures see reference:
k_{OH}* = (4.18–4.56) × 10^{-11} cm^3 $molecule^{-1}$ s^{-1} at 298 K, measured range 257–419 K (flash photolysis-resonance fluorescence, Wine et al. 1984)
Hydrolysis:
Biodegradation:
Biotransformation:
Bioconcentration and Uptake and Elimination Rate Constants (k_1 and k_2):

Half-Lives in the Environment:

TABLE 16.1.8.8.1
Reported vapor pressures of 1-propanethiol at various temperatures and the coefficients for the vapor pressure equations

log P = A – B/(T/K) (1)
log P = A – B/(C + t/°C) (2)
log P = A – B/(C + T/K) (3)
log P = A – B/(T/K) – C·log (T/K) (4)
ln P = A – B/(T/K) (1a)
ln P = A – B/(C + t/°C) (2a)

Stull 1947		Pennington et al. 1956		Zwolinski & Wilhoit 1971	
summary of literature data		ebulliometry		selected values	
t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa
–56.0	133.3	24.275	18820	–25.0	1333
–36.3	666.6	29.563	25007	–14.3	2666
–26.3	1333	34.891	31160	–7.60	4000
–15.4	2666	40.254	38547	–2.50	5333
–3.20	5333	45.663	47359	1.65	6666
4.60	7999	51.113	57803	5.13	7999
15.3	13332	56.605	70109	10.84	10666
31.5	26664	62.139	84525	15.47	13332
49.2	53329	67.719	101325	24.369	19998
67.4	101325	73.341	120798	31.092	26664
		79.004	143268	36.562	33331
mp/°C	–112	84.710	169052	41.208	39997
		90.464	198543	48.884	53329
		96.225	232087	55.151	66661
		102.088	270110	60.489	79993
				65.163	93326
		bp/°C	67.72	66.034	95992
		Antoine eq.		66.886	98659

TABLE 16.1.8.8.1 (*Continued*)

Stull 1947		Pennington et al. 1956		Zwolinski & Wilhoit 1971	
summary of literature data		ebulliometry		selected values	
t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa
		eq. 2	P/mmHg	67.720	101325
		A	6.92846	25.0	20558
		B	1183.307		
		C	224.824	eq. 2	P/mmHg
				A	6.92846
		data also fitted to Cox eq.		B	1193.307
				C	224.624
				bp/°C	67.72
				$\Delta H_V/(kJ\ mol^{-1})$ =	
				at 25°C	31.88
				at bp	29.53

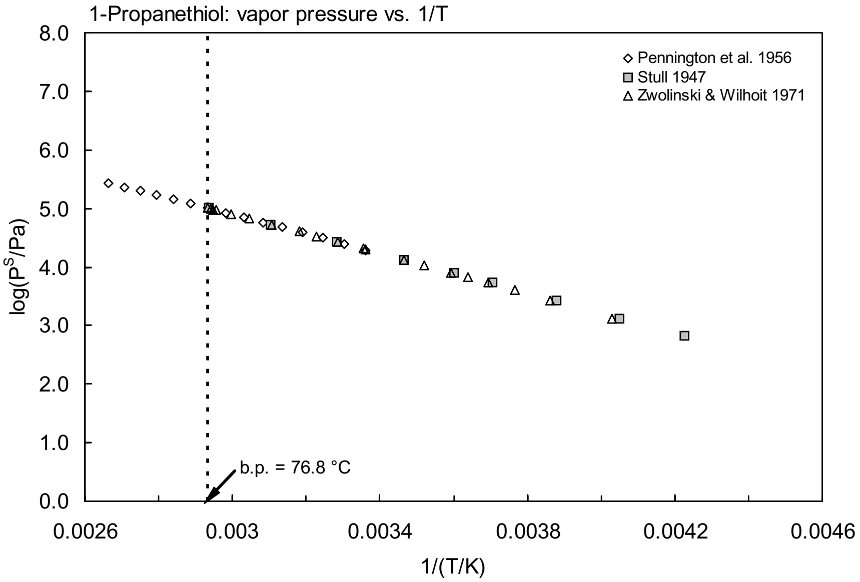
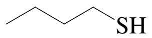


FIGURE 16.1.8.8.1 Logarithm of vapor pressure versus reciprocal temperature for 1-propanethiol.

16.1.8.9 1-Butanethiol (Butyl mercaptan)



Common Name: 1-Butanethiol
Synonym: butyl mercaptan, *n*-butyl mercaptan
Chemical Name: 1-butanethiol
CAS Registry No: 109-79-5
Molecular Formula: $C_4H_{10}S$, $CH_3(CH_2)_3SH$
Molecular Weight: 90.187
Melting Point (°C):
–115.7 (Weast 1982–83; Riddick et al. 1986; Stephenson & Malanowski 1987; Lide 2003)
Boiling Point (°C):
98.5 (Lide 2003)
Density (g/cm³ at 25°C):
0.8337 (20°C, Weast 1982–83)
0.84159, 0.83674 (20°C, 25°C, Riddick et al. 1986)
Molar Volume (cm³/mol):
107.8 (calculated-density, Stephenson & Malanowski 1987)
121.8 (calculated-Le Bas method at normal boiling point)
Dissociation Constant pK_a:
Enthalpy of Vaporization, ΔH_V (kJ/mol):
36.53, 32.225 (25°C, bp, Riddick et al. 1986)
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
10.46 (Riddick et al. 1986)
Entropy of Fusion, ΔS_{fus} (J/mol K):
Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F: 1.0

Water Solubility (g/m³ or mg/L at 25°C):
597 (Riddick et al. 1986)
600 (selected, Yaws et al. 1990)

Vapor Pressure (Pa at 25°C and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):
19920* (51.409°C, ebulliometry, measured range 51.4–135.7°C, Scott et al. 1957)
$\log (P/mmHg) = 6.92754 - 1281.018/(T/K + 218.100)$ (Antoine eq., Osborn & Douslin 1966)
5330*, 6070 (22.4°C, interpolated-Antoine eq., Zwolinski & Wilhoit 1971)
$\log (P/mmHg) = 6.92754 - 1281.018/(218.10 + t/°C)$; temp range –2.0 to 123.37°C (liquid, Antoine eq., Zwolinski & Wilhoit 1971)
$\log (P/kPa) = 6.05296 - 1281.344/(218.139 + t/°C)$, temp range 51.409–135.7°C (Antoine eq. derived from Scott et al. 1957 data, Boublik et al. 1984)
6070 (Riddick et al. 1986)
$\log (P/kPa) = 6.05244 - 1281.018/(218.10 + t/°C)$, temp range not specified (Antoine eq., Riddick et al. 1986)
$\log (P_L/kPa) = 6.05011 - 1279.95/(-55.132 + T/K)$, temp range 323–409 K (Antoine eq., Stephenson & Malanowski 1987)
$\log (P/mmHg) = 6.92754 - 1281.018/(218.10 + t/°C)$, temp range –2 to 123°C (Antoine eq., Dean 1992)
$\log (P/mmHg) = 36.2672 - 3.0452 \times 10^3/(T/K) - 9.9743 \cdot \log (T/K) - 9.1432 \times 10^{-11} \cdot (T/K) + 3.2087 \times 10^{-6} \cdot (T/K)^2$; temp range 157–569 K (vapor pressure eq., Yaws 1994)

Henry's Law Constant (Pa m³/mol at 25°C or as indicated and reported temperature dependence equations):
460.7 (distilled water, headspace-GC/FID, measured range 25–70°C, data in graph, Przyjazny et al. 1983)
$\log (1/K_{AW}) = 1655.9/(T/K) - 4.823$; temp range 25–70°C (headspace-GC, Przyjazny et al. 1983)
911.4 (computed-vapor-liquid equilibrium VLE data, Yaws et al. 1991)
363 (20°C, selected from literature experimentally measured data, Staudinger & Roberts 1996, 2001)
$\log K_{AW} = 4.823 - 1656/(T/K)$ (van't Hoff eq. derived from literature data, Staudinger & Roberts 2001)

Octanol/Water Partition Coefficient, log K_{OW}:

2.28	(shake flask, Log P Database, Hansch & Leo 1987)
2.28	(recommended, Sangster 1989)
2.28	(recommended, Hansch et al. 1995)

Octanol/Air Partition Coefficient, log K_{OA}:

Bioconcentration Factor, log BCF:

Sorption Partition Coefficient, log K_{OC}:

Environmental Fate Rate Constants, k, or Half-Lives, $t_{½}$:

Volatilization:

Photolysis:

Oxidation: rate constant k, for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO3} with NO_3 radical and k_{O3} with O_3 or as indicated, *data at other temperatures see reference:

$k_{OH} = 4.21 \times 10^{-11}$ cm^3 molecule^{-1} s^{-1} and $k_{OH} = 4.55 \times 10^{-11}$ cm^3 molecule^{-1} s^{-1} at 298 K (flash photolysis-resonance fluorescence, Wine et al. 1984)

$k_{OH} = 5.82 \times 10^{-11}$ cm^3 molecule^{-1} s^{-1} at 300 K (relative rate method, Barnes et al. 1986)

$k_{OH} = 5.11 \times 10^{-11}$ cm^3 molecule^{-1} s^{-1} at 298 K (recommended, Atkinson 1989)

Hydrolysis:

Biodegradation:

Biotransformation:

Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants:

Half-Lives in the Environment:

TABLE 16.1.8.9.1

Reported vapor pressures of 1-butanethiol at various temperatures and the coefficients for the vapor pressure equations

$\log P = A - B/(T/K)$ (1) $\ln P = A - B/(T/K)$ (1a)
$\log P = A - B/(C + t/°C)$ (2) $\ln P = A - B/(C + t/°C)$ (2a)
$\log P = A - B/(C + T/K)$ (3)
$\log P = A - B/(T/K) - C \cdot \log (T/K)$ (4)

Scott et al. 1957		Zwolinski & Wilhoit 1971			
ebulliometry		selected values			
t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa
51.409	19920	–2.0	1333	95.687	93326
57.130	25007	9.60	2666	96.630	95992
62.897	31169	16.9	4000	97.553	98659
68.710	38547	22.4	5333	98.456	101325
74.567	47359	26.9	6666	25.0	7399
80.472	57803	30.67	7999	eq. 2	P/mmHg
86.418	70109	36.86	10666	A	6.92854
92.414	84525	41.87	13332	B	1281.018
98.454	101325	51.506	19998	C	218.100
104.544	120798	58.786	26664	bp/°C	98.456
110.682	143268	64.170	33331	ΔH_V/(kJ mol^{-1}) =	
116.863	169052	69.742	39997	at 25°C	36.53
123.088	198530	78.056	53329	at bp	32.23
129.362	232087	84.844	66661		
135.678	170110	90.625	79993		

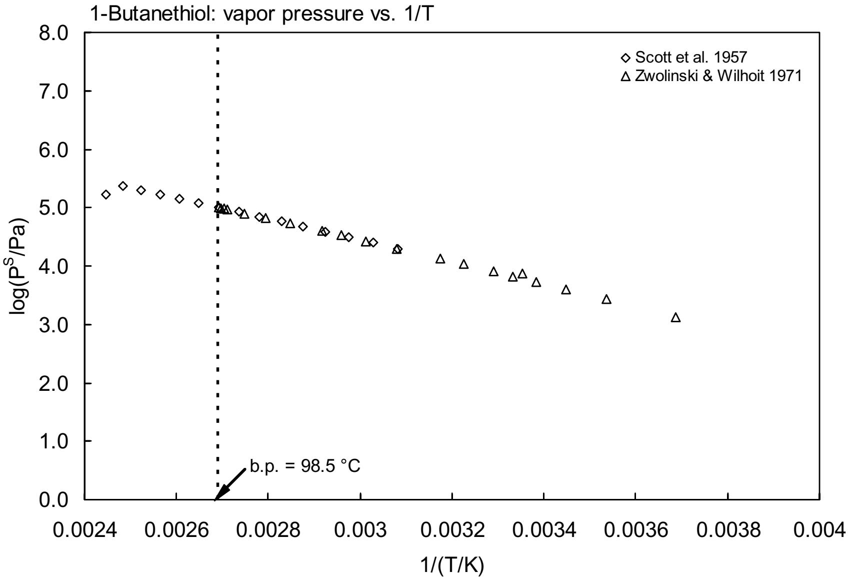
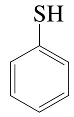


FIGURE 16.1.8.9.1 Logarithm of vapor pressure versus reciprocal temperature for 1-butanethiol.

16.1.8.10 Benzenethiol



Common Name: Benzenethiol
Synonym: thiophenol, phenyl mercaptan, mercaptobenzene
Chemical Name: benzenethiol
CAS Registry No: 108-98-5
Molecular Formula: C_6H_6S, C_6H_5SH
Molecular Weight: 110.177
Melting Point (°C):
–14.93 (Lide 2003)
Boiling Point (°C):
169.1 (Lide 2003)
Density (g/cm^3):
1.0766 (20°C, Weast 1982–83)
Dissociation Constant, pK_a:
6.615 (Riddick et al. 1986)
Molar Volume (cm^3/mol):
102.7 (calculated-density, Stephenson & Malanowski 1987)
106.8 (calculated-Le Bas method at normal boiling point)
Enthalpy of Vaporization, ΔH_V (kJ/mol):
45.35, 36.97 (25°C, bp, Riddick et al 1986)
Enthalpy of Sublimation, ΔH_{subl} (kJ/mol):
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
11.45 (calorimetry at triple pt 258.27 K, Scott et al. 1956)
11.447 (Riddcik et al. 1986)
Entropy of Fusion, ΔS_{fus} (J/mol K):
Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F: 1.0

Water Solubility (g/m^3 or mg/L at 25°C):

Vapor Pressure (Pa at 25°C or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):
133* (18.6°C, summary of literature data, temp range 18.6–168°C, Stull 1947)
1333* (51.5°C, ebulliometry, measured range 51.5–167.0°C, Vonterres et al. 1955)
19920* (114.543°C, ebulliometry, measured range 114.543–7212.160°C, Scott et al. 1956)
$\log (P/mmHg) = 6.99019 - 1529.454/(230.048 + t/°C)$; temp range 114.5–212°C (comparative ebulliometry, data fitted to Antoine eq., Scott et al. 1956)
$\log (P/mmHg) = A \pm [1 - 442.298/(T/K)]$, where $\log A = 0.87370 - 6.4975 \times 10^{-4} \pm (T/K) + 5.2309 \times 10^{-7} \pm (T/K)^2$; measured range 114.5–212°C (data fitted to Cox eq., comparative ebulliometry, Scott et al. 1956)
1333* (52.28°C, derived from compiled data, temp range 52.3–198°C, Zwolinski & Wilhoit 1971)
$\log (P/mmHg) = 6.99019 - 1529.454/(230.048 + t/°C)$; temp range 52.3–198°C (Antoine eq., Zwolinski & Wilhoit 1971)
$\log (P/kPa) = 6.11539 - 1529.668/(203.074 + t/°C)$, temp range 114.54–212.16°C (Antoine eq. derived from Scott et al. 1956 data, Boublik et al. 1984)
397 (selected, Riddick et al. 1986)
$\log (P/kPa) = 6.11509 - 1529.46/(t/°C + 258.21)$; temp range not specified (Antoine eq., Riddick et al. 1986)
$\log (P_L/kPa) = 6.11531 - 1530.286/(-69.948 + T/K)$; temp range 385–486 K (Antoine eq., Stephenson & Malanowski 1987)
$\log (P/mmHg) = -5.4919 - 2.8549 \times 10^3/(T/K) + 8.1770 \cdot \log (T/K) - 1.9494 \times 10^{-2} \cdot (T/K) + 9.2817 \times 10^{-6} \cdot (T/K)^2$; temp range 258–69 K (vapor pressure eq., Yaws et al. 1994)

Henry's Law Constant (Pa m^3/mol at 25°C):

Octanol/Water Partition Coefficient, log K_{OW}:

2.52	(shake flask, Log P Database, Hansch & Leo 1987)
2.52	(recommended, Sangster 1989)
2.52	(recommended, Hansch et al. 1995)

Octanol/Air Partition Coefficient, log K_{OA}:

Bioconcentration Factor, log BCF or log K_B:

Sorption Partition Coefficient, log K_{OC}:

Environmental Fate Rate Constants, k, and Half-Lives, $t_{½}$:

Half-Lives in the Environment:

TABLE 16.1.8.10.1
Reported vapor pressures of benzenethiol at various temperatures and the coefficients for the vapor pressure equations

$\log P = A - B/(T/K)$ (1) $\quad \ln P = A - B/(T/K)$ (1a)
$\log P = A - B/(C + t/°C)$ (2) $\quad \ln P = A - B/(C + t/°C)$ (2a)
$\log P = A - B/(C + T/K)$ (3)
$\log P = A - B/(T/K) - C \cdot \log (T/K)$ (4)

Stull 1947		**Vonterres et al. 1955**		**Scott et al. 1956**		**Zwolinski & Wilhoit 1971**	
summary of literature data		**ebulliometry**		**comparative ebulliometry**		**selected values**	
t/°C	**P/Pa**	**t/°C**	**P/Pa**	**t/°C**	**P/Pa**	**t/°C**	**P/Pa**
18.6	133.3	51.5	1333	114.543	19920	52.28	1333
43.7	666.6	71.5	5333	121.191	25007	65.79	2666
56.0	1333	87.8	6666	127.897	31160	74.38	4000
69.7	2666	97.4	9999	134.649	38547	80.81	5333
84.2	5333	105.5	13332	141.447	47359	86.01	6666
93.9	7999	116.3	19998	148.294	57803	90.40	7999
106.6	13332	124.5	26664	155.194	70109	97.61	10666
125.8	26664	131.3	33330	162.140	84525	103.444	13332
146.7	53329	136.5	39997	176.188	120789	114.655	19998
168.0	101325	141.5	46663	183.278	143268	123.120	26664
		146.0	53329	190.426	169052	130.003	33331
mp/°C	-	149.7	59995	197.623	198530	135.847	39997
		153.0	66661	204.867	232087	145.496	53329
		156.0	73327	212.160	270110	153.367	66661
		159.0	79993			160.067	79993
		162.0	86659	mp/K	258.27	165.932	93326
		165.0	93325	$\Delta H_{fus}/(kJ\ mol^{-1})$ =	11.447	167.024	95992
		167.0	101325	bp/K	416.9	168.092	98659
						169.138	101325

(Continued)

TABLE 16.1.8.10.1 (*Continued*)

Stull 1947		Vonterres et al. 1955		Scott et al. 1956		Zwolinski & Wilhoit 1971	
summary of literature data		ebulliometry		comparative ebulliometry		selected values	
t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa
				eq. 2	P/mmHg	169.653	102658
				A	6.99019	170.163	103991
				B	1529.454	171.167	106658
				C	203.048		
				temp range 114–212°C		eq. 2	P/mmHg
						A	6.99019
						B	1529.454
						C	203.048
						bp/°C	
						$\Delta H_V/(kJ\ mol^{-1})$ = 40.6	
							at normal bp

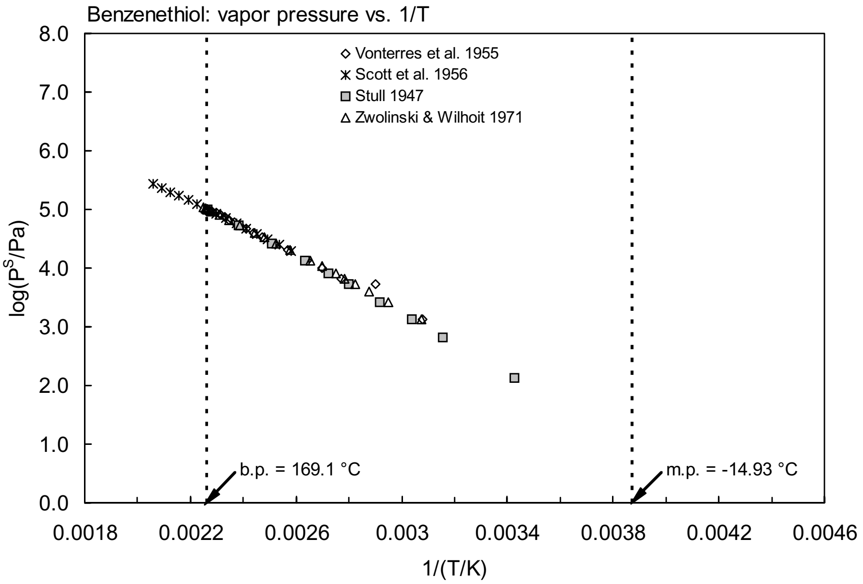
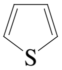


FIGURE 16.1.8.10.1 Logarithm of vapor pressure versus reciprocal temperature for benzenethiol.

16.1.8.11 Thiophene



Common Name: Thiophene
Synonym: thiofuran
Chemical Name: thiophene, thiofuran
CAS Registry No: 110-02-1
Molecular Formula: C_4H_4S
Molecular Weight: 84.140
Melting Point (°C):
–38.21 (Lide 2003)
Boiling Point (°C):
84.0 (Lide 2003)
Density (g/cm^3 at 20°C):
1.06485, 1.05887 (20°C, 25°C, Dreisbach 1955)
1.0649 (Weast 1982–83)
1.06482, 1.05884 (20°C, 25°C, Riddick et al. 1986)
Molar Volume (cm^3/mol):
79.0 (20°C, calculated from density)
88.10 (calculated-Le Bas method at normal boiling point)
Dissociation Constant pK_a:
Enthalpy of Vaporization, ΔH_V (kJ/mol):
34.6, 31.472 (25°C, bp, Riddick et al. 1986)
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
5.088 (Riddick et al. 1986)
Entropy of Fusion, ΔS_{fus} (J/mol K):
Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F: 1.0

Water Solubility (g/m^3 or mg/L at 25°C):
3015 (shake flask-GC, Price 1976)
3900 (estimated-activity coefficient by headspace-GC, Przyjazny et al. 1983)
3600 (18°C, Verschueren 1983)
3020 (selected, Yaws et al. 1990)

Vapor Pressure (Pa at 25°C or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):
9670* (interpolated-regression of tabulated data, temp range –40.7 to 81.4°C, Stull 1947)
7998 (20.1°C, Stull 1947)
10622* (ebulliometry and manometry, measured range 0–84.155°C, Waddington et al. 1949)
10620 (calculated from determined data, Dreisbach 1955)
log (P/mmHg) = 6.95926 – 1246.038/(221.354 + t/°C), temp range 5–155°C (Antoine eq. for liquid state, Dreisbach 1955)
482307* (148.89°C, static-Bourdon gauge, measured range 148.89–304.44°C, Kobe et al. 1956)
44930* (60.3 °C, isoteniscope/manometry, measured range 60.3–100.3 °C, Eon et al. 1971)
10670, 10660* (25.09°C, interpolated-Antoine eq., Zwolinski & Wilhoit 1971)
log (P/mmHg) = 6.95926 – 1246.01/(221.35 + t/°C); temp range –12.3 to 108.1°C (Antoine eq., Zwolinski & Wilhoit 1971)
log (P/mmHg) = [–0.2185 × 8748.3/(T/K)] + 8.273276; temp range –40.7 to 84.4°C (Antoine eq., Weast 1972–73)
2450 (calculated-Cox eq., Chao et al. 1983)
log (P/atm) = [1 – 394.395/(T/K)] × 10^{0.901276 – 10.3229 × 10^{-4} ± (T/K) + 21.9193 × 10^{-7} ± $(T/K)^2$}; temp range: 278.35–443.60 K (Cox eq., Chao et al. 1983)

7998, 13330 (20°C, 30°C, quoted, Verschueren 1983)
10622, 10620 (quoted exptl., calculated-Antoine eq., Boublik et al. 1984)
log (P/kPa) = 6.1336 – 1260.606/(222.787 + t/°C), temp range 0–40°C (Antoine eq. from reported exptl. data, Boublik et al. 1984)
log (P/kPa) = 6.0723 – 1138.803/(220.477 + t/°C), temp range 39.9–119.79°C (Antoine eq. from reported exptl. data, Boublik et al. 1984)
10620 (calculated-Antoine eq., Dean 1985, 1992)
log (P/mmHg) = 6.95926 – 1246.02/(221.35 + t/°C), temp range –12 to 108°C (Antoine eq., Dean l985, 1992)
10620 (selected, Riddick et al. 1986)
log (P/kPa) = 6.08416 – 1246.02/(221.35 + t/°C), temp range not specified (Antoine eq., Riddick et al. 1986)
10600 (extrapolated-Antoine eq., Stephenson & Malanowski 1987)
log (P_S/kPa) = 9.84733 – 2447.236/(T/K), temp range 195–228 K (solid, Antoine eq.-I, Stephenson & Malanowski 1987)
log (P_L/kPa) = 6.06132 – 1232.35/(–53.438 + T/K), temp range 311–393 K (liquid, Antoine eq.-II, Stephenson & Malanowski 1987)
log (P/mmHg) = 36.6016 – 2.9794 × 10^3/(T/K) – 10.104·log (T/K) + 1.1445 × 10^{-9}·(T/K) + 3.2472 × 10^{-6}·$(T/K)^2$; temp range 235–579 K (vapor pressure eq., Yaws et al. 1994)

Henry's Law Constant (Pa·m^3/mol at 25°C or as indicated and reported temperature dependence equations):
224, 236, 230 (headspace-GC, concn. of 10, 1.0 and 0.1 ppm by weight, measured range 25–70°C, data presented in graph, Przyjazny et al. 1983)
log (1/K_{AW}) = 1563.6/(T/K) – 4.199; temp range 25–70°C (headspace-GC, concn of 10 ppm by weight, Przyjazny et al. 1983)
log (1/K_{AW}) = 1580.0/(T/K) – 4.277; temp range 25–70°C (headspace-GC, concn of 1.0 ppm by weight, Przyjazny et al. 1983)
log (1/K_{AW}) = 1661.9/(T/K) – 4.542; temp range 25–70°C (headspace-GC, concn of 0.1 ppm by weight, Przyjazny et al. 1983)
223.3 (calculated-P/C with selected values)
296 (computed-vapor-liquid equllibrium VLE data, Yaws et al. 1991)
182 (20°C, selected from literature experimentally measured data, Staudinger & Roberts 1996, 2001)
log K_{AW} = 4.542 – 1662/(T/K), (van't Hoff eq. derived from literature data, Staudinger & Roberts 2001)

Octanol/Water Partition Coefficient, log K_{OW}:
1.81 ± 0.01 (shake flask-UV, Iwasa et al. 1965)
1.79 (calculated-f const., Rekker 1977)
1.74 (HPLC-RV correlation, Garst 1984)
1.82 (shake flask, Log P Database, Hansch & Leo 1987)
1.81 (recommended, Sangster 1989, 1993)
1.82 (shake flask-UV, Yamagami & Takao 1992)
1.81 (recommended, Hansch et al. 1995)

Octanol/Air Partition Coefficient, log K_{OA}:

Bioconcentration Factor, log BCF:

Sorption Partition Coefficient, log K_{OC}:

Environmental Fate Rate Constants, k, or Half-Lives, $t_{½}$:
Volatilization:
Photolysis:
Oxidation: rate constant k, for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO3} with NO_3 radical and k_{O3} with O_3 or as indicated, *data at other temperatures and the Arrhenius expression see reference:

k_{OH} = (9.58 ± 0.38) × 10^{-12} cm^3 $molecule^{-1}$ s^{-1} with calculated atmospheric lifetime τ ~ 28 h; and $k_{O3} < 6 \times 10^{-20}$ cm^3 $molecule^{-1}$ s^{-1} at 298 ± 2 K and $k_{O(3P)}$ = 4.9 × 10^{-12} cm^3 $molecule^{-1}$ s^{-1} for reaction with $O(^3P)$ atom at room temp. (relative rate method, Atkinson et al 1983)

$k_{O3} < 6 \times 10^{-20}$ cm^3 $molecule^{-1}$ s^{-1} with a loss rate of < 0.004 d^{-1}, k_{OH} = 9.6 × 10^{-12} cm^3 $molecule^{-1}$ s^{-1} with a loss rate of 0.8 d^{-1}; k_{NO3} = 3.2 × 10^{-14} cm^3 $molecule^{-1}$ s^{-1} with a loss rate of 0.7 d^{-1} at room temp. (review, Atkinson & Carter 1984)

k_{OH}* = (9.37, 9.57) × 10^{-12} cm^3 $molecule^{-1}$ s^{-1} at 298 K, measured range 255–425 K (flash photolysis-resonance fluorescence, Wine & Thompson 1984)

k_{OH} = 9.49 × 10^{-12} cm^3 $molecule^{-1}$ s^{-1} at 298 K (recommended, Atkinson 1985)

$k_{O3} < 6 \times 10^{-20}$ cm^3 $molecule^{-1}$ s^{-1} with a loss rate of < 0.004 d^{-1}, k_{OH} = 9.70 × 10^{-12} cm^3 ± $molecule^{-1}$ s^{-1} with a loss rate of 0.4 d^{-1}, and k_{NO3} = 3.2 × 10^{-14} cm^3 $molecule^{-1}$ s^{-1} with a loss rate of 0.7 d^{-1} at room temp. (review, Atkinson 1985)

k_{NO3} = (3.2 ± 0.7) × 10^{-14} cm^3 $molecule^{-1}$ s^{-1} with a calculated lifetime of 36 h and a loss rate of 0.7 d^{-1} assuming 2.4 × 10^8 NO_3 radicals/cm^3 in nighttime air at 295 ± 1 K in the atmosphere (relative rate technique, Atkinson et al. 1985)

$k_{O3} < 6 \times 10^{-20}$ cm^3 $molecule^{-1}$ s^{-1} with a calculated tropospheric lifetime $\tau > 270$ d, k_{OH} = 9.70 × 10^{-12} cm^3 $molecule^{-1}$ s^{-1} with a calculated lifetime of 29 h during daytime hours, and k_{NO3} = 3.2 × 10^{-14} cm^3 $molecule^{-1}$ s^{-1} with a calculated lifetime of 36 h at room temp. (review, Atkinson 1985)

k_{OH}* = 9.53 × 10^{-12} cm^3 $molecule^{-1}$ s^{-1} at 298 K (recommended, Atkinson 1989)

k_{NO3} = 3.93 × 10^{-14} cm^3 $molecule^{-1}$ s^{-1}, independent of temperature over the range 272–296 K (recommended, Atkinson 1991)

k_{OH}(calc) = 14.81 × 10^{-12} cm^3 $molecule^{-1}$ s^{-1} at room temp. (molecular orbital calculations, (Klamt 1993)

Hydrolysis:

Biodegradation:

Biotransformation:

Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants:

Half-Lives in the Environment:

Air: atmospheric lifetime of ~28 h due to reactions with OH radical (Atkinson et al. 1983);

calculated gas-phase lifetime of 29 h for the reaction with OH radical during daytime hours, calculated lifetime of 36 h for reaction with NO_3 radical and a calculated lifetime > 270 d for reaction with O_3 at room temp. (Atkinson et al. 1985)

TABLE 16.1.8.11.1
Reported vapor pressures of thiophene at various temperatures and the coefficients for the vapor pressure equations

log P = A – B/(T/K) (1)
log P = A – B/(C + t/°C) (2)
log P = A – B/(C + T/K) (3)
log P = A – B/(T/K) – C·log (T/K) (4)
ln P = A – B/(T/K) (1a)
ln P = A – B/(C + t/°C) (2a)

Stull 1947		Waddington et al. 1949		Kobe et al. 1956		Zwolinski & Wilhoit 1971	
summary of literature data		manometry and ebulliometry		static-Bourdon gauge		selected values	
t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa
		static method					
–40.7	133	0	2858	148.89	482307	–12.3	1333
–20.8	666.6	15	6497	154.44	585659	–1.10	2666
–10.9	1333	20	8355	160.00	620109	5.94	4000
0.0	2666	25	10627	165.56	730351	11.24	5333
12.5	5333	30	13398	171.11	813032	15.52	6666
20.1	7999	35	16733	176.67	895713	19.14	7999

(*Continued*)

TABLE 16.1.8.11.1 (*Continued*)

Stull 1947		**Waddington et al. 1949**		**Kobe et al. 1956**		**Zwolinski & Wilhoit 1971**	
summary of literature data		**manometry and ebulliometry**		**static-Bourdon gauge**		**selected values**	
t/°C	**P/Pa**	**t/°C**	**P/Pa**	**t/°C**	**P/Pa**	**t/°C**	**P/Pa**
30.5	13332	40	20736	182.22	992174	25.09	10666
46.5	26664	ebulliometric method		187.78	1088636	29.90	13332
64.7	53329	39.061	19920	193.33	1198877	39.15	19998
81.4	101325	44.560	25007	198.89	1316009	46.14	26664
		50.094	31160	204.44	1440031	51.82	33331
mp/°C	–38.3	55.663	38547	210.00	1584723	56.65	39997
		61.276	47359	215.56	1722525	64.62	53329
		66.931	57903	221.11	1874107	71.12	66661
Eon et al. 1971		72.629	70109	226.67	2039470	76.66	79993
isoteniscope-manometer		78.370	84525	232.22	2211722	81.51	93326
t/°C	**P/Pa**	84.155	101325	237.78	2397755	82.41	95992
				243.33	2590678	83.30	98659
60.3	44930	mp/°C	–38.1	248.89	2797381	84.16	101325
70.3	64795	bp/°C	84.16	254.44	3010974		
80.3	91459			260.00	3238347	bp/°C	84.16
90.3	126790	eq. 2	P/mmHg	265.56	3472610		
100.3	172519	A	6.95926	271.11	3727544	eq. 2	P/mmHg
		B	1246.038	276.67	3996258	A	6.95926
ΔH_V/(kJ mol^{-1}) =34.77		C	221.354	282.22	4251192	B	1246.02
				287.78	4540576	C	221.35
		ΔH_V/(kJ mol^{-1}) =		293.33	4836850		
		at 45.36°C	33.61	298.89	5146905	ΔH_V/(kJ mol^{-1}) =	
		at 63.08°C	32.67	304.44	5463849	at 25°C	34.60
		at bp	31.47			at bp	31.47

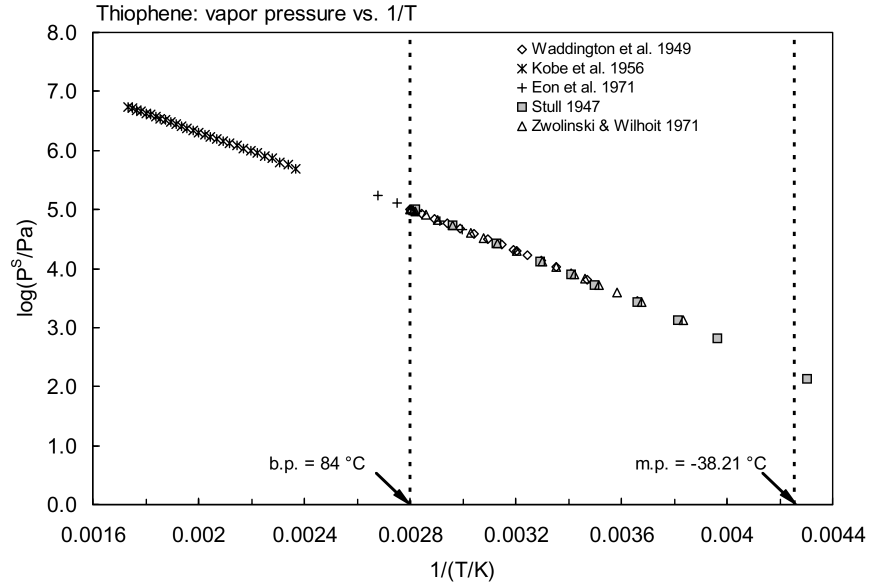
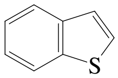


FIGURE 16.1.8.11.1 Logarithm of vapor pressure versus reciprocal temperature for thiophene.

16.1.8.12 Benzo[*b*]thiophene



Common Name: Benzo[*b*]thiophene
Synonym: thianaphthene, thionaphthene, 1-benzothiophene
Chemical Name:
CAS Registry No: 95-15-8
Molecular Formula: C_8H_6S
Molecular Weight: 134.199
Melting Point (°C):
  32 (Lide 2003)
Boiling Point (°C):
  221 (Lide 2003)
Density (g/cm^3 at 20°C):
  1.1500 (Verschueren 1983)
Molar Volume (cm^3/mol):
  139.7 (calculated-Le Bas method at normal boiling point)
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
Entropy of Fusion, ΔS_{fus} (J/mol K):
Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F: 0.854 (mp at 32°C)

Water Solubility (g/m^3 or mg/L at 25°C or as indicated):
  130.0 (20°C, shake flask, Smith et al. 1978)
  130.2 (Mill et al. 1981)
  216* (59.05°C, equilibrium cell-GC, measured range 332.2–490.5 K, Leet et al. 1987)

Vapor Pressure (Pa at 25°C or as indicated):
  26.7 (20°C, estimated from naphthalene, Smith et al. 1978)
  14.80 (calculated-bp, Mackay et al. 1982)
  $\log (P/\text{mmHg}) = -9.5352 - 2.6947 \times 10^3/(T/K) + 8.8858 \cdot \log (T/K) - 1.5478 \times 10^{-2} \cdot (T/K) + 6.5159 \times 10^{-6} \cdot (T/K)^2$;
    temp range 305–754 K (vapor pressure eq., Yaws 1994)

Henry's Law Constant (Pa·m^3/mol at 25°C):
  28.0 (calculated-P/C, Smith & Bomberger 1980)
  24.1 (calculated-P/C, this work)

Octanol/Water Partition Coefficient, log K_{OW}:
  3.09 (shake flask-UV, pH 7.4, Rogers & Cammarata 1969)
  3.05 (HPLC-RT correlation, De Voogt et al. 1988)
  3.12 (recommended, Sangster 1989, 1993)
  3.26 (shake flask-HPLC, De Voogt et al. 1990)
  3.18 (HPLC-RT correlation, Ritter et al. 1994)
  3.17 (shake flask-dialysis tubing-HPLC/UV, both phases, Andersson & Schrăder 1999)

Octanol/Air Partition Coefficient, log K_{OA}:

Bioconcentration Factor, log BCF:
  2.08 (mixed microbial populations, Steen & Karickhoff 1981)

Sorption Partition Coefficient, log K_{OC}:
  1.77 (Coyote Creek sediment, Smith et al. 1978)
  2.30 (lab. mixture of microorganisms, Smith et al. 1978)
  3.49, 3.0 (soil, quoted, calculated-MCI χ and fragment contribution, Meylan et al. 1992)

Environmental Fate Rate Constants, k, or Half-Lives, $t_{½}$:

Volatilization: estimated $t_{½}$ = 45 h in river, $t_{½}$ = 230 h in eutrophic pond, $t_{½}$ = 180 hours in eutrophic lake and oligotrophic lake by the one compartment model (Smith et al. 1978).

Photolysis: rate constant of transformation and transport of $(6.9 \pm 0.7) \times 10^{-7}$ s^{-1} exposed to 12 h sunlight per day in late May with estimated $t_{½}$ = 1200 h in river, $t_{½}$ = 2900 h in eutrophic pond, $t_{½}$ = 3500 h in eutrophic lake and $t_{½}$ = 600 h in oligotrophic lake by the one compartment model (Smith et al. 1978).

Oxidation:

laboratory investigated k = 83 M^{-1} s^{-1} for the reaction with RO_2 radical and estimated $t_{½}$ = 10^5 h in river, eutrophic pond, eutrophic lake and oligotrophic lake by the one compartment model (Smith et al. 1978)

k = 5.7×10^{-6} s^{-1} with $t_{½}$ = 34 h under natural sunlight conditions, k = 83 M^{-1} s^{-1} with $t_{½}$ = 96 d for free-radical oxidation in air-saturated water (NRCC 1983)

Hydrolysis:

Biodegradation: estimated $t_{½}$ > 20 h in river, $t_{½}$ < 20 h in eutrophic pond, $t_{½}$ = 20 h in eutrophic lake and very long half-life in oligotrophic lake, based on the biodegradation rate in the presence of alternative carbon sources will be one-half the biodegradation rate of quinoline when quinoline is the only carbon source by the one compartment model (Smith et al. 1978).

Biotransformation:

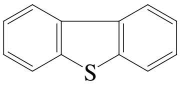
Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants:

Half-Lives in the Environment:

Surface water: estimated volatilization $t_{½}$ = 45 h in river, $t_{½}$ = 230 h in eutrophic pond, $t_{½}$ = 180 h in eutrophic lake and oligotrophic lake by the one compartment model (Smith et al. 1978);

photolysis rate constant of transformation and transport of $(6.9 \pm 0.7) \times 10^{-7}$ s^{-1} exposed to 12 h sunlight per day in late May with estimated photolysis $t_{½}$ = 1200 h in river, $t_{½}$ = 2900 h in eutrophic pond, $t_{½}$ = 3500 h in eutrophic lake and $t_{½}$ = 600 h in oligotrophic lake by the one compartment model (Smith et al. 1978).

16.1.8.13 Dibenzothiophene



Common Name: Dibenzothiophene
Synonym:
Chemical Name: dibenzothiophene
CAS Registry No: 132-65-0
Molecular Formula: $C_{12}H_8S$
Molecular Weight: 184.257
Melting Point (°C):
98.2 (Lide 2003)
Boiling Point (°C):
332.5 (Lide 2003)
Density (g/cm^3 at 20°C):
Molar Volume (cm^3/mol):
191.3 (calculated-Le Bas method at normal boiling point)
Entropy of Fusion, ΔS_{fus} (J/mol K):
Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F: 0.191 (mp at 98.2°C)

Water Solubility (g/m^3 or mg/L at 25°C or as indicated):
1.11 ± 0.09 (28°C, measured, Smith et al. 1978)
1.470 (24°C, shake flask-LSC, Means et al. 1980)
1.106 (Mill et al. 1981)
1.500 (Steen & Karickhoff 1981)
1.032 (literature average, Pearlman et al. 1984)

Vapor Pressure (Pa at 25°C or as indicated and reported temperature dependence equations):
0.267 (20°C, estimated, Aubry et al. 1975)
log (P/mmHg) = 22.90 – 10910/(T/K), temp range 60–00°C (solid, gas saturation, Edward & Prausnitz 1981)
log (P/mmHg) = 21.10 – 8353/(T/K), temp range 100–130°C (liquid, gas saturation, Edward & Prausnitz 1981)
0.263, 0.0083 (20°C, quoted, calculated-bp, Mackay et al. 1982)
0.893 (static apparatus-extrapolated from Chebyshev polynomials, Sivaraman & Kobayashi 1982)
0.586 (extrapolated-Cox eq., Chao et al. 1983)
log (P/atm) = [1– 605.160/(T/K)] × 10^{0.865373 – 5.51221 × 10^{-4} ± (T/K) + 6.05701 × 10^{-7} ± $(T/K)^2$}; temp range: 424.81–607.53 K (Cox eq., Chao et al. 1983)
log (P_L/kPa) = 7.18577 – 3140.15/(T/K), temp range 385–574 K (Antoine eq., Stephenson & Malanowski 1987)

Henry's Law Constant (Pa·m^3/mol at 25°C):
44.3 (calculated-P/C, Smith & Bomberger 1980)

Octanol/Water Partition Coefficient, log K_{OW}:
4.38 (shake flask-LSC, Means et al. 1980)
4.33 (HPLC-RT correlation, De Voogt et al. 1988)
4.38 (recommended, Sangster 1989, 1993)
4.49 (shake flask-HPLC, De Voogt et al. 1990)
4.38 (recommended, Hansch et al. 1995)
4.41 ± 0.19, 4.43 ± 0.61 (HPLC-k′ correlation: ODS-65 column, Diol-35 column, Helweg et al. 1997)
4.36 (shake flask-dialysis tubing-HPLC/UV, both phases, Andersson & Schräder 1999)

Octanol/Air Partition Coefficient, log K_{OA}:

Bioconcentration Factor, log BCF:

3.20	(mixed microbial populations, Steen & Karickhoff 1981)

Sorption Partition Coefficient, log K_{OC}:

3.14	(Coyote Creek sediment, Smith et al. 1978)
4.05	(soil, Hassett et al. 1980)
4.05	(average of 3 sediment/soil samples, equilibrium sorption isotherm, Means et al. 1980)
4.00	(soil, calculated-MCI χ, Sabljic 1987)
4.00	(soil, calculated-MCI χ, Sabljic 1987)
4.17	(soil, calculated-K_{OW}, model of Karickhoff et al. 1979, Sabljic 1987)
3.75	(soil, calculated-K_{OW}, model of Kenaga & Goring 1980, Sabljic 1987)
2.92	(soil, calculated-K_{OW}, model of Briggs 1981, Sabljic 1987)
4.00	(soil, calculated-K_{OW}, model of Means et al. 1982, Sabljic 1987)
3.60	(soil, calculated-K_{OW}, model of Chiou et al. 1983, Sabljic 1987)
4.59	(humic acid, HPLC-k′ correlation, Nielsen et al. 1997)
3.87	(soil: organic carbon OC ≥ 0.1%, average, Delle Site 2001)
4.02, 4.04	(sediments: organic carbon OC ≥ 0.1%, OC ≥ 0.5%, average, Delle Site 2001)
4.07	(Askov soil, a Danish agricultural soil, Sverdrup et al. 2002)

Environmental Fate Rate Constants, k, or Half-Lives, $t_{1/2}$:

Volatilization: estimated $t_{1/2}$ = 140 h in river, $t_{1/2}$ = 720 h in eutrophic pond, $t_{1/2}$ = 580 h in eutrophic lake and oligotrophic lake by the one compartment model (Smith et al. 1978).

Photolysis: solar photolysis $k = 1.5 \times 10^{-8}$ s^{-1} over 24-h day; rate constant of transformation and transport of $(2.04 \pm 0.08) \times 10^{-6}$ s^{-1} exposed to 12 h sunlight per day in early March with estimated $t_{1/2}$ = 380 h in river, $t_{1/2}$ = 950 h in eutrophic pond and eutrophic lake and $t_{1/2}$ = 190 h in oligotrophic lake from average photolysis rates on a summer day at 40°N latitude by the one compartment model (Smith et al. 1978); $t_{1/2}$ = 4–8 h for disappearance via direct photolysis in aquatic media (Harris 1982).

Oxidation: laboratory investigated $k < 7.5$ M^{-1} s^{-1} for the reaction with RO_2 radical and estimated $t_{1/2} > 10^5$ h in river, eutrophic pond, eutrophic lake and oligotrophic lake by the one compartment model (Smith et al. 1978). $k = 1.5 \times 10^{-6}$ s^{-1} with $t_{1/2}$ = 128 h under natural sunlight conditions, $k < 7.5$ M^{-1} s^{-1} with $t_{1/2}$ > 3.5 yr for free-radical oxidation in air-saturated water (NRCC 1983)

Hydrolysis:

Biodegradation: $k = 5.3 \times 10^{-7}$ mL $cell^{-1}$ h^{-1} and the estimated $t_{1/2}$ = 13 h in river, eutrophic pond, and eutrophic lake and $t_{1/2} > 10^4$ h in oligotrophic lake by the one compartment model (Smith et al. 1978)

Biotransformation:

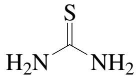
Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants:

Half-Lives in the Environment:

Surface water: $t_{1/2}$ = 0.5 h from river water, $t_{1/2}$ = 13 h from pond water, $t_{1/2}$ = 13 h from eutrophic lake and $t_{1/2}$ = 140 h from oligotrophic lake predicted by one-compartment model for all processes; estimated volatilization $t_{1/2}$ = 140 h in river, $t_{1/2}$ = 720 h in eutrophic pond, $t_{1/2}$ = 580 h in eutrophic lake and oligotrophic lake; photolysis rate constant of transformation and transport $k = (2.04 \pm 0.08) \times 10^{-6}$ s^{-1} exposed to 12 h sunlight per day in early March with estimated photolysis $t_{1/2}$ = 380 h in river, 950 h in eutrophic pond and eutrophic lake and $t_{1/2}$ = 190 h in oligotrophic lake; biodegradation $t_{1/2}$ = 13 h in river, eutrophic pond water and $t_{1/2}$ = 140 h in oligotrophic lake (Smith et al. 1978);

$t_{1/2}$ = 4–8 h for disappearance via direct photolysis in aqueous media (Harris 1982).

16.1.8.14 Thiourea



Common Name: Thiourea
Synonym: thiocarbamide
Chemical Name: thiourea
CAS Registry No: 62-56-6
Molecular Formula: CH_4N_2S, H_2NCSNH_2
Molecular Weight: 76.121
Melting Point (°C):
  178 (Lide 2003)
Boiling Point (°C):
  decomposes (Verschueren 1983)
Density (g/cm^3 at 20°C):
  1.045 (Weast 1982–83; Verschueren 1983, Dean 1992)
Dissociation Constant, pK:
  2.03 (pK_1, Dean 1985)
Molar Volume (cm^3/mol):
  76.2 (calculated-Le Bas method at normal boiling point)
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
  14.42 (Donnelly et al. 1990)
  12.55 (Kim et al. 1994)
  15.64, 14.92, 15.17 (differential scanning calorimetry in three types of crucibles, Gatta et al. 2000)
Entropy of Fusion, ΔS_{fus} (J/mol K):
  35.2, 33.7, 34.1 (Gatta et al. 2000)
Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F: 0.0315 (mp at 178°C)

Water Solubility (g/m^3 or mg/L at 25°C or as indicated):
  91000 (20–25°C, shake flask-gravimetric, Dehn 1917)
  91800 (13°C, Verschueren 1983)
  89800 (Windholz 1983)
  110000 (Budavari 1989)
  90000 (Dean 1985)

Vapor Pressure (Pa at 25°C):

Henry's Law Constant (Pa m^3/mol at 25°C):

Octanol/Water Partition Coefficient, log K_{OW}:
  –1.02 (Leo et al. 1971)
  –0.95 (shake flask, Cornford 1982)
  –2.38, –0.95 (calculated, Verschueren 1983)
  –1.17 (shake flask, OECD 1981 Guidelines, Geyer et al. 1984)
  –1.08, –1.03 (pH 6.5, pH 12, shake flask-HPLC, Govers et al. 1986)
  –1.14, –1.02 (shake flask, Log P Database, Hansch & Loe 1987)
  –0.99 (recommended, Sangster 1993)
  –1.02 (recommended, Hansch et al. 1995)

Octanol/Air Partition Coefficient, log K_{OA}:

Bioconcentration Factor, log BCF:
  1.73 (alga *chlorella fusca*, wet wt. basis, Geyer et al. 1984)
  –0.699 (alga *chlorella fusca*, calculated-K_{OW}, Geyer et al. 1984)

Sorption Partition Coefficient, log K_{OC}:

Environmental Fate Rate Constants, k, and Half-Lives, $t_{½}$:

Volatilization:

Photolysis:

Oxidation: photooxidation $t_{½}$ = 1.6–16 h in air, based on rate constant for the vapor-phase reaction with OH radical and photooxidation $t_{½}$ = 2048–81927 h in water, based on estimated rate data for reaction with OH radical in aqueous solution (Howard et al. 1991).

Hydrolysis:

Biodegradation: aqueous aerobic biodegradation $t_{½}$ = 24–168 h, based on aqueous aerobic screening test data and aqueous anaerobic biodegradation $t_{½}$ = 96–672 h, based on aqueous aerobic degradation half-life (Howard et al. 1991).

Biotransformation:

Bioconcentration Uptake (k_1) and Elimination (k_2) Rate Constants:

Half-Lives in the Environmental Compartments:

Air: $t_{½}$ = 1.6–16 h, based on estimated photooxidation half-life in air (Howard et al. 1991).

Surface water: $t_{½}$ = 24–168 h, based on estimated aqueous aerobic biodegradation half-life (Howard et al. 1991).

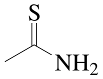
Ground water: $t_{½}$ = 48–336 h, based on estimated unacclimated aqueous aerobic biodegradation half-life (Howard et al. 1991).

Sediment:

Soil: $t_{½}$ = 24–168 h, based on estimated aqueous aerobic biodegradation half-life (Howard et al. 1991)

Biota:

16.1.8.15 Thioacetamide



Common Name: Thioacetamide
Synonym: ethanethioamide, acetothioamide
Chemical Name: thioacetamide
CAS Registry No: 62-55-5
Molecular Formula: C_2H_5NS, CH_3CSNH_2
Molecular Weight: 75.133
Melting Point (°C):
  115.5 (Lide 2003)
Boiling Point (°C):
Density (g/cm^3 at 20°C):
Molar Volume (cm^3/mol):
  84.2 (calculated-Le Bas method at normal boiling point)
Dissociation Constant pK_a:
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
Entropy of Fusion, ΔS_{fus} (J/mol K):
Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F: 0.129 (mp at 115.5°C)

Water Solubility (g/m^3 or mg/L at 25°C):
  163000 (Dean 1985)
  163000 (Budavari 1989)

Vapor Pressure (Pa at 25°C):

Henry's Law Constant (Pa·m^3/mol at 25°C):

Octanol/Water Partition Coefficient, log K_{OW}:
  –0.46, 0 36 (Verschueren 1983)
  –0.26 (shake flask, Log P Database, Hansch & Leo 1987)
  –0.26 (recommended, Sangster 1993)
  –0.26 (recommended, Hansch & Leo 1995)

Octanol/Air Partition Coefficient, log K_{OA}:

Bioconcentration Factor, log BCF:

Sorption Partition Coefficient, log K_{OC}:

Environmental Fate Rate Constants, k, or Half-Lives, $t_{1/2}$:
  Volatilization:
  Photolysis:
  Oxidation: atmospheric $t_{1/2}$ = 3.2–31.7 h, based on estimated rate data for OH radical in air (Howard et al. 1991).
  Hydrolysis: first-order rate constant k = 8.6×10^{-1} h^{-1} at pH 7 and 25°C (Ellington et al. 1987), corresponding to a $t_{1/2}$ = 8064 h (Howard et al. 1991);
    acid rate constant k = 6.0×10^{-2} M^{-1} ± h^{-1}, corresponding to a $t_{1/2}$ = 333 d and base rate constant k = 1.4 M^{-1} ± h^{-1}, corresponding to a $t_{1/2}$ = 289 d (Howard et al. 1991).
  Biodegradation: aerobic biodegradation $t_{1/2}$ = 24–168 h, based on aqueous aerobic screening test data and anaerobic biodegradation $t_{1/2}$ = 96–672 h, based on estimated aqueous aerobic biodegradation half-life (Howard et al. 1991).
  Biotransformation:
  Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants:

Half-Lives in the Environment:

Air: $t_{1/2}$ = 3.2–31.7 h, based on estimated photooxidation half-life in air (Howard et al. 1991).

Surface water: $t_{1/2}$ = 24–268 h, based on estimated aqueous aerobic biodegradation half-life (Howard et al. 1991).

Groundwater: $t_{1/2}$ = 48–336 h, based on estimated unacclimated aqueous aerobic biodegradation half-life (Howard et al. 1991).

Sediment:

Soil: $t_{1/2}$ = 24–168 h, based on estimated aqueous aerobic biodegradation half-life (Howard et al. 1991).

Biota:

16.2 SUMMARY TABLES

TABLE 16.2.1
Summary of physical properties of nitrogen and sulfur containing compounds

Compound	CAS no.	Molecular formula	Molecular weight, MW g/mol	m.p. °C	b.p. °C	Fugacity ratio, F at 25°C*	Molar volume, V_M cm³/mol		pK_a or pK_b
							MW/ ρ at 20°C	Le Bas	
Nitriles:									
Acetonitrile	75-05-8	CH_3CN	41.052	–43.82	81.65	1	52.25	56.3	
Propionitrile	107-12-0	C_2H_5CN	55.079	–92.78	97.14	1	70.45	78.5	
Butyronitrile	109-74-0	C_3H_7CN	69.106	–111.9	117.6	1	87.35	100.7	
Acrylonitrile (2-Propenitrile)	107-13-1	C_2H_3CN	53.063	–83.48	77.3	1	65.83	71.1	
Benzonitrile	100-47-0	C_6H_5CN	103.122	–13.99	191.1	1		107.9	
Adiponitrile	111-69-3	$CN(CH_2)_4CN$	108.141	1	295	1		149.6	
Aliphatic amines:									
Methylamine	74-89-5	CH_3NH_2	31.058	–93.5	–6.32	1		43.8	
Dimethylamine	124-40-3	$(CH_3)_2NH$	45.084	–92.18	6.88	1	68.77	67.5	10.77
Trimethylamine	75-50-3	$(CH_3)_3N$	59.110	–117.1	2.87	1	93.00	93.3	9.8
Ethylamine	75-04-7	$CH_3CH_2NH_2$	45.084	–80.5	16.5	1	66.02	66.0	10.63
Diethylamine	109-89-7	$(C_2H_5)_2NH$	73.137	–49.8	55.5	1	103.45	111.9	10.8
Triethylamine	121-44-8	$(C_2H_5)_3N$	101.910	–114.7	89	1		154.8	10.78
n-Propylamine	107-10-8	$C_3H_7NH_2$	59.110	–84.75	47.22	1	82.41	88.2	10.568
Dipropylamine	142-84-7	$(C_3H_7)_2NH$	101.190	–63	109.3	1			
Diisopropylamine	108-18-9	$i(C_3H_7)_2NH$	101.190	–61	83.9	1			
Tripropylamine	102-69-2	$(C_3H_7)_3N$	143.270	–93.5	156	1			10.66
n-Butylamine	109-73-9	$C_4H_9NH_2$	73.137	–49.1	77.0	1	98.94	110.4	10.64
Isobutylamine	78-81-9	$iC_4H_9NH_2$	73.137	–86.7	67.75	1		110.4	10.41
tert-Butylamine	75-64-9	$(CH_3)_3CNH_2$	73.137	–66.94	44.04	1		110.4	1.685
Di-*n*-butylamine	111-92-2	$(C_4H_9)_2NH$	129.244	–62	159.6	1		199.2	11.25
Tributylamine	102-82-9	$(C_4H_9)_3N$	185.349	–70	216.5	1		288	9.93
Ethylenediamine	107-15-3	$H_2NCH_2CH_2NH_2$	60.098	11.14	117	1			
Ethanolamine	141-43-5	$HOCH_2CH_2NH_2$	61.098	10.5	171	1	60.21	73.4	9.48
Diethanolamine	111-42-2	$(HOCH_2CH_2)_2NH$	105.136	28	268.8	0.934	95.87	126.7	8.88
Triethanolamine	102-71-6	$(HOCH_2CH_2)_3N$	149.188	20.5	335.4	1	132.71	182.1	7.76
Cyclohexylamine	108-91-8	$C_6H_{12}NH$	99.174	–17.8	134	1		117.4	10.66

(*Continued*)

TABLE 16.2.1 (*Continued*)

Compound	CAS no.	Molecular formula	Molecular weight, MW g/mol	m.p. °C	b.p. °C	Fugacity ratio, F at 25°C*	Molar volume, V_M cm³/mol		pK_a or pK_b
							MW/ ρ at 20°C	Le Bas	
Aromatic amines:									
Aniline	62-53-3	$C_6H_5NH_2$	93.127	–6.02	184.17	1	91.15	110.2	4.596
2-Chloroaniline	95-51-2	$Cl(C_6H_4)NH_2$	127.572	–1.9	208.8	1	105.21	131.1	2.661
3-Chloroaniline	108-42-9	$Cl(C_6H_4)NH_2$	127.572	–10.28	230.5	1	104.91	131.1	3.5
4-Chloroaniline	106-47-8	$Cl(C_6H_4)NH_2$	127.572	70.5	232	0.358		131.1	3.982
3,4-Dichloroaniline	95-76-1	$Cl_2C_6H_3NH_2$	162.017	72	272	0.346		152.0	
2,4,6-Trichloroaniline	634-93-5	$C_6H_4Cl_3N$	196.462	78.5	262	0.299		172.9	
o-Toluidine	95-53-4	$CH_3C_6H_4NH_2$	107.153	–14.41	200.3	1	107.32	132.4	4.45
m-Toluidine	108-44-1	$CH_3C_6H_4NH_2$	107.153	–31.3	203.3	1	108.36	132.4	4.71
p-Toluidine	106-49-0	$CH_3C_6H_4NH_2$	107.153	43.6	200.4	0.657	111.40	132.4	5.08
N,N′-Dimethylaniline	121-69-7	$C_6H_5N(CH_3)_2$	121.180	2.42	194.15	1	126.80	154.6	5.15
2,4-Xylidine	95-68-1	$(CH_3)_2C_6H_3NH_2$	121.180	–14.3	214	1		154.6	4.89
2,5-Xylidine	95-78-3	$(CH_3)_2C_6H_3NH_2$	121.180	15.5	214	1		154.6	4.54
2,6-Xylidine	87-62-7	$(CH_3)_2C_6H_3NH_2$	121.180	11.2	215	1	123.12	154.6	3.95
2-Ethylaniline	578-54-1	$C_2H_5C_6H_4NH_2$	121.180	–43	209.5	1		139.6	4.42
3-Ethylaniline	587-02-0	$C_2H_5C_6H_4NH_2$	121.180	–64	214	1		139.6	4.70
4-Ethylaniline	589-16-2	$C_2H_5C_6H_4NH_2$	121.180	–2.4	217.5	1		139.6	5.00
N,N′-Diethylaniline	91-66-7	$C_6H_5N(C_2H_5)_2$	149.233	–38.8	216.3	1		199.0	6.56
Diphenylamine	122-39-4	$(C_6H_5)_2NH$	169.222	53.2	302	0.529	145.88	200.3	0.90
4-Aminobiphenyl	92-67-1	$C_6H_5C_6H_4NH_2$	169.222	53.5	302	0.525		168.8	4.27
Benzidine	92-87-5	$NH_2(C_6H_4)_2NH_2$	184.236	120	401	0.117		213.0	4.66
3,3′-Dichlorobenzidine	91-94-1	$C_{12}H_{10}Cl_2N_2$	253.126	132.5		0.0882		254.8	11.7
α-Naphthylamine	134-32-7	$C_{10}H_7NH_2$	143.185	49.2	300.7	0.579		161.8	3.92
β-Naphthylamine	91-59-8	$C_{10}H_7NH_2$	143.185	113	306.2	0.137		161.8	4.15
N,N′-Bianiline	122-66-7	$(C_6H_5)_2(NH)_2$	184.236	131		0.0912		213.0	13.2
2-Nitroaniline	88-74-4	$C_6H_6N_2O_2$	138.124	71.0	284	0.354		138.7	–0.28
3-Nitroaniline	99-09-2	$C_6H_6N_2O_2$	138.124	113.4	306 dec	0.136		138.7	2.46
4-Nitroaniline	100-01-6	$C_6H_6N_2O_2$	138.124	147.5	332	0.0628	97.00	138.7	1.01
2,4-Dinitroaniline	97-02-9	$(O_2N)_2C_6H_3NH_2$	183.122	180.0		0.0301		167.2	–4.25
2,6-Dinitroaniline	606-22-4	$(O_2N)_2C_6H_3NH_2$	183.122	141		0.0728		167.2	–5.23
3,5-Dinitroaniline	618-87-1	$(O_2N)_2C_6H_3NH_2$	183.122	163		0.0443		167.2	0.229

Nitroaromatic compounds:									
Nitrobenzene	98-95-3	$C_6H_5NO_2$	123.110	5.7	210.8	1	102.28	112.0	
1,2-Dinitrobenzene	528-29-0	$C_6H_4(NO_2)_2$	168.107	116.5	318	0.127		149.4	
1,3-Dinitrobenzene	99-65-0	$C_6H_4(NO_2)_2$	168.107	90.3	291	0.229		149.4	
1,4-Dinitrobenzene	100-25-4	$C_6H_4(NO_2)_2$	168.107	173.5	297	0.0349		149.4	
2-Nitrotoluene	88-72-2	$CH_3C_6H_4NO_2$	137.137	–10.4	222	1	117.93	153.0	
3-Nitrotoluene	99-08-1	$CH_3C_6H_4NO_2$	137.137	15.5	232	1		153.0	
4-Nitrotoluene	99-99-0	$CH_3C_6H_4NO_2$	137.137	51.63	238.3	0.548		153.0	
2,4-Dinitrotoluene (DNT)	121-14-2	$CH_3C_6H_3(NO_2)_2$	182.134	70.5	300 dec	0.358		175.2	
2,6-Dinitrotoluene	606-20-2	$CH_3C_6H_3(NO_2)_2$	182.134	66.0	285	0.396		175.2	
2,4,6-Trinitrotoluene (TNT)	118-96-7	$CH_3C_6H_2(NO_2)_3$	227.131	80.5	240 exp	0.285	137.32	203.7	
1-Nitronaphthalene	86-57-7	$C_{10}H_7NO_2$	173.169	61	304	0.443		176.1	
2-Nitronaphthalene	581-89-5	$C_{10}H_7NO_2$	173.169	79	314	0.295		176.1	
4-Nitrobiphenyl	92-93-3	$C_{12}H_9NO_2$	199.205	114	340	0.134		211.3	
5-Nitro-acenaphthene	602-87-9	$C_{12}H_9NO_2$	199.205	103		0.172		211.3	
Amide and ureas:									
Acetamide	60–35-5	CH_3CONH_2	59.067	80.16	222	0.288		66.9	7.62
Acrylamide	79-06-1	$H_2C{=}CHCONH_2$	71.078	84.5	192.5	0.261		80.8	
Benzamide	55-21-0	$C_6H_5CONH_2$	121.137	127.3	290	0.0992		132.4	
Urea	57-13-6	H_2NCONH_2	60.055	133	dec	0.0872	45.39	58.0	
Nitrosoamines:									
N-Nitrosodimethylamine	62-75-9	$(CH_3)_2NNO$	74.081		152			87.7	
N-Nitrosodiethylamine	55-18-5	$(C_2H_5)_2NNO$	120.134		176.9			130.6	
Di-*n*-propyl nitrosamine	621-64-7	$(C_3H_7)_2NNO$	130.187		206			176.5	
Diphenylnitrosamine	86-30-6	$(C_6H_5)_2NNO$	198.219	66.5	152	0.392		220.5	
Heterocyclic compounds:									
1*H*-Pyrrole	109-97-7	C_4H_5N	67.090	–23.39	129.79	1	69.18	78.2	
1-Methylpyrrole	96-54-8	C_5H_7N	81.117	–56.32	112.81	1		104.0	
Pyrrolidine	123-75-1	C_4H_8NH	71.121	–57.79	86.56	1		96.6	4.453
Imidazole	288-32-4	$C_3H_4N_2$	68.077	89.5	257	0.233		78.9	11.305
Indazole	271-44-3	$C_7H_6N_2$	118.136	148	269	0.0621		130.5	
Indole	120-72-9	C_8H_7N	117.149	52.5	253.6	0.537		133.4	
Indoline	496-15-1	C_8H_9N	119.164		229			140.8	
Pyridine	110-86-1	C_5H_5N	79.101	–41.70	115.23	1	80.56	93.0	5.17
2-Methylpyridine	109-06-8	C_6H_7N	93.127	–66.68	129.38	1	98.61	115.2	5.96
3-Methylpyridine	108-99-6	C_6H_7N	93.127	–18.14	144.14	1	97.35	115.2	5.68
4-Methylpyridine	108-89-4	C_6H_7N	93.127	3.67	145.36	1		115.2	6.00

(*Continued*)

TABLE 16.2.1 *(Continued)*

Compound	CAS no.	Molecular formula	Molecular weight, MW g/mol	m.p. °C	b.p. °C	Fugacity ratio, F at 25°C*	Molar volume, V_M cm^3/mol		pK_a or pK_b
							MW/ ρ at 20°C	Le Bas	
2,3-Dimethylpyridine	583-61-9	C_7H_9N	107.153	–15.5	161.12	1		135.9	6.6
2,4-Dimethylpyridine	108-47-4	C_6H_9N	107.153	–64	158.38	1		135.9	
2,6-Dimethylpyridine	108-48-5	C_7H_9N	107.153	–6.1	144.01	1		135.9	6.72
2,4,6-Trimethylpyridine	108-75-8	$C_8H_{11}N$	121.180	-46	170.6	1		158.1	7.43
Quinolines:									
Quinoline	91-22-5	C_9H_7N	129.159	–14.78	237.16	1		144.7	4.90
Isoquinoline	119-65-3	C_9H_7N	129.159	26.47	243.22	0.967		144.7	5.4
3-Methyl-isoquinoline	1125-80-0	$C_{10}H_9N$	143.185	68	249	0.379		166.9	
2,7-Dimethylquinoline	93-37-8	$C_{11}H_{11}N$	157.212	61	264.5	0.443		189.1	
Benzo[*f*]quinoline	85-02-9	$C_{13}H_9N$	179.217	94	352	0.210		196.3	
Benzo(*h*)quinoline	230-27-3	$C_{13}H_9N$	179.217	52	339	0.543		196.3	
9*H*-Carbazole	86-74-8	$C_6H_4NHC_6H_4$	167.206	246.3	354.69	0.00674		192.9	
7*H*-Dibenzo[*c*,*g*]carbazole	194-59-2	$(C_{10}H_6)_2NH$	267.324	158		0.0496		296.1	
Acridine	260-94-6	$C_{13}H_9N$	179.217	110	344.86	0.147		196.3	5.60
Benz[*a*]acridine	225-11-6	$C_{17}H_{11}N$	229.276					244.8	
Benz[*c*]acridine	225-51-4	$C_{17}H_{11}N$	229.276	132		0.0892		244.8	
Dibenz[*a*,*h*]acridine	53–70–3	$C_{22}H_{14}$	278.346	269.5	524	0.00399		300.0	
Sulfur compounds:									
Carbon disulfide	75-15-0	CS_2	76.141	–112.1	46	1	60.28	66.0	
Dimethyl sulfate	77-78-1	$(CH_3O)_2SO_2$	126.132	–27	188 dec	1		109.7	
Diethyl sulfate	64-67-5	$(C_2H_5O)_2SO_2$	154.185	–24	208	1		138.4	
Dimethyl sulfite	616-42-2	$(CH_3O)_2SO$	110.132		126			100.5	
Dimethyl sulfoxide (DMSO)	67-68-5	$(CH_3)_2SO$	78.133	17.89	189	1		85.7	
Dimethyl sulfone	67-71-0	$(CH_3)_2SO_2$	94.133	108.9	238	0.150		94.0	
Dimethyl sulfide	75-18-3	$(CH_3)_2S$	62.134	–98.24	37.33	1	73.77	77.4	
Dimethyl disulfide	624-92-0	$C_2H_6S_2$	94.199	–84.67	109.74	1	58.78	103.0	
Diethyl sulfide	352-93-2	$C_4H_{10}S$	90.187	–103.91	92.1	1		128.1	
Diethyl disulfide	110-81-6	$C_4H_{10}S_2$	122.252	–101.5	154.0	1		147.4	
Thiols:									
Methanethiol	74-93-1	CH_3SH	48.108	–123	5.9	1	55.52	55.2	10.7
Ethanethiol	75-08-1	C_2H_5SH	62.134	–147.88	35.0	1	74.05	77.4	10.61
Propanethiol	107-03-9	C_3H_7SH	76.161	–113.13	67.8	1	90.55	99.6	
1-Butanethiol (Butyl mercaptan)	109-79-5	$CH_3(CH_2)_3SH$	90.187	–115.7	98.5	1	107.16	121.8	

2-Butanethiol	513-53-1	C_4H_7SH	90.187	–165	85.0	1		121.8	
Benzenethiol	108-98-5	C_6H_5SH	110.177	-14.93	169.1	1	102.34	106.8	6.5
2-Methylbenzenethiol	137-06-4	C_7H_8S	124.204	15	195	1		129.0	
3-Methylbenzenethiol	108-40-7	C_7H_8S	124.204	–20	195	1		129.0	
4-Methylbenzenethiol	106-45-6	C_7H_8S	124.204	43	195	0.666		129.0	
Thiophenes:									
Thioazole	288-47-1	C_3H_3NS	85.128	–33.62	118	1		85.2	
Thiophene	110-02-1	C_4H_4S	84.140	–38.21	84.0	1	79.02	88.1	
2-Methylthiophene	554-14-3	C_5H_6S	98.167	–63.4	112.6	1		110.3	
3-Methylthiophene	616-44-4	C_5H_6S	98.167	–69	115.5	1		110.3	
Benzo[*b*]thiophene	95-15-8	C_8H_6S	134.199	32	221	0.854		139.7	
Dibenzothiophene	132-65-0	$C_{12}H_8S$	184.257	98.2	332.5	0.191		191.3	
Thianthrene	92-85-3	$(C_6H_4)_2S_2$	216.322	159.3	365	0.0481		210.9	
Thiobenzamide	2227-79-4	$C_6H_5CSNH_2$	137.203	117		0.125		135.8	
Thiourea	62-56-6	H_2NCSNH_2	76.121	178		0.0315	72.84	76.2	2.03
Thioacetamide	62-55-5	CH_3CSNH_2	75.133	115.5		0.129		84.2	

* Assuming ΔS_{fus} = 56 J/mol K

TABLE 16.2.2
Summary of selected physical-chemical properties of nitrogen and sulfur containing compounds at 25°C.

Compound	Selected properties						Henry's law constant	
	Vapor pressure		Solubility				H/(Pa·m³/mol)	
	P^S/Pa	P_L/Pa	S/(g/m³)	C^S/(mol/m³)	C_L/(mol/m³)	log K_{OW}	calcd P/C	exptl
Nitriles:								
Acetonitrile	11840	11840	miscible			–0.34		2.75
Propionitrile	5950	5950	103000	1870.0	1870.0	0.16	3.182	3.8
Butyronitrile	2546	2546	33000	477.5	477.5			5.263
Benzonitrile	100	100	2000	19.39	19.39	1.55	5.156	
Acrylonitrile (2-Propenitrile)	11000	11000	75500	1423	1423	0.25	7.731	11.14
Adiponitrile	0.3066	0.3066	8000	73.96	73.96	–0.32	0.0041	
Aliphatic amines:								
Methylamine	357300	357300	miscible			–0.57		1.125
Dimethylamine	206200	206200	miscible			–0.38		1.8
Trimethylamine	219300	219300	miscible			0.27		6.67
Ethylamine	141650	141650	miscible			–0.13		1.012
Diethylamine	31490	31490	miscible			0.43		2.60
Triethylamine	7610	7610	55000	540	540	1.64	14.099	
n-Propylamine	40740	40740	miscible			0.48		1.274
Dipropylamine			53000	520	520			
Diisopropylamine			12390	122				
Tripropylamine			220	1.536	1.54	2.79		
n-Butylamine	13650	13650	miscible			0.97		1.526
Isobutylamine	18760	18760	miscible			0.73		
t-Butylamine	48260	48260	miscible			0.4		
Di-*n*-butylamine	304	304	4700	36.37	36.37	2.83	8.359	
Tributylamine	5330	5330	40	0.216	0.216		2.47×10^4	
Ethanolamine	34.66	34.66	miscible			–1.31		
Diethanolamine	0.0373	0.0399	miscible			–1.43		
Triethanolamine	4.79×10^{-4}	4.79×10^{-4}	miscible			–1.59		
Cyclohexylamine	1173	1173	miscible			1.49		
Diphenylamine	0.0612	0.115	300	1.773	3.338	3.45	0.035	
α-Naphthylamine	0.254	0.45				2.23		
β-Naphthylamine	0.035	0.248	6.4	0.045	0.317	2.34		
4-Aminobiphenyl						2.83		

Aromatic amines:								
Aniline	65.19	65.19	36070	387.4	387.35	0.90	0.168	12.16
2-Chloroaniline	22.66	22.66	3800	29.79	29.79	1.90	0.761	
3-Chloroaniline	9.53	9.530	5440	42.64	42.64	1.88	0.223	
4-Chloroaniline	2.33	6.873	3000	23.52	69.37	1.83	0.099	
3,4-Dichloroaniline	1.3	3.746	92.05	0.568	1.637	2.67	2.289	
2,4,6-Trichloroaniline	0.00626	0.021				3.694		
o-Toluidine	13.3	13.30	15000	139.98	139.98		0.095	
m-Toluidine	36	36.0	15030	140.26	140.26	1.44	0.257	
p-Toluidine	45	61.48	7350	68.59	93.70	1.4	0.656	
N,N′-Dimethylaniline	107	107.0	1105	9.119	9.119	2.31	11.734	
2,4-Xylidine	20.5	20.50	5900	48.69	48.69		0.421	
2,5-Xylidine			5000	41.26	41.26			
2,6-Xylidine	670	670.0	4700	38.79	38.79	1.94	17.275	
2-Ethylaniline			7500	61.89	61.89	1.93		
4-Ethylaniline	13.5	13.50	5100	42.09	42.09	1.96	0.321	
N,N′-Diethylaniline	9.7	9.70	670	4.49	4.49		2.161	
Benzidine	1.0×10^{-6}	1.06×10^{-5}	400	2.17	23.1	1.81	4.61×10^{-7}	
3,3′-Dichlorobenzidine	5.6×10^{-5}	6.41×10^{-4}	3.1	0.0122	0.140	3.51	0.005	
N,N′-Bianiline	0.0035		0.252	0.0014	0.0154	3.82	3.45×10^{-4}	
2-Nitroaniline	0.62	1.851	1200	8.687	25.93	1.78		
4-Nitroaniline	0.035	0.589	800	5.792	97.50	1.31		
2,4-Dinitroaniline						4.1		
Nitroaromatic compounds:								
Nitrobenzene	20	20.0	1900	15.43	15.43	1.85	1.296	
1,2-Dinitrobenzene	0.0052	0.0433						
1,3-Dinitrobenzene	0.0081	0.0348	546	3.25	13.94	1.49	0.002	
1,4-Dinitrobenzene	13.3	386.63	442	2.63	76.43	2.37	5.059	
2-Nitrotoluene	17.9	17.90	651.42	4.75	4.75	2.30	3.768	
3-Nitrotoluene	27.2	27.20	499.19	3.64	3.64	2.45	7.473	
4-Nitrotoluene	0.653	1.2004	254.4	1.86	3.41	2.37	0.352	
2,4-Dinitrotoluene (DNT)	0.133	0.3705	270	1.48	4.13	2.01	0.090	
2,6-Dinitrotoluene	0.0767	0.1952	200			1.72	0.070	
2,4,6-Trinitrotoluene (TNT)	0.00107	0.0038	210	0.925	3.29			
1-Nitronaphthalene	0.702 0.0312	0.072	9.82	0.057	0.132	3.19	3.50	
2-Nitronaphthalene			9.24	0.053	0.183			
4-Nitrobiphenyl			1.231	6.18×10^{-3}	0.045	3.78		
5-Nitro-acenaphthene			0.91	4.57×10^{-3}	0.026			

(*Continued*)

TABLE 16.2.2 *(Continued)*

	Selected properties						Henry's law constant	
	Vapor pressure		Solubility				H/(Pa·m³/mol)	
Compound	P^S/Pa	P_L/Pa	S/(g/m³)	C^S/(mol/m³)	C_L/(mol/m³)	log K_{OW}	calcd P/C	exptl
Amides: RCONH2								
Acetamide (ethanamide)	2.44	8.3562	408000	6907.1	23650	–1.26	3.53×10^{-4}	
Acrylamide	0.415	1.5900	2050000	2884	11050	–0.9	1.44×10^{-4}	
Benzamide	0.00522	0.0544	14000	1692	17630	0.64	4.52×10^{-5}	
Urea: (NH2)2C=O								
Urea	0.0016	0.0186	1000000	16650	$1.93\text{x}10^5$	–2.11	9.61×10^{-8}	
Nitrosoamines:								
N-Nitrosodimethylamine			miscible			–0.57		3.343
Di-*n*-propyl nitrosamine	27		9900	76.04		1.31	0.355	
Diphenyl nitrosamine	13.33	34.27	35.10	0.116	0.299	3.13	114.6	
Heterocyclic compounds:								
1*H*-Pyrrole	1100	1100	45000	670.7	670.7	0.75	1.640	
1-Methylpyrrole	3312							
Indazole			827	7.00	100.43			
Indole	2.24	4.187	1874	16.00	29.90	2	0.140	
Indoline			10800	90.63				
Pyridine	2775	2775	miscible			0.65		0.895
2-Methylpyridine	1496	1496	miscible			1.11		1.01
3-Picoline	1333	1333	miscible			1.2–1.24		0.788
4-Picoline	757	757	miscible			1.22		0.601
2,3-Dimethylpyridine	426		104000	970.6				0.725
2,4-Dimethylpyridine	456	456	miscible					0.678
2,6-Dimethylpyridine	746	746	miscible					1.06
2,4,6-Trimethylpyridine	5170	5170	35700	294.6	294.6		17.549	
Quinolines:								
Quinoline	1.21	1.21	6110	47.31	47.31	2.06	0.026	
Isoquinoline	670	693	4521	35.00	36.20	2.08	19.141	
2,7-Dimethylquinoline			1795	11.42	24.77			
Benzo[*f*]quinoline		0.0067	76.1	0.42	2.02	3.20	0.0096	
Benzo[*h*]quinoline	0.03	0.0555						
9*H*-Carbazole	0.0933	14.976	1.03	0.006	0.989	3.80	15.146	
7*H*-Dibenzo[*c,g*]carbazole	1.3×10^{-7}	2.5×10^{-6}	0.063	0.236	4.532	5.75		

Acridine	0.0065	0.0451	38.5	0.215	1.492	3.4	0.030	
Benz[*a*]acridine						4.45		
Sulfur compounds:								
Carbon disulfide	48210	48210	2100	27.584	27.584		1747.75	
Dimethyl sulfate	128	128						
Diethyl sulfate	49.1	49.1						
Dimethyl sulfoxide (DMSO)	80.0	80.0	253000	354.8	354.8	–1.35	0.225	
Dimethyl sulfone	5.16	34.17				–1.41	200.83	
Dimethyl sulfide	64650	64650	20000	321.9			7.72	
Dimethyl disulfide	4000	4000	6300	66.88	66.88		59.81	
Diethyl sulfide	7782	7782				1.95		
Diethyl disulfide	689	689						
Thiols:								
Methanethiol	201980	201980						
Ethanethiol	70000		15000				289.94	
Propanethiol	20635	20635				1.81		
1-Butanethiol	6070	6070	597	6.62	6.62	2.28	916.94	
2-Butanethiol	10790	10790						
Benzenethiol	397	397				2.52		
2-Methylbenzenethiol	87.4	87.4						
3-Methylbenzenethiol	76.6	76.60						
4-Methylbenzenethiol	85.2	128.3						
Thiophenes:								
Thioazole	2287							
Thiophene	10620	8000	3015	35.833	35.833	1.81	223.3	224
2-Methylthiophene	3318							
3-Methylthiophene	2953							
Benzo[*b*]thiophene	26.66	26.7	130	0.969	1.107	3.12	24.1	
Dibenzothiophene	0.267		1.11	0.006		4.38	44.3	
Thiourea			90000	1182	36833	–0.99		
Thioacetamide			163000	2170	15722	–0.26		

TABLE 16.2.3
Suggested half-life classes for nitrogen and sulfur containing compounds in various environmental compartments at 25°C

Compound	Air class	Water class	Soil class	Sediment class
Acetonitrile	6	5	5	6
Propionitrile	6	5	5	6
Acrylonitrile (2-Propenitrile)	3	4	4	5
Dimethylamine	1	3	4	5
Ethylamine	2	3	4	5
Eiethylamine	1	2	2	3
n-Butylamine	2	3	3	4
Ethanolamine	1	3	3	4
Diethanolamine	1	4	4	5
Cyclohexylamine	1	3	3	4
Aniline	1	4	4	6
2-Chloroaniline	3	4	5	6
4-Chloroaniline	1	4	4	5
o-Toluidine	1	3	3	4
N,N'-Dimethylaniline	1	4	5	6
2,6-Xylidine	1	4	5	6
Diphenylamine	1	4	5	6
Benzidine	1	4	4	5
3,3'-Dichlorobenzidine	1	1	5	6
N,N'-Bianiline	1	3	3	4
α-Naphthylamine	1	4	4	6
β-Naphthylamine	1	4	4	6
Nitrobenzene	1	6	6	7
2-Nitrotoluene	2	3	6	7
4-Nitrotoluene	2	3	6	7
2,4-Dinitrotoluene (DNT)	2	3	6	7
2,4,6-Trinitrotoluene (TNT)	1	2	6	7
Acetamide	2	4	4	5
Benzamide	2	4	4	5
n-Nitrosodimethylamine	1	2	6	7
n-Nitrosodiethylamine	1	2	6	7
Di-*n*-propyl nitrosoamine	1	2	6	7
Diphenyl nitrosoamine	1	2	6	7
Pyridine	5	5	6	7
3-Methylpyridine	5	5	6	7
4-Methylpyridine	5	5	6	7
Quinoline	3	4	5	6
Dimethyl sulfate	4	2	2	3
Diethyl sulfate	2	2	3	4
Thiophene	3	3	6	7
Benzo[*b*]thiophene	4	5	6	7
Thiourea	1	4	4	5
Thioacetamide	2	4	4	5

TABLE 16.2.3 (*Continued*)

where,

Class	Mean half-life (hours)	Range (hours)
1	5	< 10
2	17 (~ 1 day)	10–30
3	55 (~ 2 days)	30–100
4	170 (~ 1 week)	100–300
5	550 (~ 3 weeks)	300–1,000
6	1700 (~ 2 months)	1,000–3,000
7	5500 (~ 8 months)	3,000–10,000
8	17000 (~ 2 years)	10,000–30,000
9	~ 5 years	> 30,000

16.3 REFERENCES

Abraham, M.H. (1984) Thermodynamics of solution of homologous series of solutes in water. *J. Chem. Soc., Farad. Trans. 1* 80, 153–181.

Abraham, M.H., Le J., Acree, Jr., W.E., Carr, P.W., Dallas, A.J. (2001) The solubility of gases and vapours in dry octan-1-ol at 298 K. *Chemosphere* 44, 855–863.

Aim, K. (1994) Saturated vapor pressure measurements on isomeric mononitrotoluenes at temperatures between 380 and 460 K. *J. Chem. Eng. Data* 39, 591–594.

Albersmeyer, W. (1958) Quantitative determination of aromatic hydrocarbons in aqueous solutions. *Gas-U. Wasserfach* 99, 269.

Albert, A. (1966) *The Acridines.* Edward Arnold, London.

Alcorn, C.J., Simpson, R.J., Leahy, D.E., Peters, T.J. (1993) Partition and distribution coefficients of solutes and drugs in brush border membrane vesicles. *Biochem. Pharm.* 45, 1775–1782.

Alexander, M., Lustigman, B.K. (1966) Effects of chemical structure on microbial degradation of substituted benzenes. *J. Agric. Food Chem.* 14, 410–413.

Altschuh, J., Brüggemann, Santl, H., Eichinger, G., Piringer, O.G.(1999) Henry's law constants for a diverse set of organic chemicals: Experimental determination and comparison of estimation methods. *Chemosphere* 39, 1871–1887.

Ambrose, D. Gundry, H.A. (1980) The vapour pressure of *p*-nitrotoluene. *J. Chem. Thermodyn*. 12, 559–561.

Anbar, M., Meyerstein, D., Neta, P. (1966) The reactivity of aromatic compounds toward hydroxyl radicals. *J. Phys. Chem.* 70, 2661–2662.

Anbar, M., Neta, P. (1967) A compilation of specific bimolecular rate and hydroxyl radical with inorganic and organic compounds in aqueous solution. *Int. J. Appl. Radiation Isotopes* 18, 493–523.

Anderson, T.A., Beauchamp, J.J., Walton, B.T. (1991) Organic chemicals in the environment. *J. Environ. Qual.* 20, 420–424.

Andersson, J.T., Schrăder, W. (1999) A method for measuring 1-octanol-water partition coefficients. *Anal. Chem.* 71, 3610–3614.

Andon, R.J.L., Cox, J.D. (1952) Phase relationships in pyridine series. Part I. The miscibility of some pyridine homologues with water. *J. Chem. Soc.* 4601–4606.

Andon, R.J.L., Cox, J.D., Herington, E.F.G. (1954) Phase relationships in the pyridine series. Part V. The thermo-dynamic properties of dilute solutions of pyridine bases in water at 25°C and 40°C. *J. Chem. Soc.* 3188–3196.

Appleton, H., Banerjee, S., Pack, E., Sikka, H. (1978) Fate of 3,3'-dichlorobenzidine in aquatic environment. In: *Pergamon Series in Environmental Science* 1, 473–474.

Appleton, H., Sikka, H. (1980) Accumulation, elimination and metabolism of dichlorobenzidine in bluegill sunfish. *Environ. Sci. Technol.* 14, 50–54.

Arbuckle, W.B. (1983) Estimating activity coefficients for use in calculating environmental parameters. *Environ. Sci. Technol.* 17, 537–542.

Arey, J., Atkinson, R., Aschmann, S.M., Schuetzle, D. (1990) Experimental investigation of the atmospheric chemistry of 2-methyl-1-nitronaphthalene and a comparison of predicted nitroarene concentrations with ambient air data. In: *Polycyclic Aromatic Compounds*. Vol. 1(1–2), pp. 33–50. Gordon and Breach Science Publishers, United Kingdom.

Armbrust, K.L. (2000) Pesticide hydroxyl radical rate constants: measurements and estimates of their importance in aquatic environments. *Environ. Toxicol. Chem*. 19, 2175–2180.

Ashton, J.G., Eidimoff,. M.L., Forster, W.S. (1939) The heat capacity and entropy, heats of fusion and vaporization and the vapor pressure of dimethylamine. *J. Am. Chem. Soc*. 61, 1539–1543.

Aston, J.G., Sagenkahn, M.L., Szasz, G.J., Moessen, G.W., Zuhr, H.F. (1944) The heat capacity and entropy, heats of fusion and vaporization and the vapor pressure of trimethylamine. The entropy from spectroscopic and molecular data. *J. Am. Chem. Soc*. 66, 1171–1177.

Atkinson, R. (1985) Kinetics and mechanisms of the gas-phase reactions of hydroxyl radicals with organic compounds under atmospheric conditions. *Chem. Rev.* 85, 69–201.

Atkinson, R. (1987) A structure-activity relationship for the estimation of rate constants for the gas-phase reactions of OH radicals with organic compounds. *Int. J. Chem. Kinetics* 19, 799–828.

Atkinson, R. (1989) Kinetics and mechanisms of the gas-phase reactions of the hydroxyl radical with organic compounds. *J. Phys. Chem. Ref. Data*, Monograph No. 1, 1–246.

Atkinson, R. (1991) Kinetics and mechanisms of the gas-phase reactions of NO_3 radical with organic compounds. *J. Phys. Chem. Ref. Data* 20(3), 459–507.

Atkinson, R., Aschmann, S.M., Arey, J., Zielinska, B. (1989) Gas-phase atmospheric chemistry of 1- and 2-nitronaphthalene and 1,4-naphthoquinone. *Atmos. Environ.* 23(12), 2679–2690.

Atkinson, R., Aschmann, S.M., Fitz, D.R., Winer, A.M., Pitts, Jr., J.N. (1982) Rate constants for the gas-phase reactions of O_3 with selected organics at 296 K. *Int. J. Chem. Kinet.* 14, 13–18.

Atkinson, R., Aschmann, S.M., Carter, W.P.L. (1983) Kinetics of the reactions of ozone and hydroxyl radicals with furan and thiophene at 298 ± 2 K. *Int. J. Chem. Kinetics* 15, 51–61.

Atkinson, R., Aschmann, S.M., Winer, A.M., Carter, W.P.L. (1985) Rate constants for the gas-phase reactions of the NO_3 radicals with furan, thiophene, and pyrrole at 295 ± 1 K and atmospheric pressure. *Environ. Sci. Technol.* 19, 87–90

Atkinson, R., Baulch, D.L., Cox, R.A., Hampson Jr., R.F., Kerr, J.A., Troe, J. (1992) Evaluated kinetic and photochemical data for atmospheric chemistry supplement IV. *J. Phys. Chem. Ref. Data* 21, 1125–1568.

Atkinson, R., Carter, W.P.L. (1984) Kinetics and mechanisms of the gas-phase reactions of ozone with organic compounds under atmospheric conditions. *Chem. Rev.* 84, 437–470.

Atkinson, R., Perry, R.A., Pitts, J.N., Jr. (1977) Rate constants for the reaction of the OH radical with CH_3SH and CH_3NH_2 over the temperature range 299–426 K. *J. Chem. Phys.* 66, 1578–1581.

Atkinson, R., Perry, R.A., Pitts, J.N., Jr. (1978a) Rate constants for the reaction of OH radicals with COS, CS_2, and CH_3SCH_3 over the temperature range 299–430 K. *Chem. Phys. Lett.* 54, 14–18.

Atkinson, R., Perry, R.A., Pitts, J.N., Jr. (1978b) Rate constants for the reactions of hydroxyl radical with dimethylamine, trimethylamine, and ethylamine over the temperature range 298–426 K. *J. Chem. Phys.* 68, 1850–1853.

Atkinson, R., Pitts, Jr., J.N., Aschmann, S.M. (1984) Tropospheric reactions of dimethyl sulfide with NO_3 and OH radicals. *J. Phys. Chem.* 88, 1584–1587.

Atkinson, R., Tuazon, E.C., Wallington, T.J., Aschmann, S.M., Arey, J., Winer, A.M., Pitts, J.N., Jr. (1987) Atmospheric chemistry of aniline, N,N-dimethylaniline, Pyridine, 1,3,5-triazine, and nitrobenzene. *Environ. Sci. Technol.* 21, 64–72.

Aubry, M., Mayoral, M.N., Villardry, P. (1975) Determination of the vapor pressure of low volatility compounds by gas chromatography. Application to dibenzothiophene. *Boll. Soc. Chim. Fr.* 3–4 of Pt.1, 500–502.

Bailey, G.W., White, J.L., Rothberg T. (1968) Adsorption of organic herbicides by montmorillonite: Role of pH and chemical character of adsorbate. *Soil Sci. Am. Proc.* 32, 222–234.

Baird, R., Caroma, L., Jenkins, R.L. (1977) Behavior of benzidine and other aromatic amines in aerobic waste water treatment. *J. Water Pollut. Control Fed.* 49, 1606–1615.

Banerjee, S., Howard, P.H. (1988) Improved estimation of solubility and partitioning through correction of UNIFAC-derived activity coefficients. *Environ. Sci. Technol.* 22, 839–841.

Banerjee, S., Howard, P.H., Lande, S.S. (1990) General structure-vapor pressure relationships for organics. *Chemosphere* 21, 1173–1180.

Banerjee, S., Sikka, H.C., Gray, D.A., Kelly, C.M. (1978) Photodegradation of 3,3′-dichlorobenzidine. *Environ. Sci. Technol.* 12, 1425–1427.

Banerjee, S., Yalkowsky, S.H., Valvani, S.C. (1980) Water solubility and octanol/water partition coefficients of organics. Limitations of the solubility-partition coefficient correlations. *Environ. Sci. Technol.* 14, 1227–1229.

Barnes, I., Bastian, V., Becker, K.H., Martin, D. (1989) Fourier transform IR studies of the reactions of dimethyl sulfoxide with OH, NO_3 and Cl radicals. In: *Biogenic Sulfur in the Environment*. Salzmann, E.S., Cooper, W.J., Eds. ACS Symposium Series 393, pp. 476–488

Barrows, M.E. et al. (1978) *Am. Chem. Soc. Div. Environ. Chem.* 18, 345–346.

Basu, D.K., Hsu, R.S., Neal, M.W., Santodonato, J., Sugatt, R.H., Bayard, S., Bayliss, D.L., Hiremath, C.B., Vaughn-Dellarco, V. (1983) *Health Assessment Document for Acrylonitrile*. Final Report. EPA-600/8–82–007F, U.S. E.P.A., Research Triangle Park, N.C., PB84–149152. U.S. Department of Commerce, NTIS.

Bebahani, Gh.R.R., Hogan, P., Waghorne, W.E. (2002) Ostwald concentration coefficients of acetonitrile in aqueous mixed solvents: A new rapid method for measuring the solubility of volatile solutes. *J. Chem. Eng. Data* 47, 1290–1292.

Bechalany, A., Röthlisberger, T., El Tayler, N., Testa, B. (1989) Comparison of various non-polar stationary phases used for assessing lipophilicity. *J. Chromatog*. 473, 115–124.

Becker, K.H., Biehl, H.M., Bruckmann, P., Fink, E.H., Führ, F., Klöpffer, W., Zellner, R., Zetzsch, C. (1984) Hydroxyl radical reaction rate constants and tropospheric lifetimes of selected environmental chemicals. *Kernforschungsanlage.* Jülich, GmbH. November 1984, ISSN 0343–7639.

Beneš M., Dohnal, V. (1999) Limiting activity coefficients of some aromatic and aliphatic nitro compounds in water. *J. Chem. Eng. Data* 44, 1097–1102.

Benkelberg, H.-J., Hamm, S., Warneck, P. (1995) Henry's law coefficients for aqueous solutions of acetone, acetaldehyde and acetonitrile, and equilibrium constants for the addition compounds of acetone and acetaldehyde with bisulfite. *J. Atmos. Chem.* 20, 17–34.

Berliner, J.F.T., May, O.E. (1925) Studies in vapor pressure. I. The nitro-anilines. *J. Am. Chem. Soc.* 47, 2350–2356.

Berthod, A., Han, Y.I., Armstrong, D.W. (1988) Centrifugal partition chromatography. V. Octanol-water partition coefficients, direct and indirect determination. *J. Liq. Chromatogr.* 11(7), 1441–1456.

Bintein, S., Devillers, J., Karcher, W. (1993) Nonlinear dependence of fish bioconcentration on *n*-octanol/water partition coefficient. *SAR and QSAR in Environ. Res.* 1, 29–39.

Bittrich, H.J., et al. (1962) *J. Prakt. Chem.* 17, 250.-reference in Boublik et al. 1984.

Bittrich, H.J., Kauer, E. (1962) *Z. Phys. Chem.* 219, 224.-reference in Boublik et al. 1984.

Bocek, K. (1976) Relations among activity coefficients, partition coefficients and solubilities. *Experientia Suppl.* 23, 231–240.

Boethling, R.S., Alexander, M. (1979) Microbial degradation of organic compounds at trace levels. *Environ. Sci. Technol.* 13, 989–991.

Bollag, J.M., Blattmann, P., Lannio, T. (1978) Adsorption and transformation of four substituted anilines in soil. *J. Agric. Food Chem.* 26, 1302–1306.

Booth, H.S., Everson, H.E. (1948) Hydrotropic solubilities. Solubilities in 40 per cent sodium xylenesulfonate. *Ind. Eng. Chem.* 40(8), 1491–1493.

Börnick, H., Eppinger, P., Grischek, T., Worch, E. (2001) Simulation of biological degradation of aromatic amines in river bed sediments. *Water Res*. 35, 619–624.

Boublik, T., Aim, K.I. (1972) *Collection Czech. Chem. Comm.* 37, 3513.—reference from Boublik et al. 1984.

Boublik, T., Fried, V., Hala, E. (1973) *The Vapour Pressures of Pure Substances*. Elsevier, Amsterdam, The Netherlands.

Boublik, T., Fried, V., Hala, E. (1984) *The Vapour Pressures of Pure Substances*. Second Edition, Elsevier, Amsterdam, The Netherlands.

Boyd, S.A., Kao, C.W., Suflita, J. (1984) Fate of 3,3′-dichlorobenzidine in soil: Persistence and binding. *Environ. Toxicol. Chem.* 3, 201–208.

Bridie, A.L., Wolff, C.J.M., Winter, M. (1979) BOD and COD of some petrochemicals. *Water Res.* 13, 627–630.

Briggs, G.G. (1981) Theoretical and experimental relationships between soil adsorption, octanol-water partition coefficients, water solubilities, bioconcentration factors and Parachor. *J. Agric. Food Chem.* 29, 1050–1059.

Brooke, D.N., Nielsen, I., De Bruijn, Hermens, J. (1990) An interlaboratory evaluation of the stir-flask method for the determination of octanol-water partition coefficients (LOG P_{OW}). *Chemosphere* 21, 119–133.

Brown, H.C., Barbaras, G.K. (1947) Dissociation of the compounds of trimethylboron with pyridine and the picolines; evidence for the steric nature of the ortho effect. *J. Am. Chem. Soc*. 69, 1137–1144.

Brown, I. (1952) Liquid-vapour equilibria. III. The systems benzene-heptane, hexane-chlorobenzene, and cyclohexane-nitrobenzene. *Austral. J. Sci. Res.* 5A, 530–540.—reference from Boublik et al. 1984

Budavari, S., Editor (1989) *The Merck Index. An Encyclopedia of Chemicals, Drugs and Biologicals.* 11th Edition, Merck & Co. Rahway, NJ.

Butler, J.A.V., Ramchandani, C.N. (1935) The solubility of non-electrolytes. Part II. The influence of the polar group on the free energy of hydration of aliphatic compounds. *J. Chem. Soc.* 952–955.

Buttery, R.G., Ling, J.C., Guadagni, D.G. (1969) Food volatiles. Volatilities of aldehydes, ketones, and esters in dilute water solution. *J. Agric. Food Chem.* 17, 385–389.

Buxton, G.V., Greenstock, C.L., Helman, W.P., Ross, A.B. (1986) Critical review of rate constants for reactions of hydrated electrons, hydrogen atoms and hydroxyl radicals (-OH/-O^-) in aqueous solution. *J. Phys. Chem. Ref. Data* 17, 513–817.

Bysshe, S.E. (1982) Bioconcentration factor in aquatic organisms. In: *Handbook of Chemical Property Estimation Methods: Environmental Behavior of Organic Compounds.* Lyman et al. Editors, Chapter 5, pp. 5–1 to 5–30, McGraw-Hill Book Company, New York.

Cabani, S., Conti, G., Lepori, L. (1971) Thermodynamic study on aqueous dilute solutions of organic compounds: Part 1. Cyclic amines. *Trans. Farad. Soc.* 67, 1933–1942.

Calamari, D., Da Gasso, R., Galassi, S., Provine, A., Vighi, M. (1980) Biodegradation and toxicity of selected amines on aquatic organisms. *Chemosphere* 9, 753–762.

Callahan, M.A., Slimak, M.W., Gabel, N.W., May, I.P., Fowler, C.F., Freed, J.R., Jennings, P., Durfee, R.L., Whitemore, F.C., Maestri, B., Mabey, W.R., Holt, B.R., Gould, C. (1979) *Water Related Environmental Fate of 129 Priority Pollutants.* EPA-440-4-79-029a,b. Versar, Inc., Springfield, VA.

Campbell, J.R., Luthy, R.G. (1985) Prediction of aromatic solute partition coefficient using the UNIFAC group contribution model. *Environ. Sci. Technol.* 19, 980–985.

Canton, J.H., Sloof, W., Kool, H.J., Struys, J., Pouw, T.J.M., Wegman, R.C.C., Piet, G.J. (1985) Toxicity, biodegradability and accumulation of a number of chlorine/nitrogen containing compounds for classification and establishing water quality criteria. *Regulat. Toxicol. Pharmacol.* 5, 123–131.

Capel, P.D., Larson, S.J. (1995) A chemodynamic approach for estimating losses of target organic chemicals from water during sample holding time. *Chemosphere* 30, 1097–1107

Carlier, P., Hannachi, H., Mouvier, G. (1986) The chemistry of carbonyl compounds in the atmosphere - A review. *Atmos. Environ.* 20, 2079–2099.

Carlson, R.M., Carlson, R., Kopperman, H.L. (1975) Determination of partition coefficients by liquid chromatography. *J. Chromatogr.* 107, 219–223.

Chao, J., Lin, C.T., Chung, T.H. (1983) Vapor pressure of coal chemicals. *J. Phys. Chem. Ref. Data* 12, 1033–1063.

Chao, J., Gadalla, N.A.M., Gammon, B.E., Marsh, K.N., Rodgers, A.S., Somayajulu, G.R., Wilhoit, R.C. (1990) Thermodynamic and thermophysical properties of organic nitrogen compounds. Part I. Methanamine, ethanamine, 1-and 2-propanamine, benzenamine, 2-,3-, and 4-methylbenzenamine. *J. Phys. Chem. Ref. Data* 19(6), 1547–1615.

Chessells, M., Hawker, D.W., Connell, D.W. (1992) Influence of solubility in lipid on bioconcentration of hydrophobic compounds. *Ecotoxicol. Environ. Saf.* 23, 260–273.

Chiou, C.T. (1981) Partition coefficient and water solubility in environmental chemistry. In: *Hazard Assessment of Chemicals, Current Developments.* Volume I, pp. 117–153. Academic Press, New York.

Chiou, C.T. (1985) Partition coefficients of organic compounds in lipid-water systems and correlations with fish bioconcentration factors. *Environ. Sci. Technol.* 19, 57–62.

Chiou, C.T., Schmedding, D.W. (1981) Measurement and interrelation of octanol-water partition coefficient and water solubility of organic chemicals. In: *Test Protocols for Environmental Fate and Movement of Toxicants. J. Assoc. Anal. Chem.*, Arlington, VA.

Chiou, C.T., Schmedding, D.W., Manes, M. (1982) Partitioning of organic compounds in octanol-water system. *Environ. Sci. Technol.* 16, 4–10.

Cichna, M., Markl, P., Huber, J.F.K. (1995) Determination of true octanol-water partition coefficients by means of solvent generated liquid-liquid chromatography. *J. Pharmaceu. Biomed. Anal.* 11, 339–351.

Ciusa, R. (1922) Doebner's reaction. *Gazz. Chim. Ital.* 52(II), 43–48.

Clarke, F.H. (1984) Ionization constants by curve-fitting: Application to the determination of partition coefficients. *J. Pharm. Sci.* 73, 226–230.

Clarke, F.H., Cahoon, N.M. (1987) Ionization constants by curve-fitting: Application to the determination of partition and distribution coefficients of acids and bases and their ions. *J. Pharm. Sci.* 76(8), 611–620.

Collander, R. (1951) Partition of organic compounds between higher alcohols and water. *Acta. Chem. Scand.* 5, 774–780.

Collet, A.R., Johnson, J. (1926) Solubility relations of isomeric organic compounds VI. Solubility of the nitroanilines in various liquids. *J. Phys. Chem.* 30, 70–82.

Conder, J.M., La Point, T.W., Bowen, A.T. (2004) Preliminary kinetics and metabolism of 2,4,6-trinitrotoluene and its reduced metabolites in an aquatic oligochaete. *Aqua. Toxicol.* 69, 199–213.

Cornford, E.M., (1982) Correlation between liquid partition coefficients and surface permeation in Schistosoma japonicum. *J. Membr. Biol.* 64, 217–224.

Coulson, E.A., Cox, J.D., Herington, E.F.G., Martin, J.F. (1959) The preparation and physical properties of the pure lutidines. *J. Chem. Soc.* (London) 1934–1940.

Cox, R.A., Sheppard, D. (1980) *Nature* 284, 330.

D'Amboise, M., Hanai, T. (1982) Hydrophobicity and retention in reversed phase liquid chromatography. *J. Liq. Chromatogr.* 5(2), 229–244.

Darnall, K.R., Lloyd, A.C., Winer, A.M., Pitts, Jr., J.N. (1976) Reactivity scale for atmospheric hydrocarbons based on reaction with hydroxyl radical. *Environ. Sci. Technol.* 10, 692–696.

Daubert, T.E., Danner, R.P. (1985) *Data Compilation of Properties of Pure Compounds.* pp. 450. American Institute of Chemical Engineers.

Dauble, D.D., Carlile, D.W., Hanf, Jr., R.W. (1986) Bioaccumulation of fossil fuel components during single-compound and complex-mixture exposures of *daphnia magna. Bull. Environ. Contam. Toxicol.* 37, 125–132.

Davis, E.M., Murray, H.E., Leihr, J.G., Powers, E.L. (1981) Basic microbial degradation rates and chemical byproducts of selected organic compounds. *Water Res.* 15, 1125–1127.

Dean, J.D., Editor (1985) *Lange's Handbook of Chemistry.* 13th ed. McGraw-Hill, New York.

Dean, J.D., Ed. (1992) *Lange's Handbook of Chemistry.* 14th ed. McGraw-Hill, Inc., New York.

Debnath, A.K., Hansch, C. (1992) Structure-activity relationship of genotoxic polycyclic aromatic nitro compounds. Further evidence for the importance of hydrophobicity and molecular orbital energies in genetic toxicity. *Environ. Mol. Mutagen.* 20, 140–144.

De Bruijn, J., Busser, F., Seipnen, W., Hermens, J. (1989) Determination of octanol/water partition coefficients for hydrophobic organic chemicals with the "slow-stirring" method. *Environ. Toxicol. Chem.* 8, 499–512.

Dehn, W.M. (1917) Comparative solubilities in water, in pyridine and in aqueous pyridine. *J. Am. Chem. Soc*. 29, 1399–1404.

Delle Site, A. (1997) The vapor pressure of environmentally significant organic chemicals: A review of methods and data at ambient temperature. *J. Phys. Chem. Ref. Data* 26, 157–193.

Delle Site, A. (2001) Factors affecting sorption of organic compounds in natural sorbent/water systems and sorption coefficients for selected pollutants. A review. *J. Phys. Chem. Ref. Data* 30, 187–439.

DePablo, R.S. (1976) Determination of saturated vapor pressure in range 10^{-1}–10^{-4} torr by effusion method. *J. Chem. Eng. Data* 21, 141–143.

De Voogt, P., Van Zijl, G.A., Govers, H., Brinkman, U.A.T. (1990) Reversed-phase TLC and structure-activity relationships of polycyclic (hetero) aromatic hydrocarbons. *J. Planar Chromatogr. - Mod. TLC*, 3(1–2), 24–33.

De Voogt, P., Wegener, J.W.M., Klamer, J.C., Van Zijl, G.A., Govers, H. (1988) Prediction of environmental fate and effects of heteroatomic polycyclic aromatics by QSARs: The position of *n*-octanol/water partition coefficients. *Biomed. Environ. Sci.* 1(2), 194–209.

Deneer, J.W., Sinnige, T.L., Seinen, W., Hermens, J.L.M. (1987) Quantitative structure-activity relationships for the toxicity and bioconcentration factor of nitrobenzene derivatives towards guppy *(Poecilia reticulata). Aqua. Toxicol.* 10, 115–129.

Deno, N.C., Berkheimer, H.E. (1960) Part I. Phase equilibria molecular transport thermodynamics. *J. Chem. Eng. Data* 5(1), 1–5.

Digeronimo, M.J., Boethling, R.S., Alexander, M. (1979) Effect of chemical structure and concentration on microbial degradation in model ecosystems. In: *Microbial Degradation of Pollutants in Marine Environments.* EPA-600/9–79–012. U.S. Environmental Protection Agency, Gulf Breeze, FL.

Dilling, W.L., Gonsior, S.J., Boggs, G.U., Mendoza, C.G. (1988) Organic photochemistry. 20. A method for estimating gas-phase rate constants for reactions of hydroxyl radicals with organic compounds from their relative rates of reaction with hydrogen peroxide under photolysis in 1,1,2-trichlorotrifluoroethane solution. *Environ. Sci. Technol.* 22, 1447–1453.

Dlugokencky, E. J., Howard, C.J. (1988) Laboratory studies of NO_3 radical reactions with some sulfur compounds. *J. Phys. Chem.* 92, 1188–1193.

Dojcanske, J., Heinrich, J. (1974) *Chem. Zvesti* 28, 157. - reference from Boublik et al. 1984

Dojlido, J.R. (1979) *Investigation of Biodegradability and Toxicity of Organic Compounds.* Final Report 1975–79. U.S. EPA 600/2–79–163. Municipal Environmental Research Lab., Cincinnati, OH.

Donahue, D.J., Bartell, F.E. (1952) The boundary tension at water-organic liquid interfaces. *J. Phys. Chem.* 56, 480–484.

Donberg, P.A., Odelson, D.A., Klecka, G.M., Markham, D.A. (1992) Biodegradation of acrylonitrile in soil. *Environ. Toxicol. Chem.* 11, 1583–1594.

Dorfman, L.M., Adams, G.E. (1973) *Reactivity of the Hydroxyl Radical in Aqueous Solution.* NSRD-NDB-46. NTIS COM-73–50623. National Bureau of Standards, Washington, D.C.

Douglas, T.B. (1948) Vapor pressure of methyl sulfoxide from 20 to 50°C. Calculation of the heat of vaporization. *J. Am. Chem. Soc*. 70, 2001–2002.

Dreisbach, R.R. (1955) *Physical Properties of Chemical Compounds. No. 15, Am. Chem. Soc. Adv. Chem. Series.* American Chemical Society, Washington D.C.

Dreisbach, R.R. (1961) *Physical Properties of Chemical Compounds-III.* No. 29 of the Adv. Chem. Series. American Chemical Society, Washington D.C.

Dreisbach, R.R., Martin, R.A. (1949) Physical data on some organic compounds. *Ind. Eng. Chem.* 41, 2875–2878.

Dreisbach, R.R., Shrader, S.A. (1949) Vapor pressure-temperature data on some organic compounds. *Ind. Eng. Chem*. 41, 2879–2880.

Dunlap, K.L. (1981) In: *Kirk-Othmer Encyclopedia of Chemical Technology.* Vol.15, 3rd. Edition, John Wiley & Sons, New York. pp. 925–926, 930–931.

Eadsforth, C.V. (1986) Application of reverse-phase HPLC for the determination of partition coefficients. *Pestic. Sci.* 17, 311–325.

Eadsforth, C.V., Moser, P. (1983) Assessment of reverse-phase chromatographic methods for determining partition coefficients. *Chemosphere* 12, 1459–1475.

Edney, E. et al. (1983) *Atmospheric Chemistry of Several Toxic Compounds.* US EPA-600/53–82–092.

Edwards, G. (1950) The vapour pressure of 2:4:6-trinitrotoluene. *Trans. Farad. Soc*. 46, 423-427.

Edwards, D.R., Prausnitz, J. M. (1981) Vapor pressures of some sulfur-containing, coal-related compounds. *J. Chem. Eng. Data* 26, 121–124.

Ellington, J.J., Stancil, F.E., Payne, W.D. (1987) *Measurement of Hydrolysis Rate Constants for Evaluation of Hazardous Waste Land Disposal. Vol. 1, Data on 32 Chemicals.* U.S. EPA-600/3–86–043. NTIS PB87–140 349/GAR.

Elovitz, M.S., Weber, E.J. (1999) Sediment-mediated reduction of 2,4,6-trinitrotoluene and fate of the resulting aromatic (poly)amines. *Environ. Sci. Technol*. 33, 2617–2625.

El Tayar, N., Tsai, R.-S., Vallat, P., Altomare, C., Testa, B. (1991) Measurement of partition coefficient by various centrifugal partition chromatographic techniques. A comprehensive evaluation. *J. Chromatogr.* 556, 181–194.

El Tayar, N., van de Waterbeemd, H., Grylaki, M., Testa, B., Trager, W.F. (1984) The lipophilicity of deuterium atoms. A comparison of shake-flask and HPLC (high performance liquid chromatography) methods. *Int. J. Pharm.* 19, 271–281.

Eon, C., Pommier, C., Guiochon, G. (1971) Vapor pressures and second virial coefficients of some five-membered heterocyclic derivatives. *J. Chem. Eng. Data* 16, 408–410.

Ewing, M.B., Sanchez Ochoa, J.C. (2004) Vapor pressure of acetonitrile determined by comparative ebulliometry. *J. Chem. Eng. Data* 49, 486–491.

Ezumi, K., Kubota, T. (1980) Simultaneous determination of acid dissociation constants and true partition coefficients by analyses of the apparent partition coefficient. *Chem. Pharm. Bull.* 28, 85–91.

Falbe-Hansen, H., Sorenson, S., Jensen, N.R., Pedersen, T., Hjorth, J. (2000) Atmospheric gas-phase reactions of dimethylsulphoxide and dimethyl sulphone with OH and NO_3 radicals, Cl atoms and ozone. *Atmos, Environ*. 1543–1451.

Fochtman, E.G., Eisenberg, W. (1979) *Treatability of Carcinogenic and Other Hazardous Organic Compounds.* U.S. EPA-600/S2–79–097. U.S. Environmental Protection Agency, Cincinnati, OH.

Foote, C.S. (1976) *Free Radicals in Biology.* Pryor, W.A., Editor, Academic Press, Inc., New York.

Fournier, J.C., Salle, J. (1974) Microbial degradation of 2,6-dichlorobenzamide in laboratory models. I. Degradation of 2,6-dichlorobenzamide in soil, comparison with the evolution of other benzamides with different substituents. Research of metabolic products. *Chemosphere* 3, 77–82.

Freitag, D., Geyer, H., Kraus, A., Viswanathan, R., Kotzias, D., Klein, W., Körte, F. (1982) Ecotoxicological profile analysis. VII. Screening chemicals for their environmental behavior by comparative evaluation. *Ecotoxicol. Environ. Saf.* 6, 60–81.

Freitag, D., Scheunert, I., Klein, W., Körte, F. (1982) Long-term fate of 4-chloroaniline-^{14}C in soil and plants under outdoor conditions. A contribution to terrestrial ecotoxicology of chemicals. *Ecotoxicol. Environ. Saf.* 6, 60–81.

Freitag, D., Scheunert, I., Klein, W., Körte, F. (1984) Long-term fate of 4-chloroaniline ^{14}C in soil and plants under outdoor conditions. A contribution to terrestrial ecotoxicology of chemicals. *J. Agric. Food Chem.* 32, 203–207.

Freitag, D., Ballhorn, L., Geyer, H., Körte, F. (1985) Environmental hazard profile of organic chemicals. An experimental method for assessment of the behavior of organic chemicals in the ecosphere by means of simple laboratory tests with ^{14}C labelled chemicals. *Chemosphere* 14, 1589–1616.

Fu, J.-K., Luthy, R.G. (1985) *Pollutant Sorption to Soils and Sediments in Organic/Aqueous Solvent Systems.* EPA/600/3–85/050. Environmental Research Laboratory, Office of Research and Development, U.S. Environmental Protection Agency, Athens, GA.

Fu, J.-K., Luthy, R.G. (1986) Aromatic compound solubility in solvent/water mixtures. *J. Chem. Eng.* 112, 328–345.

Fujita, T., Iwasa, J., Hansch, C. (1964) A new substituent constant derived from partition coefficients. *J. Am. Chem. Soc.* 86(23), 5175–5180.

Fujisawa, S., Masuhara, E. (1980) Binding of methyl methacrylate to bovine albumin. *J. Dent. Res.* 59, 2056–2061.

Fujisawa, S., Masuhara, E. (1981) Determination of partition coefficients of acrylates, methacrylates, and vinyl monomers using high performance liquid chromatography (HPLC). *J. Biomed. Mat. Res.* 15, 787–793.

Gaffney, J.S., Streit, W.D., Hall, J.H. (1987) Beyond acid rain. Do soluble oxidants and organic toxins interact with SO_2 and NO_2 to increase ecosystem effects? *Environ. Sci. Technol.* 21(6), 519–524.

Garst, J.E. (1984) Accurate, wide range, automated, high-performance liquid chromatographic method for the estimation of octanol/water partition coefficients. II: Equilibrium in partition coefficient measurements, additivity of substituent constants, and correlation of biological data. *J. Pharm. Sci.* 73, 1623–1629.

Garst, J.E., Wilson, W.C. (1984) Accurate, wide range, automated, high-performance liquid chromatographic method for the estimation of octanol/water partition coefficients. I: Effect of chromatographic conditions and procedure variables on accuracy and reproducibility of the method. *J. Pharm. Sci.* 73, 1616–1623.

Gatta, G.D., Jóźwiak, M., Brunetti, B., Abate, L. (2000) Enthalpies and entropies of fusion and of sublimation at the temperature 298.15 K of thiourea and seven N-alkylthioureas. *J. Chem. Thermodyn*. 32, 979–997.

Gawlik, B.M., Feicht, E.A., Karcher, W., Kettrup, A., Muntau, H. (1998) Application of the European soil set (Eurosoils) to a HPLC-screening method for the estimation of soil adsorption coefficients of organic compounds. *Chemosphere* 36, 2903–2919.

Gawlik, B.M., Kettrup, A., Muntau, H. (1999) Characterisation of a second generation of European reference soils for sorption studies in the framework of chemical testing - Part II: soil adsorption behaviour of organic chemicals. *Sci. Total Environ*. 229, 109–120.

Gawlik, B.M., Kettrup, A., Muntau, H. (2000) Estimation of soil adsorption coefficients of organic compounds by HPLC screening using the second generation of the European reference soil set. *Chemosphere* 41, 1337–1347.

Ge, J., Liu, W., Dong, S. (1987) Determination of partition coefficient with chemically bonded omega-hydroxysilica as HPLC column packing. *Sepu* 5(3), 182–185.

Gehring, P.J., Torkelson, T.R., Oyen, F. (1967) A comparison of the lethality of chlorinated pyridines and a study of the acute toxicity of 2-chloropyridine. *Toxicol. Appl. Pharmacol.* 11, 361–371.

GEMS (1986) *Graphical Exposure Modeling System.* FAP. Fate of Atmospheric Pollutants.

GEMS (1987) *Graphical Exposure Modeling System.* FAP. Fate of Atmospheric Pollutants.

Gerike, P., Fischer, W.K. (1979) A correlation study of biodegradability determinations with various chemicals in various tests. *Ecotoxicol. Environ. Safety* 3, 159–73.

Gerstl, Z., Helling, C.S. (1987) Evaluation of molecular connectivity as a predictive method for the adsorption of pesticides in soil. *J. Environ. Sci. Health* B22, 55–69.

Geyer, H., Politzki, G., Freitag, D. (1984) Prediction of ecotoxicological behaviour of chemicals: Relationship between *n*-octanol/water partition coefficient and bioaccumulation of organic chemicals by Alga *Chlorella. Chemosphere* 13, 269–284.

Gluck, S.J., Martin, E.J. (1990) Extended octanol-water partition coefficient determination by dual-mode centrifugal partition chromatography. *J. Liq. Chromatogr.* 13, 3559–3570.

Go, M.L., Ngiam, T.L. (1988) Hydrophobicity change on *N*-oxidation of some 4-aminoquinolines. *Chem. Pharm. Bull.* 36(4), 1393–1398.

Going, J., Kuykendahl, P., Long, S., Onstol, J., Thomas, K. (1979) *Environmental Monitoring Near Industrial Sites. Acrylonitrile.* U.S. EPA 560/6–79–003. U.S. Environmental Protection Agency, Washington, DC.

Govers, H., Ruepert, C., Stevens, T.J., van Leeuwen, C.J. (1986) Experimental determination and prediction of partition coefficients of thioureas and their toxicity to photobacterium phosphoreum. *Chemosphere* 15, 383–393.

Graveel, J.G., Sommers, L.E., Nelson, D.W. (1986) Decomposition of benzidine, α-naphthalamine, and *p*-toluidine in soils. *J. Environ. Qual.* 15(1), 53–59.

Greene, S., Alexander, M., Leggett, D. (1981) Formation of N-nitrosodimethylamine during treatment of municipal waste water by simulated land application. *J. Environ. Qual.* 10, 416–421.

Gross, P. M., Saylor, J.H., Gorman, A. (1933) Solubilities studies. IV. The solubilities of certain slightly soluble organic compounds in water. *J. Am. Chem. Soc.* 55, 650.

Gudkov, A.N., Fermor, N.A., Smirnov, N.I. (1964) *Zh. Prikl. Kh.* 37, 2204.- ref see Boublik et al. 1984.

Güesten, H., Filby, W.G., Schoop, S. (1981) Prediction of hydroxyl radical reaction rates with organic compounds in the gas phase. *Atmos. Environ.* 15, 1763–1765.

Günther, F.A., Westlake, W.E., Jaglan, P.S. (1968) Reported solubilities of 738 pesticide chemicals in water. *Residue Rev.* 20, 1–148.

Hakuta, T., Negishi, A., Goto, T., Ishizaka, S. (1977) Vapor-liquid equilibriums of some pollutants in aqueous and saline solutions. Part I. Experimental results. *Desalination* 21, 11–21.

Haky, J.E., Leja, B. (1986) Evaluation of octanol-water partition coefficients using capillary gas chromatography with cold on-column injection. *Anal. Lett.* 19, 123–134.

Haky, J.E., Young, A.M. (1984) Evaluation of a simple HPLC correlation method for the estimation of the octanol-water partition coefficients of organic compounds. *J. Chromatogr.* 7, 675–689.

Hale, V.Q., Stanford, T.B., Taft, L.G. (1979) Evaluation of the environmental fate of munition compound in soil. Final Report AD-A082874, US Army Medical Research and Development Command, Fort Detrick, Frederick, MD. 1979.

Hammers, W.E., Meurs, G.J., De Ligny, C.L. (1982) Correlations between liquid chromatographic capacity ratio data on Lichrosorb RP-18 and partition coefficients in the octanol-water system. *J. Chromatogr.* 247, 1–13.

Hanai, T., Hubert, J. (1982) Hydrophobicity and chromatographic behaviour of aromatic acids found in urine. *J. Chromatogr.* 239, 527–536.

Hansch, C., Fujita, T. (1964) ρ-σ-π Analysis: Method for the correlation of biological activity and chemical structure. *J. Am. Chem. Soc*. 86, 1616–1626.

Hansch, C., Anderson, S. (1967) The effect of intermolecular hydrophobic bonding on partition coefficients. *J. Org. Chem.* 32, 2583.

Hansch, C., Leo, A. (1979) *Substituent Constants for Correlation Analysis in Chemistry and Biology.* Wiley, New York.

Hansch, C., Leo, A. (1983) *Medchem Project.* Pomona College, Claremont, CA.

Hansch, C., Leo, A. (1985) *Medchem Project.* Pomona College, Claremont, CA.

Hansch, C., Leo, A. (1987) *Medchem Project.* Pomona College, Claremont, CA.

Hansch. C., Leo, A.J., Hoekman, D. (1995) *Exploring QSAR, Hydrophobic, Electronic, and Steric Constants*. ACS Professional Reference Book, American Chemical Society, Washington, DC.

Hansch, C., Quinlan, J.E., Lawrence, G.L. (1968) The linear free-energy relationship between partition coefficients and the aqueous solubility of organic liquids. *J. Org. Chem.* 33, 347–350.

Hanst, P.L., Spence, J.W., Miller, M. (1977) Atmospheric chemistry of *N*-nitrosodimethylamine. *Environ. Sci. Technol.* 11, 403–405.

Haque, R., Falco, J., Cohen, S., Riordan, C. (1980) Role of transport and fate studies in the exposure, assessment and screening of toxic chemicals. pp. 47–67. In: *Dynamics, Exposure and Hazard Assessment of Toxic Chemicals.* Haque, R., Editor, Ann Arbor Science Publishers Inc., Ann Arbor, MI.

Harnish, M., Möckel, H.J., Schulze, G. (1983) Relationship between log P_{OW} shake flask values and capacity factors derived from reversed phase HPLC for *n*-alkylbenzenes and some OECD reference substances. *J. Chromatogr.* 282, 315–332.

Harris, J.C. (1982) Rate of aqueous photolysis. In: *Handbook of Chemical Property Estimation Methods. Environmental Behavior of Organic Compounds.* Lyman, W.J., Reehl, W.F., Rosenblatt, D.H., Eds., Chapter 8, McGraw-Hill Book Co., New York.

Harris, G.W., Kleindienst, T.E., Pitts, J.N., Jr. (1981) Rate constants for the reaction of OH radicals with CH_3CN, C_2H_5CN and CH_2=CH-CN in the temperature range 298–424 K. *Chem. Phys. Lett.* 80, 479–483.

Hasegawa, K., Murase, M., Kuboshita, M., Saida, H., Shinoda, M., Miyamoto, M., Shimasaki, C., Yoshimura, T., Tsukurimichi, E., Takeuchi, S. (1993) Photooxidation of naphthaleneamines adsorbed on particles under simulated atmospheric conditions. *Environ. Sci. Technol.* 27, 1819–1825.

Hashimoto, Y., Tokura, K., Kishi, H., Strachan, W.M.J. (1984) Prediction of seawater solubility of aromatic compounds. *Chemosphere* 13, 881–888.

Hashimoto, Y., Tokura, K., Ozaki, K., Strachan, W.M.J. (1982) A comparison of water solubilities by the flask and micro-column methods. *Chemosphere* 11, 991–1001.

Hatton, W.E., Hildenbrand, D.L., Sinke, G.C., Stull, D.R. (1962) Chemical thermodynamic properties of aniline. *J. Chem. Eng. Data* 7, 229–231.

Hawthorne, S.B., Sievers, R.E., Barkley, R.M. (1985) Organic emissions from shale oil wastewaters and their implications for air quality. *Environ. Sci. Technol.* 19, 992–997.

Helweg, C., Nielsen, T., Hansen, P.E. (1997) Determination of octanol-water partition coefficients of polar polycyclic aromatic compounds (N-PAC) by high performance liquid chromatography. *Chemosphere* 34, 1673–1684.

Hendry, D.G., Mill, T., Piszkiewicz, L., Howard, J.A., Eigenmann, H. K. (1974) Critical review of hydrogen-atom transfer in the liquid phase. Chlorine atom, alkyltrichloromethyl, alkoxy, and alkyl peroxy radicals. *J. Phys. Chem. Ref. Data* 3, 937–978.

Herington, E.F.G., Martin, J.F. (1953) Vapour pressures of pyridine and its homologues. *Trans. Faraday Soc.* 49, 154–162.

Hill, A.E., Macy, R.J. (1924) Ternary system. II. Silver perchlorate, aniline and water. *J. Am. Chem. Soc.* 46, 1132.

Hine, J., Haworth, H.W., Ramsay, O.B. (1963) Polar effects on rates and equilibria. VI. The effect of solvent on the transmission of polar effects, *J. Am. Chem. Soc.* 85, 1473–1476.

Hine, J., Mookerjee, P.K. (1975) The intrinsic hydrophilic character of organic compounds. Correlations in terms of structural contributions. *J. Org. Chem.* 40, 292–298.

Hodson, J., Williams, N.A. (1988) The estimation of the adsorption coefficient (Koc) for soils by high performance liquid chromatography. *Chemosphere* 17, 67–77.

Hoigné, J., Bader, H. (1983) Rate constants of reactions of ozone with organic compounds in water-I. Non-dissociating organic compounds. *Water Res.* 17, 173–183.

Holmes, H.L., Lough, C.E. (1976) *Effect of Intramolecular Hydrogen Bonding on Partition Coefficients.* Suffield Tech. Note No. DRES-TN-365. Defence Res. Establishment Suffield/Information Canada. U.S. NTIS Report No. AD-A030683.

Hong, H., Wang, L., Han, S. (1996) Prediction adsorption coefficients (KOC) for aromatic compounds by HPLC retention factors (K'). *Chemosphere* 32, 343–351.

Hopke, E.R., Sears, G.W. (1951) Vapor pressures below 1 mm Hg of several aromatic compounds. *J. Chem. Phys.* 19(11), 1345–1351.

Howard, J.A. (1972) Absolute rate constants for reactions of oxy radicals. *Adv. Free Radical Chem.* 4, 49–173.

Howard, P.H., Editor (1989) *Handbook of Environmental Fate and Exposure Data for Organic Chemicals. Vol. I, Large Production and Priority Pollutants*. Lewis Publishers, Chelsea, MI.

Howard, P.H., Editor (1990) *Handbook of Environmental Fate and Exposure Data for Organic Chemicals. Vol. II, Solvents.* Lewis Publishers, Chelsea, MI.

Howard, P.H., Editor (1993) *Handbook of Environmental Fate and Exposure Data for Organic Chemicals. Vol. IV, Solvents 2.* Lewis Publishers, Chelsea, MI.

Howard, P.H., Boethling, R.S., Jarvis, W.F., Meylan, W.M., Michalenko, E.M. (1991) *Handbook of Environmental Degradation Rates.* Lewis Publishers, Chelsea, MI.

Howard, P.H., Hueber, A.E., Mulesky, B.C., Crisman, J.S., Meylan, W., Crosby, E., Gray, D.A., Sage, G.W., Howard, K.P., LaMacchia, A., Boethling, R.S., Troast, R. (1986) BIOLOG, BIODEG, and FATE/EXPOS: New files on microbial degradation and toxicity as well as environmental fate/exposure of chemicals. *Environ. Toxicol. Chem.* 5, 977–988.

Hoy, K.L. (1970) New values of the solubility parameters from vapor pressure data. *J. Paint Technol.* 42(541), 76–118.

Hoyer, Von H., Peperle, W. (1958) Dampfdruckmessungen an organischen substanzen und ihre sublimationswärmen. *Zeit. für Elcktrochemie* 62(1), 61–66.

Hsu, Y.-C., Chem., D.-S., Lee, Y.-P. (1987) Rate constant for the reaction of OH radicals with dimethyl sulfide. *Int. J. Chem. Kinet.* 19, 1073–1082.

Huang, J.-D. (1990) Comparative drug adsorption in the perfused rat intestine. *J. Pharm. Pharmacol.* 42, 167–170.

Hwang, H.M., Hodson, R.E., Lee, R.F. (1987) Degradation of aniline and chloroanilines by sunlight and microbes in estuarine water. *Water Res.* 21, 309–316.

Hynes, A.J. Wine, P.H., Semmes, D.H. (1986) Kinetics and mechanism of OH reactions with organic sulfides. *J. Phys. Chem.* 90, 4148–4156.

Hynes, A.J., Wine, P.H. (1996) The atmospheric chemistry of dimethylsulfoxide (DMSO) kinetics and mechanism of the OH + DMSO reaction. *J. Atmos. Chem.* 24, 23–37.

IARC (1975) *IARC Monographs on the Evaluation of Carcinogenic Risk of Chemicals to Man. Vol. 8, Some Aromatic Azo Compounds.* Internal Agency for Research on Cancer, Lyon, France. 357p.

Ichikawa, Y., Yamano, T., Fujishima, H. (1969) Relationships between the interconversion of cytochrome P540 and its activities in hydroxylations and demethylations by P450 oxidase systems. *Biochem. Biophys. Acta* 171, 32–46.

Ingerslev, F., Nyholm, N. (2000) Shake-flask test for determination of biodegradation rates of C-14-labeled chemicals at low concentrations in surface water systems. *Ecotoxicol. Environ. Saf.* 45, 274–283.

Isnard, P., Lambert, S. (1988) Estimation bioconcentration factors from octanol-water partition coefficient and aqueous solubility. *Chemosphere* 17, 21–34.

Isnard, P., Lambert, S. (1989) Aqueous solubility/*n*-octanol water partition coefficient correlations. *Chemosphere* 18, 1837–1853.

Iwasa, J., Fujita, T., Hansch, C. (1965) Substituent constants for aliphatic functions obtained from partition coefficients. *J. Med. Chem.* 8, 150–153.

Jäckel, H., Klein, W. (1991) Prediction of mammalian toxicity by quantitative-structure-activity relationships: Aliphatic amines and anilines. *Quant.-Strut.-Act. Relat.* 10, 198–204.

Jakli, G., Van Hook, W.A. (1972) The vapor pressures of dimethyl sulfoxide and hexadeuterodimethyl sulfoxide from about 313 to 453 K. *J. Chem. Thermodyn.* 4, 857–864.

Jaworska, J.S., Schultz, T.W. (1993) Quantitative relationships of structure-activity and volume fraction for selected nonpolar and polar narcotic chemicals. *SAR and QSAR in Environ. Res.* 1, 3–19.

Jenke, D.R., Hayward, D.S., Kenley, R.A. (1990) Liquid chromatographic measurement of solute/solvent partition coefficients: Application to solute/container interactions. *J. Chromatogr. Sci.* 28(12), 609–612.

Jia, Z., Mei, L., Lin, F., Huang, S., Killion, R.B. (2003) Screening of octanol-water partition coefficients for pharmaceuticals by pressure-assisted microemulsion electrokinetic chromatography. *J. Chromatog.* A, 1007, 203–208.

Jiménez, P., Moux, M.V., Turrión, C. (1990) Thermochemical properties of *N*-heterocyclic compounds. III. Enthalpies of combustion, vapour pressures and enthalpies of sublimation, and enthalpies of formation of 9H-carbazole, 9-methylcarbazole, and 9-ethylcarbazole. *J. Chem. Thermodyn.* 22, 721–726.

Johnson, C.A., Westall, J.C. (1990) Effect of pH and KCl concentration on octanol-water distribution of methylanilines. *Environ. Sci. Technol.* 24(12), 1869–1875.

Jori, A., Calamari, D., Cattabeni, F., Domenico, A.D., Galli, C.L., Galli, E., Silano, V. (1983) Ecotoxicological profile of pyridine. *Ecotoxicol. Environ. Saf.* 7, 251–275.

Kahlbaum, G.W.A. (1898) Studien über dampfspannkraftmessungen. II. *Z. Phys. Chem.* 26, 577–658.

Kakinuma, H. (1941) The solubility of urea in water. *J. Phys. Chem.* 45, 1045–1046.

Kalsch, W., Nagel, R., Urich, K. (1991) Uptake, elimination, and bioconcentration of ten anilines in zebrafish (*Brachydanio rerio). Chemosphere* 22, 351–363.

Kamlet, M.J., Doherty, R,M., Abboud, J.-L.M., Abraham, M.H., Taft, R.W. (1986) Linear solvation energy relationships: 36. Molecular properties governing solubilities of organic nonelectrolytes in water. *J. Pharm. Sci.* 75(4), 338–349.

Kamlet, M.J., Doherty, R.M., Abraham, M.H., Carr, P.W., Doherty, R.F., Taft, R.W. (1987) Linear solvation energy relationships: 41. Important differences between aqueous solubility relationships for aliphatic and aromatic solutes. *J. Phys. Chem.* 91, 1996–2004.

Kamlet, M.J., Doherty, R.M., Taft, R.W., Abraham, M.H., Veith, G.D., Abraham, D.J. (1987) Solubility properties in polymers and biological media. 8. An analysis of the factors that influence toxicities of organic nonelectrolytes to the golden orfe fish (*leuciscus idus melanotus). Environ. Sci. Technol.* 21(2), 149–155.

Karickhoff, S.W. (1985) Chapter 3, Pollutant sorption in environmental systems. In: *Environmental Exposure from Chemicals.* Vol. I, Neely, W.B., Blau, G.E., Editors, CRC Press, Boca Raton, FL. pp. 49–64.

Karickhoff, S.W., Brown, D.S., Scott, T.A. (1979) Sorption of hydrophilic organic pollutants on natural sediments. *Water Res.* 13, 241–248.

Kawasaki, M. (1980) Experiences with test scheme under the chemical control law of Japan: An approach to structure-activity correlations. *Ecotoxicol. Environ. Saf.* 4, 444–454.

Kelly, T.J., Mukund, R., Spicer, C.W., Pollack, A.J. (1994) Concentrations and transformations of hazardous air pollutants. *Environ. Sci. Technol.* 28, 378A-387A.

Kenaga, E.E. (1980) Predicted bioconcentration factors and soil sorption coefficients of pesticides and other chemicals. *Ecotoxicol. Environ. Saf.* 4, 26–38.

Kenaga, E.E., Goring, C.A.I. (1980) In: *Aquatic Toxicology.* Eaton, J.G., Parrish, P.R., Hendricks, A.C., Editors, *ASTM STP* 707, pp. 78–115, Am. Soc. for Testing and Materials, Philadelphia, PA.

Killian, H., Bittrich, H.J. (1965) *Z. Phys. Chem.* 230, 3831.-reference in Boublik et al. 1984.

Kim, K.-J., Lee, C.-H., Ryu, S.-K. (1994) Solubility of thiourea in C_1 to C_6 1-alcohol. *J. Chem. Eng. Data* 39, 228–230.

Kilzer, L., Scheunert, I., Geyer, H., Klein, W., Körte, F. (1979) Laboratory screening of the volatilization rates of organic chemicals from water and soil. *Chemosphere* 8, 751–761.

Kincannon, D.F., Lin, Y.S. (1985) Microbial degradation of hazardous wastes by land treatment. *Proc. Ind. Waste Conference* 40, 607–619.

Klamt, A. (1993) Estimation of gas-phase hydroxyl radical rate constants of organic compounds from molecular orbital calculations. *Chemosphere* 26(7), 1273–1289.

Klara, C.M., Mohamed, R.S., Dempsey, D.M., Holder G.D. (1987) Vapor-liquid equilibria for the binary systems of benzene/toluene, diphenylmethane/toluene, *m*-cresol/1,2,3,4-tetrahydronaphthalene and quinoline/benzene. *J. Chem. Eng. Data* 32, 143–147.

Klečka, G.M. (1985) Biodegradation. In: *Environmental Exposure from Chemicals.* Vol I. Neely, W.B., Blau, G.E., Eds., pp. 110–155, CRC Press Inc., Boca Raton, FL.

Klein, E., Weaver, J.W., Weber, B.G. (1957) Solubility of acrylonitrile in aqueous bases and alkali salts. *Chem. Eng. Data Ser.* 2, 72–75.

Klusen, J., Tröber, S.P., Haderlein, S.B. Schwarzenbach, R.P. (1995) Reduction of substituted nitrobenzenes by Fe(II) in aqueous mineral suspensions. *Environ. Sci. Technol*. 29, 2396–2404.

Kobe, K.A., Okabe, T.S., Ramstad, M.T., Huemmer, P.M. (1941) *p*-Cymene studies. VI. Vapor pressure of *p*-cymene, some of its derivatives and related compounds. *J. Am. Chem. Soc*. 63, 3251–3252.

Kobe, K.A., Ravicz, A.E., Vohra, S.P. (1956) Critical properties and vapor pressures of some ethers and heterocyclic compounds. *Ind. Eng. Chem*. 1, 50–56.

Kochany, J., Maguire, R.J. (1994) Photodegradation of quinoline in water. *Chemosphere* 28(6), 1097–1110.

Kollig, H.P., Ed. (1993) *Environmental Fate Constants for Organic Chemicals under Consideration of EPA's Hazardous Waste Identification Projects.* EPA Report EPA/600/R-93/132, U.S. Environmental Research Lab., Athens GA.

Könemann, H., Zelle, R., Busser, F., Hammers, W.E. (1979) Determination of log P_{OCT} values of chloro-substituted benzenes, toluenes and anilines by high-performance liquid chromatography on ODS-silica. *J. Chromatogr.* 178, 559–565.

Kördel, W., Stutte, J., Kotthoff, G. (1993) HPLC-screening method for the determination of the adsorption-coefficient on soil-comparison of different stationary phases. *Chemosphere* 27, 2341–2352.

Korenman, I.M. (1971) Extraction of homologous compounds. *Russ. J. Phys. Chem*. 45(6), 795–797.

Korenman, I.M., Gurevich, Yu. N., Kulagina, T.G. (1973) Extraction of some *n*-alkylamines from aqueous solutions. *Zh. Prikl. Khim.* (Leningrad) 46(3), 683–684.

Korenman, Ya.I., Polumestnaya, E.I. (1982) Principles of interfacial distribution of certain substituted naphthalenes. *J. Appl. Chem.* USSR (English translation) 55(2), 364–367.

Körte, F., Freitag, D., Geyer, H., Klein, W., Kraus, A.G., Lahaniatis, E. (1978) Ecotoxicologic profile analysis-a concept for establishing ecotoxicologic priority lists for chemicals. *Chemosphere* 1, 79–102.

Kramer, C.R., Henze, U. (1990) Partitioning properties of benzene derivatives. I. Temperature dependence of the partitioning of monosubstituted benzenes and nitrobenzenes in the *n*-octanol/water system. *Z. Phys. Chem.* (Leipzig) 271(3), 503–513.

Kühne, R., Ebert, R.-U., Kleint, F., Schmidt, G., Schüürmann, G. (1995) Group contribution methods to estimate water solubility of organic chemicals. *Chemosphere* 30, 2061–2077.

Kurylo, M.J. (1978) Flash photolysis resonance fluorescence investigation of the reaction of OH radicals with dimethyl radicals. *Chem. Phys. Lett*. 37, 323.

Kurylo, M.J., Knable, G.L. (1984) A kinetic investigation of the gas-phase reactions of atomic chlorine (^{2}P) and hydroxyl (X^2) with acetonitrile: Atmospheric significance and evidence of decreased reactivity between strong electrophiles. *J. Phys. Chem*. 88, 3305–3308.

Leahy, D.E. (1986) Intrinsic molecular volume as a measure of the cavity term in linear solvation energy relationships: Octanol-water partition coefficients and aqueous solubilities. *J. Pharm. Sci.* 75(7), 629–636.

Leahy, D.E., De Meere, A.L.J., Wait, A.R., Taylor, P.J., Tomenson, J.A. (1989) A general description of water -oil partitioning ratios using the rotating diffusion cell. *Int. J. Pharm.* 50, 117–132.

Lee, B.I., Erbar, J.H., Edmister, W.C. (1972) Thermodynamic properties at low temperatures. *Chem. Eng. Prog.* 68(9), 83–84.

Lee, J.H., Tang, I.N. (1983) Absolute rate constants for the hydroxyl radical reactions with CH_3SH and C_2H_5SH at room temperature. *J. Chem. Phys.* 78, 6646–6649.

Lee, M.L., Later, D.W., Rollins, D.K., Eatough, D.J., Hansen, L.D. (1980) Dimethyl and monomethyl sulfate: Presence in coal fly ash and airborne particulate matter. *Science* 207, 186–188.

Leet, W.A., Lin, H.-M., Chao, K.-C. (1987) Mutual solubilities in six binary mixtures of water + a heavy hydrocarbon or a derivative. *J. Chem. Eng. Data* 32, 37–40.

Leggett, D.C., Jenkins, T.F., Miyares, P.H. (1990) Salting-put solvent extraction for preconcentration of neutral organic solutes form water. *Anal. Chem.* 62, 1355–1356.

Leggett, D.C., Miyares, P.H., Jenkins, T.F. (1992) Apparent donor-acceptor interaction between nitroaromatics and acetonitrile. *J. Sol. Chem.* 21, 105–108.

Lenchitz, C., Velicky, R.W. (1970) Vapor pressure and heat of sublimation of three nitrotoluenes. *J. Chem. Eng. Data* 15(3), 401–403.

Łencka, M. (1990) Measurements of vapour pressures of pyridine, 2-methyl pyridine, 2,4-dimethylpyridine, 2,6-dimethylpyridine, and 2,4,6-trimethylpyridine from 0.1 kPa to atmospheric pressure using a modified -wietos-awski ebulliometer. *J. Chem. Thermodyn.* 22, 473–480.

Leo, A., Hansch, C., Elkins, D. (1971) Partition coefficients and their uses. *Chem. Rev.* 71, 525–616.

Leo, A., Hansch, C., Church, C. (1969) Comparison of parameters currently used in the study of structure-activity relationships. *J. Med. Chem.* 12, 766–771.

Lewis, S.J., Mirrlees, M.S., Taylor, P.J. (1983) Rationalizations among heterocyclic partition coefficients. Part 2. The azines. *Quant. Struct.-Act. Relat. Pharmacol. Chem. Biol.* 2, 100–111.

Li, H., Lee, L.S., Fabrega, J.R., Jafvert, C.T. (2001) Role of pH in partitioning and cation exchange of aromatic amines on water saturated soils. *Chemosphere* 44, 627-635.

Lide, D.R., Editor (2003) *Handbook of Chemistry and Physics*. 84th Edition, CRC Press, LLC. Boca Raton, FL.

Liu, D.H.W. et al. (1983) *Aquatic Toxicology Hazard Assessment.* ASTM Spec. Tech. Publication 802. pp. 135–150.

Loekke, H. (1985) Degradation of 4-nitrophenol in two Danish Soils. *Environ. Pollut. Ser. A*. 38, 171–181.

Lu, P.Y., Metcalf, R.L. (1975) Environmental fate and biodegradability of benzene derivatives as studies in a model aquatic ecosystem. *Environ. Health Prospect.* 10, 269–284.

Lu, P.Y., Metcalf, R.L., Plummer, N., Mandel, D. (1977) The environmental fate of three carcinogens: benzo(*a*)pyrene, benzidine, and vinyl chloride evaluated in laboratory model ecosystems. *Arch. Environ. Contam. Toxicol.* 6, 129–142.

Lu, P.Y., Walton, B.T., Lewis, E.B., Kine, B.W., Scott, J.H., Groover, G.E. (1986) *Chemical Information Profile of Selected Resource Conservation and Recovery Act Chemicals.* ORNL Internal Report to Robert S. Kerr Res. Lab., U.S. Environmental Protection Agency, Oak Ridge, TN.

Ludzack, F.J., Schaffer, R.B., Bloomhuff, R.N., Ettinger, M.B. (1958) Biochemical oxidation of some commercially important organic cyanides. I. River oxidation. In: *Proc. 13th Industrial Waste Conference Eng. Bull. Purdue Univ. Eng. Ext. Ser.* pp. 297–312.

Lyman, W.J., Reehl, W.F., Rosenblatt, D.H., Editors (1982) *Handbook on Chemical Property Estimation Methods. Environmental Behavior of Organic Compounds.* McGraw-Hill, New York.

Lynch, E.J., Wilke, C.R. (1960) Vapor pressure of liquid nitrobenzene at low temperature. *J. Chem. Eng. Data* 5, 300.

Lynch, J.C., Myer, K.F., Brannon, J.M., Delfino, J.J. (2001) Effects of pH and temperature on the aqueous solubility and dissolution rate of 2,4,6-trinitrotoluene (TNT), hexahydro-1,3,5-trinitro-1,3,5-triazine (RDX), and octahydro-1,3,5,7-tetranitro-1,3,5,7-tetrazocine (HMX). *J. Chem. Eng. Data* 46, 1549–1555.

Lyons, C.D., Katz, S., Bartha, R. (1984) Mechanisms and pathways of aniline elimination from aquatic environments. *Appl. Environ. Microbiol.* 48(3), 491–496.

Ma, K.C., Shiu, W.Y., Mackay, D. (1990) *A Critically Reviewed Compilation of Physical and Chemical and Persistence Data for 110 Selected EMPPL Substances.* A report prepared for the Ontario Ministry of Environment, Water Resources Branch, Toronto, ON.

Mabey, W.R., Mill, T. (1978) Critical review of hydrolysis of organic compounds in water under environmental conditions. *J. Phys. Chem. Ref. Data* 7, 383–415.

Mabey, W.R., Smith, J.H., Podoll, R.T., Johnson, H.L., Mill, T., Chou, T.-W., Cates, J., Waight Partridge, I., Jaber, H., Vandenberg, D. (1982) *Aquatic Fate Process Data for Organic Priority Pollutants.* EPA Report No. 440/4–81–014, U.S. EPA, Office of Water Regulations and Standards, Washington D.C.

Mabey, W.R., Tse, D., Baraze, A., Mill, T. (1983) Photolysis of nitroaromatics in aquatic systems. I. 2,4,6-Trinitrotoluene. *Chemosphere* 12, 3–16.

Mackay, D. (1982) Correlation of bioconcentration factors. *Environ. Sci. Technol.* 16, 274–278.

Mackay, D. (1984) Air/water exchange coefficients. In: *Environmental Exposure from Chemicals*, Vol. 1, Neely, W.B., Blau, G.E., Eds., pp. 92–108. CRC Press, Boca Raton, FL.

Mackay, D., Bobra, A., Chan, D.W., Shiu, W.Y. (1982) Vapor pressure correlations for low-volatility environmental chemicals. *Environ. Sci. Technol.* 16(10), 645–649.

Mackay, D., Leinonen, P.J. (1975) Rate of evaporation of low-solubility contaminants from water to atmosphere. *Environ. Sci. Technol.* 7, 1178–1180.

Mac Leod, H., Jourdain, J.L., Poulet, G, Le Bras, G. (1983b) Absolute rate constant for the reaction of OH with thiophene between 293 and 473 K. *Chem. Phys. Lett*. 98, 381–385.

Mac Leod, H., Jourdain, J.L., Poulet, G., Le Bras, G. (1984) Kinetic study of reactions of some organic sulfur compounds with OH radicals. *Atmos. Environ*. 18, 2621–2626.

Mac Leod, H., Poulet, G., Le Bras, G. (1983a) Etude cinétique des réactions du radical OH avec CH_3SCH_3, CH_3SH et C_2H_5SH. *J. Chim. Phys.* 80, 287–292.

Maczynski, A., Maczynska, Z. (1965) Vapor-liquid equilibrium in binary system quinoline-water. *Bull. Acad. Pol. Sci.* 13, 299–302.

Makovskaya, V., Dean, J.R., Tomlinson, W.R., Comber, M. (1995) Determination of octanol-water partition coefficients using gradient liquid chromatography. *Anal. Chim. Acta* 315, 183–192.

Malaney, G.W. (1960) Oxidative abilities of aniline-acclimated activated sludge. *J. Water Pollut. Control Fed.* 32, 1300–1311.

Malaney, G.W., Gerhold, R.W. (1962) Structural determinants in the oxidative breakdown of aliphatic compounds by domestic activated sludge. In: *Proc. 17th Indust. Waste Conf. Purdue Univ. Ext. Ser.* 112, 249–257.

Malaney, G.W., Gerhold, R.W. (1969) Structural determinants in the oxidation of aliphatic compounds by activated sludge *J. Water Pollut. Control Fed.* 41, R18–R33.

Mallik, M.A.B., Tesfai, K. (1981) Transformation of nitrosoamines in soil and in vitro by soil organisms. *Bull. Environ. Contam. Toxicol.* 27, 115–121.

Marin, M., Baek, I., Taylor, A.J. (1999) Volatile release from aqueous solutions under dynamic headspace dilution conditions. *J. Agric. Food Chem.* 47, 4750–4755.

Martin-Villodre, A., Pla-Delfina, J.M., Moreno, J., Perez-Buendia, M.D., Miralles, J., Collado, E.F., Sanchez-Moyano, E., Del Pozo, A. (1986) Studies on the reliability of a bihyperbolic functional absorption model. I. Ring-substituted anilines. *J. Pharmacokinet. Biopharm.* 14, 615–633.

Matthews, J.B., Sumner, J.F., Moelwyn-Huges, E.A. (1950) The vapor pressure of certain liquid. *Trans. Farad. Soc.* 46, 797–803.

Matzner, R.A., Bales, R.C. (1994) Transport of acridine in saturated porous media. *Chemosphere* 29, 1755–1773.

Matzner, R.A., Hunter, D.R., Bales, R.C. (1991) The effects of pH and anions on the solubility and sorption behavior of acridine. In: *Organic Substances and Sediments in Water. Vol. 2, Processes and Analytical Methods*. Baker, R.A., Editor, Lewis Publishers, Chelsea, MI.

McCall, J.M. (1975) Liquid-liquid partition coefficients by high-performance liquid chromatography. *J. Med. Chem.* 18(6), 549–552.

McCullough, J.P., Douslin, D.R., Messerly, J.F., Hossenlopp, I.A., Kincheloe, T.C., Waddington, G. (1957) Pyridine: Experimental and calculated chemical thermodynamic properties between 0 and 1500 K; a revised vibrational assignment. *J. Am. Chem. Soc*. 79, 4289–4295.

McCullough, J.P., Scott, D.W., Finke, H.L., Gross, M.E., Williamson, K.D., Pennington, R.E., Waddington, G., Huffman, H.M. (1952) Ethanethiol (ethyl mercaptan): Thermodynamic properties in the solid, liquid and vapor states. Thermodynamic functions to 1000 K. *J. Am. Chem. Soc*. 74, 2801–2804.

McDonald, R.A., Shrader, S.A., Stull, D.R. (1959) Vapor pressures and freezing points of 30 organics. *J. Chem. Eng. Data* 4, 311–313.

McDuffie, B. (1981) Estimation of octanol/water partition coefficients for organic pollutants using reversed-phase HPLC. *Chemosphere* 10, 73–83.

McEachern, D.M., Iniguez, J.C., Ornelas (1975) Enthalpies of combustion and sublimation and vapor pressures of three benzoquinolines. *J. Chem. Eng. Data* 20, 226–228.

McEachern, D.M., Sandoval, O., Iniguez, J.C. (1975) The vapor pressures, derived enthalpies of sublimation, enthalpies of fusion, and resonance energies of acridine and phenazine. *J. Chem. Thermodyn*. 7, 299–306.

McGowan, J.C., Atkinson, P.N., Ruddle, L.H. (1966) The physical toxicity of chemicals. V. Interaction terms for solubilities and partition coefficients. *J. Appl. Chem.* 16, 99–102.

McLeese, D.W., Zitko, V., Peterson, M.R. (1979) Structure lethality relationships for phenols, anilines and other aromatic compounds in shrimp and clams. *Chemosphere* 2, 53–57.

Means, J.C. (1983) Am. Chem. Soc. 186th Nat′l. Meeting Preprints Div. Environ. Chem. 23, 250–251. Washington, D.C.

Means, J.C., Hassett, J.J., Wood, S.G., Banwart, W.L., Ali, S., Khan, A. (1980) Sorption properties of polynuclear aromatic hydrocarbons and sediments: Heterocyclic and substituted compounds. In: *Polynuclear Hydrocarbons: Chemistry and Biological Effects*. Bjorseth, A., Dennis, A.J., Editors, pp. 395–404, Ann Arbor Sci. Publishers, Ann Arbor, MI.

Means, J.C., Wood, S.G., Hassett, J.J., Banwart, W.L. (1982) Sorption of amino- and carboxy-substituted polynuclear aromatic hydrocarbons by sediments and soils. *Environ. Sci. Technol.* 16, 93–98.

Medvedev, V.A., Davidov, V.D. (1981) The transformation of various coke industry products in Chernozem soil. In: *Decomposition of Toxic and Nontoxic Compounds in Soil.* Overcash, M.R., Editor, pp. 245–254., Ann Arbor Science Publishers, Ann Arbor, MI.

Meyer, E.F., Hotz, C.A. (1976) Cohesive energies in polar organic liquids. 3. Cyclic ketones. *J. Chem. Eng. Data* 21, 274–279.

Meyer, E.F., Renner, T.A., Stee, K.S. (1971) Cohesive energies in polar organic liquids. II. The *n*-alkyl nitriles and the 1-chloroalkanes. *J. Phys. Chem.* 75, 642–649.

Meylan, W.M., Howard, P.H. (1991) Bond contribution method for estimating Henry's law constants. *Environ. Toxicol. Chem.* 10, 1283–1291.

Meylan, W.M., Howard, P.H., Boethling, R.S. (1992) Molecular topology/fragment contribution method for predicting soil sorption coefficients. *Environ. Sci. Technol*. 26(8), 1560–1567.

Milazzo, G. (1956) *Annali Di Chemica* 46, 1105.—reference from Boublik et al. 1984

Mill, T. (1979) *Structure Reactivity Correlations for Environmental Reactions*. EPA Final Report, EPA 560/11–79–012.

Mill, T. (1982) Hydrolysis and oxidation processes in the environment. *Environ. Toxicol. Chem.* 1, 135–141.

Mill, T., Mabey, W.R. (1985) Photochemical transformations. *Environ. Exposure Chem.* 1, 175–216.

Mill, T., Hendry, D.G., Richardson, H. (1980) Free-radical oxidants in natural waters. *Science* 207, 886–887.

Mill, T., Mabey, W.R., Lan, B.Y., Baraze, A. (1981) Photolysis of polycyclic aromatic hydrocarbons in water. *Chemosphere* 10, 1281–1290.

Mills, W.B., Dean, J.D., Porcella, D.B., Gherini, S.A., Hudson, R.J.M., Frick, W.E., Rupp, G.L., Bowie, G.L. (1982) *Water Quality Assessment: A Screening Procedure for Toxic and Conventional Pollutants.* Part 1, EPA Report No. EPA-600/6–82–004a, Environmental Research Lab., US EPA, Athens, GA.

Minero, C., Pelizzetti, E., Piccinini, P., Vincenti, M. (1994) Photocatalyzed transformation of nitrobenzene on TiO_2 and ZnO. *Chemosphere* 28(6), 1229–1244.

Minick, D.J., Frenz, J.H., Patrick, M.A., Brent, D.A. (1988) A comprehensive method for determining hydrophobicity constants by reversed-phase high-performance liquid chromatography. *J. Med. Chem.* 31, 1923–1933.

Mirrlees, M.S., Moulton, J.J., Murphy, C.T., Taylor, P.J. (1976) Direct measurement of octanol-water partition coefficients by high-pressure liquid chromatography. *J. Med. Chem.* 19, 615–619.

Mirvish, S.S., Issenberg, P., Sornson, H.C. (1976) Air-water and ether-water distribution of N-nitroso compounds: Implications for laboratory safety, analytic methodology, and carcinogenicity for the rat esophagus, nose, and liver. *J. Nat'l. Cancer Inst.* 56(6), 1125–1129.

Miyake, K., Kitaura, F., Mizuno, N., Terada, H. (1987) Determination of partition coefficient and acid dissociation constant by high-performance liquid chromatography on porous polymer gel as stationary phase. *Chem. Pharm. Bull.* 35(1), 377–388.

Miyake, K., Mizuno, N., Terada, H. (1986) Method for determination of partition coefficient by high-performance liquid chromatography on an octadecylsilane column. Examination of its applicability. *Chem. Pharm. Bull.* 34(11), 4787–4796.

Miyake, K., Tereda, H. (1982) Determination of partition coefficients of very hydrophobic compounds by high-performance liquid chromatography on glyceryl-coated controlled-pore glass. *J. Chromatogr.* 240, 9–20.

Moreale, A., Van Bladel, R. (1976) Influence of soil properties on adsorption of pesticide-derived aniline and *p*-chloroaniline. *J. Soil Sci.* 27, 48–57.

Mousa, A.H.N. (1981) Vapour pressure and saturated-vapour volume of acetonitrile. *J. Chem. Thermodyn.* 13, 201–202.

Müller, M., Klein, W. (1991) Estimating atmosphere degradation processes by SARs. *Sci. Total Environ.* 109/110, 261–273.

Müller, M., Klein, W. (1992) Comparative evaluation of methods predicting water solubility for organic compounds. *Chemosphere* 25, 769–782.

Müller, M., Kördel, W. (1996) Comparison of screening methods for the estimation of adsorption coefficients on soil. *Chemosphere* 32, 2493–2504.

Nakagawa, Y., Izumi, K., Oikawa, N., Sotomatsu, T., Shigemura, M., Fujita, T. (1992) Analysis and prediction of hydrophobicity parameters of substituted acetanilides, benzamides, and related aromatic compounds. *Environ. Toxicol. Chem.* 11, 901–916.

Naik, M.N., Jackson, R.B., Stokes, J., Swaby, R.J. (1972) Microbial degradation and phytotoxicity of picloram and other substituted pyridines. *Soil Biol. Biochem.* 4, 13–23.

Neely, W.B., Blau, G.E. (1985) Chapter 1, Introduction to environmental exposure from chemicals. In: *Environmental Exposure from Chemicals.* Volume I., Neely, W.B., Blau, G.E., Editors, CRC Press Inc., Boca Raton, FL. pp. 1–11.

Neely, W.B., Branson, D.R., Blau, G.E. (1974) Partition coefficient to measure bioconcentration potential of chemicals in fish. *Environ. Sci. Technol.* 8, 1113–1115.

Neish, W.J.P. (1948) Solubilization of aromatic amines by purines. *Rec. Trav. Chim. Pays-Bas* 67, 361–373.

Nielsen, T., Silgur, K., Helweg, C., Jørgensen, O., Hansen, P.E., Kirso, U. (1997) Sorption of polycyclic aromatic compounds to humic acid as studied by High-Performance Liquid Chromatography. *Environ. Sci. Technol.* 31, 1102–1108.

Nipper, M., Qian, Y., Carr, R.S., Miller, K. (2004) Degradation of picric acid and 2,6-DNT in marine sediments and waters: the role of microbial activity and ultra-violet exposure. *Chemosphere* 56, 519–530.

Norrington, F.E., Hyde, R.M., Williams, S.G., Wootton, R. (1975) Physicochemical-activity relations in practice. 1. A rational and self-consistent data bank. *J. Med. Chem.* 18, 604–607.

NRCC (1983) Polycyclic aromatic hydrocarbons in the aquatic environment: Formation, sources, fate and effects on aquatic biota. NRCC/CNRC, Ottawa, Canada.

OECD (1981) *OECD Guidelines for Testing of Chemicals.* Section 1: Physical-Chemical Properties. Organization for Economic Co-operation and Development. OECD, Paris.

Oliver, J.E. (1981) Pesticide-derived nitrosoamines. Occurrence and environmental fate. *Agric. Symp. Ser.* 74, 349–362.

Oliver, J.E., Kearney, P.C., Kontson, A. (1979) Degradation of herbicide-related nitrosoamines in aerobic soils. *J. Agric. Food Chem.* 27, 887–891.

Osborn, A.G, Douslin, D.R. (1966) Vapor pressure relations of 36 sulfur compounds present in petroleum. *J. Chem. Eng. Data* 11, 502–509.

Osborn, A.G., Douslin, D.R. (1968) Vapor pressure relations of 13 nitrogen compounds related to petroleum. *J. Chem. Eng. Data* 13(4), 534–537.

Osborn, A.G., Scott, D.W. (1980) Vapor pressures of 17 miscellaneous organic compounds. *J. Chem. Thermodyn.* 12, 429–438.

Osborn, D.W., Doescher, R.N., Yost, D.M. (1942) The heat capacity, heats of fusion and vaporization, vapor pressure and entropy of dimethyl sulfide. *J. Am. Chem. Soc.* 64, 169–172.

Paris, D.F., Wolfe, N.L. (1987) Relationship between properties of a series of anilines and their transformation by bacteria. *Appl. Environ. Microbiol.* 53, 911–916.

Pearlman, R.S., Yalkowsky, S.H., Banerjee, S. (1984) Water solubilities of polynuclear aromatic and heteroaromatic compounds. *J. Phys. Chem. Ref. Data* 13, 555–562.

Peijnendburg, W.J.G.M., de Beer, K.G.M., den Hollander, H.A., Stegeman, M.H.L., Verboom, H. (1993) Kinetics, products, mechanisms and QSARs for the hydrolytic transformation of aromatic nitriles in anaerobic sediment slurries. *Environ. Toxicol. Chem.* 12, 1149–1161.

Pella, P.A. (1977) Measurement of the vapor pressures of TNT, 2,4-DNT, 2,6-DNT, and EGDN. *J. Chem. Thermodyn*. 9, 301–305.

Pennington, R.E., Scott, D.W., Finke, H.L., McCullough, J.P., Messerly, J.F., Hossen-Lopp, I.A., Waddington, G. (1956) The chemical thermodynamic properties and rotational tautomerism of 1-propanethiol. *J. Am. Chem. Soc*. 78, 3266–3272.

Perrin, D.D. (1965) *Dissociation Constants of Organic Bases in Aqueous Solutions*. Butterworth, London.

Perrin, D.D. (1972) *Dissociation Constants of Organic Bases in Aqueous Solutions*. IUPAC Chemical Data Series; Supplement. Butterworth, London.

Phelan, J.M., Barnett, J.L. (2001) Solubility of 2,4-dinitrotoluene and 2,4,6-trinitrotoluene in water. *J. Chem. Eng. Data* 46, 373–376.

Philpot, J.P., Rhodes, E.C., Davies, C.W. (1940) The determination of mobilities and dissociation constants by means of conductivity titrations. *J. Chem. Soc.* 84–87.

Piacente, V., Scardala, P., Gigli, R. (1985) Vaporization study of *o*-, *m*-, and *p*-chloroaniline by torsion-weighing effusion vapor pressure measurements. *J. Chem. Eng. Data* 30, 372–376.

Pinck, L.A., Kelly, M.A. (1925) The solubility of urea in water. *J. Am. Chem. Soc*. 47, 2170–21772.

Pillai, P., Helling, C.S., Dragun, J. (1982) Soil catalyzed oxidation of aniline. *Chemosphere* 11, 299, 317.

Pinck, L.A., Kelly, M.A. (1925) The solubility of urea in water. *J. Am. Chem. Soc*. 47, 2170–2172.

Poole, S.K., Durham, D., Kibbey, C. (2000) Rapid method for estimation the octanol-water partition coefficient (log P_{OW}) by microemulsion electrokinetic chromatography. *J. Chromatog*. B, 745, 117–126.

Poulet, G., Laverdet, G., Jourdain, J.L., Le Bras, G. (1984) Kinetic study of the reactions of acetonitrile with Cl and OH radicals. *J. Phys. Chem*. 88, 6259–6263.

Pratesi, P., Villa, L., Ferri, V., de Micheli, C., Grana, E., Grieco, C., Silipo, C., Victtoria, A. (1979) On the additive-constitutive properties of substituent hydrophobic parameters in a set of muscarinic agents. *Il Farmaco Ed. Sci.* 34(7), 579–587.

Price, L.C. (1976) Aqueous solubility of petroleum as applied to its origin and primary migration. *Am. Assoc. Petrol. Geol. Bull.* 60, 213–244.

Przyjazny, A., Janicki, W., Chrzanowski, W., Staszewski, R. (1983) Headspace gas chromatographic determination of distribution coefficients of selected organosulphur compounds and their dependence on some parameters. *J. Chromatogr.* 280, 249–260.

Puck, T.T., Wise, H. (1946) Studies in vapor-liquid equilibria. I. A new dynamic method for the determination of vapor pressures of liquids. *J. Phys. Chem*. 50, 329–339.

Putnam, W.E., McEachern, Jr., D.M., Kilpatrick, J.E. (1965) Entropy and related thermodynamic properties of acetonitrile (methyl cyanide). *J. Chem. Phys*. 42, 740–755.

Radchenko, L.G., Kitiagorodskii, A.I. (1974) The vapour pressures and heats of sublimation of naphthalene, biphenyl, octafluoronaphthalene, decafluorobiphenyl, acenaphthene and α-nitronaphthalene. *Russian J. Phys. Chem.* 48(11), 1595–1597.

Radding, S.B., Liu, D.H., Johnson, H.L., Mill, T. (1977) *Review of the Environmental Fate of Selected Chemicals.* EPA 560/5–77–003. US. Environmental Protection Agency, Office of Toxic Substance, Washington, D.C. pp. 147.

Rao, P.S.C., Davidson, J.M. (1982) *Retention and Transformation of Selected Pesticides and Phosphorus in Soil-Water System. A Critical Review.* EPA-600/S3–82–060.

Rekker, R.F. (1977) *The Hydrophobic Fragmental Constant.* Its Derivation and Application. A Means of Characterizing Membrane Systems. Vol. 1, Pharmacochemistry Library, Nauta, W.T., Rekker, R.F., Editors. Elsevier Scientific Publishing Company, Oxford, U.K.

Rekker, R.F., De Kort, H.M. (1979) The hydrophobic fragment constant: An extension to a 1000 data point set. *Eur. J. Med. Chem.* 14, 479–488.

Riddick, J.A., Bunger, W.B., Sakano, T.K. (1986) *Organic Solvents.* 4th Edition. John Wiley and Sons, New York.

Rinke, M., Zetzsch, C. (1984) Rate constants for the reactions of hydroxyl radicals with aromatics: benzene, phenol, aniline, and 1,2,4-trichlorobenzene. *Ber. Bunsen-Ges. Phys. Chem.* 88, 55–62.

Ritter, S., Hauthal, W.H., Maurer, G. (1994) Partition coefficients of some environmentally important organic compounds between 1-octanol and water from reversed-phase high-performance liquid chromatography. *J. Chem. Eng. Data* 39, 414–417.

Ro., K.S., Venugopal, A., Adrian, D.D., Constant., D., Qaisi, K., Valsaraj, K., Thbodeaux, L.J., Roy, D. (1996) Solubility of 2,4,6-trinitrotoluene (TNT) in water. *J. Chem. Eng. Data* 41, 758–761.

Roberts, M.S., Kowaluk, E.A., Polack, A.E. (1991) Prediction of solute sorption by polyvinylchloride plastic infusion bags. *J. Pharm. Sci.* 80, 449–455.

Rogers, J.E., Li, S.W., Felice, L.J. (1984) *Microbial Transformation Kinetics of Xenobiotics in Aquatic Environment.* EPA-600/3–84–043. (NTIS-PB84–162866). Battelle Pacific West Labs., Richland, WA.

Rogers, K.S. (1969) Rabbit erythrocyte hemolysis by lipophile aryl molecules. *Proc. Soc. Exp. Biol. Med.* 130(4), 1140–1142.

Rogers, K.S., Cammarata, A. (1969) Superdelocalizability and charge density. A correlation with partition coefficients. *J. Med. Chem.* 12, 692–693.

Rohrschneider, L. (1973) Solvent characterization by gas-liquid partition coefficients of selected solutes. *Anal. Chem.* 45(7), 1241–1247.

Rott, B., Viswanathan, R., Freitag, D., Korte, F. (1982) Vergleichende untersuchung der anwendbrakeit von umweltchemikalien. *Chemosphere* 11, 531–538.

Ruppert, G., Bauer, R., Heisler, G., Novalic, S. (1993) Mineralization of cyclic organic water contaminants by the photo-Fenton reaction-Influence of structure and substituents. *Chemosphere* 27(8), 1339–1347.

Russell, C.J., Dixon, S.L., Jurs, P.C. (1992) Computer-assisted study of the relationship between molecular structure and Henry's law constant. *Anal. Chem.* 64, 1350–1355.

Russell, Jr., H., Osborne, D.W., Yost, D.M. (1942) The heat capacity, entropy, heats of fusion, transition, and vaporization and vapor pressures of methyl mercaptan. *J. Am. Chem. Soc.* 64, 165–169.

Ryan, J.A., Bell, R.M., Davidson, J.M., O'Connor, G.A. (1988) Plant uptake of non-ionic organic chemicals from soils. *Chemosphere* 17(12), 2299–2323.

Sabljic, A. (1987) On the prediction of soil sorption coefficients of organic pollutants from molecular structure: Application of molecular topology model. *Environ. Sci. Technol.* 21, 358–366.

Sabljic, A., Güsten, H. (1990) Predicting the night-time NO_3 radical reactivity in the troposphere. *Atmos. Environ.* 24A(1), 73–78.

Sabjic, A., Güsten, H., Verhaar, H., Hermens, J. (1995) QSAR modelling of soil sorption. Improvements and systematics of log K_{OC} vs. log K_{OW} correlations. *Chemosphere* 31, 4489–4514.

Sandell, K.B. (1962) Distribution of aliphatic amines between water and mixture of organic solvents. *Naturwissenschaften* 49, 12–13.

Sangster, J. (1989) Octanol-water partition coefficients of simple organic compounds. *J. Phys. Chem. Ref. Data* 18(3), 1111–1230.

Sangster, J. (1993) *LOGKOW Database,* Sangster Research Lab., Montreal, Canada.

Sasaki, S. (1978) The scientific aspects of the chemical substance control law in Japan. In: *Aquatic Pollutants: Transformation and Biological Effects.* Hutzinger, O. et al., Editors, Pergamon Press, Oxford, U.K. pp. 283–298.

Schauerte, W., Lay, J.P., Klein, W., Korte, F. (1982) Long-term fate xenobiotics in aquatic ecosystems. *Ecotoxicol. Environ. Safety* 6, 560–569.

Schmidt-Bleek, F., Haberland, W., Klein, A.W., Caroli, S. (1982) Steps towards environmental hazard assessment of new chemicals. *Chemosphere* 11(4), 383–415.

Schnell, S., Bak, F., Pfennig, N. (1989) Anaerobic degradation of aniline and dihydroxybenzenes by newly isolated sulfate-reducing bacteria and description of *Desulfobacterium anilini. Arch. Microbiol.* 152, 556–563.

Schultz, Q.E., Jung, C., Moller, K.E. (1970) Schätzung des verteilungkoeffizienten mit hilfe quantenchemischer molekülgröβen. *Z. Naturforsch.* 25B, 1024–1026.

Schultz, T.W., Moulton, B.A. (1985) Structure-activity relationships for nitrogen-containing aromatic molecules. *Environ. Toxicol. Chem.* 4, 353–359.

Scott, D.W., Berg. W.T., Hossenlopp, I.A., Hubbard, W.N., Messerly, J.F., Todd, S.S., Douslin, D.R., McCullough, J.P., Waddington, G. (1967) Pyrrole: Chemical thermodynamic properties. *J. Phys. Chem.* 71, 2263–2270.

Scott, D.W., Finke, H.L., Gross, M.E., Guthrie, G.B., Huffman, H.M. (1950) 2,3-Dithiabutane: low temperature heat capacity, heat of fusion, heat of vaporization, vapor pressure, entropy and thermodynamic functions. *J. Am. Chem. Soc.* 72, 2424–2430.

Scott, D.W., Finke, H.L., McCullough, J.P., Messerly, J.F., Pennington, R.E., Hossenlopp, I.A., Waddington, G. (1957) 1-Butanethiol and 2-thiapentane. Experimental thermodynamic studies between 12 and 500 K: thermodynamic functions by a refine method of increments. *J. Am. Chem. Soc.* 79, 1062.

Scott, D.W., McCullough, J.P., Hubbard, W.N., Messerly, J.F., Hossenlopp, I.A., Frow, F.R., Waddington, G. (1956) Benzenethiol: Thermodynamic properties in the solid, liquid, and vapor states; internal rotation of the thiol group. *J. Am. Chem. Soc.* 78, 5457–5463.

Scott, D.W., Hubbard, W.N., Messerly, J.F., Todd, S.S., Hossenlopp, I.A., Good, W.D., Douslin, D.R., McCullough, J.P. (1963a) Chemical thermodynamic properties and internal rotation of methylpyridines. I. 2-Methylpyridine. *J. Phys. Chem.* 67, 680–685.

Scott, D.W., Good, W.D., Gurthrie, G.B., Todd, S.S., Hossenlopp, IA., Douslin, D.R., McCullough, J.P. (1963b) Chemical thermodynamic properties and internal rotation of methylpyrines. II. 3-Methylpyridine. *J. Phys. Chem.* 67, 685–689.

Scow, K.M. (1982) Chapter 9, Rate of biodegradation. In: *Handbook of Chemical Property Estimation Methods. Environmental Behavior of Organic Compounds.* Lyman, W.J., Reehl, W.F., Rosenblatt, D.H., Editors, pp. 9–1 to 9–85, McGraw-Hill Book Co., New York.

Seidell, A. (1941) *Solubilities of Organic Compounds.* Van Nostrand Co., New York.

Seidell, A. (1952) *Solubilities of Organic Compounds.* Van Nostrand Co., New York.

Seip, H.M., Alstad, J., Carlberg, G.E., Martinsen, K., Skaane, P. (1986) Measurements of mobility of organic compounds in soils. *Sci. Total Environ.* 50, 87–101.

Shnidman, L., Sunier, A.A. (1932) The solubility of urea in water. *J. Phys. Chem.* 35, 1232–1240

Shriner, C.D. et al. (1978) *Reviews of the Environmental Effects of Pollutants. II. Benzidine.* U.S. EPA-600/1–78–024.

Sikka, H.C., Appleton, H.T., Banerjee, S. (1978) *Fate of 3,3′-Dichlorobenzidine in Aquatic Environment.* EPA-600/3–78–068. Syracuse Research Corp., Syracuse, NY.

Simmons, M.S., Zepp, R.G. (1986) Influence of humic substances on photolysis of nitroaromatic compounds in aquatic systems. *Water Res.* 20, 899–904.

Sims, G.K., O'Loughlin, E.J. (1989) Degradation of pyridines in the environment. *Critical Rev. Environ. Control.* 19, 309–340.

Sims, G.K., Sommers, L.E. (1985) Degradation of pyridine derivatives in soil. *J. Environ. Qual.* 14, 580–584.

Singer, G.M., Taylor, H.W., Lijinsky, W. (1977) Lipophilicity as an aspect of nitrosamine carcinogenicity: quantitative correlations and qualitative observation, *Chem.-Biol. Interact*. 19, 133–142.

Sivaraman, A., Kobayashi, R. (1982) Investigation of vapor pressures and heats of vaporization of condensed aromatic compounds at elevated temperatures. *J. Chem. Eng. Data* 27, 264–269.

Sivaraman, A., Kobayashi, R. (1983) Vapor pressures and enthalpies of vaporization of thianthrene, acridine, and 9-methylanthracene at elevated temperatures. *J. Chem. Thermodyn.* 15, 1127–1135.

Slagle, I.R., Balocchi, F., Gutman, D. (1978) Study of the reactions of oxygen atoms with hydrogen sulfide, methanethiol, ethanethiol and methyl sulfide. *J. Phys. Chem.* 82(12), 1333–1336.

Slater, B., McCormack, A., Avdeef, A., Comer, J.E.A. (1994) pH-metric log P. 4. Comparison of partition coefficients determined by HPLC and potentiometric methods to literature values. *J. Pharm. Sci*. 83, 1280–1283.

Smith, J.H., Bomberger, D.C. (1980) Prediction of volatilization rate of chemicals in water. In: *Hydrocarbons and Halogenated Hydrocarbons in the Environment*, Afghan, B.K., Mackay, D., Eds., pp. 445–451, Plenum Press, New York.

Smith, J.H., Bomberger, D.C., Jr., Haynes, D.L. (1981) Volatilization rates of intermediate and low volatility chemicals from water. *Chemosphere* 10(5), 281–289.

Smith, J.H., Mabey, W.R., Bahonos, N. Holt, B.R., Lee, S.S., Chou, T.W., Venberger, D.C., Mill, T. (1978) *Envirnmental Pathways of Selected Chemicals in Fresh Water Systems: Part II. Laboratory Studies.* Interagency Energy-Environment Research Program Report. EPA-600/7–78–074. Environmental Research Laboratory Office of Research and Development. U.S. Environment Protection Agency, Athens, GA.

Smith, J.H., Mackay, D., Ng, C.W.K. (1983) Volatilization of pesticides from water. *Residue Rev.* 85, 73–88.

Snider, J.R., Dawson, G.A. (1985) Tropospheric light alcohols, carbonyls, and acetonitrile: concentrations in the southwestern United States and Henry's law data. *J. Geophys. Res.* 90(D2), 3797–3805.

SOGC (1987) *Dinitrotoluenes: BUA Substance Report 12.* The Advisory Board for Environmentally Significant Hazardous Waste (BUA) of the Society of German Chemists, Editors. Weinheim, Fed. Republic of Germany: VCH Verlagsgesellschaft p.2.

Son, H.-S., Lee, S.-J., Cho, I.-H., Zoh, K.-D. (2004) Kinetics and mechanism of TNT degradation in TiO_2 photocatalysis. *Chemosphere* 57, 309–317.

Sonnefeld, W.J., Zoller, W.H., May, W.E. (1983) Dynamic coupled-column liquid chromatographic determination of ambient temperature vapor pressures of polynuclear aromatic hydrocarbons. *Anal. Chem.* 55, 275–280.

Sotomatsu, T., Nakagawa, N., Fujita, T. (1987) Quantitative structure-activity studies of benzoylphenylurea larvicides. IV. Benzoyl ortho substituent effects and molecular conformation. *Pestic. Biochem. Physiol*. 27, 156–164.

Southworth, G.R., Beauchamp, J.J., Schmieder, P.K. (1978) Bioaccumulation potential and acute toxicity of synthetic fuels in freshwater biota: azarenes. *Environ. Sci. Technol.* 12, 1062–1066.

Spanggord, R.J., Mabey, W.R., Mill, T., Chou, T.W., Smith, J.H. (1981) *Environmental Fate Studies on Certain Munitions Wastewater Constituents. Part 1. Model Validation.* NTIS AD-A129 373/7. SRI International, Menlo Park, CA. 79 pp.

Spanggord, R.J., Mill, T., Chou, T.W., Mabey, W.R., Smith, J.H., Lee, S. (1980) *Environmental Fate Studies on Certain Munitions Wastewater Constituents. Final Report. Phase I-Literature Review.* SRI Project No. LSU-7934. Contract No. DAMD 17–78-C-8081. US. Army Medical Research and Development Command, Fort Detrick, MD.

Spanggord, R.J., Mabey, W.R., Mill, T., Chou, T.W., Smith, J.H., Lee, S., Robert, D. (1983) *Environmental Fate Studies on Certain Munitions Wastewater Constituents*. LSU-7934, AD-A138550; SRI International: Menlo Park, CA.

Speyers, (1902) *Am. J. Sci.* 14, 293.

Staudinger, J., Roberts, P.V. (1996) A critical review of Henry's law constant for environmental applications. *Crit. Rev. Environ. Sci. Technol.* 26, 205–297.

Staudinger, J., Roberts, P.V. (2001) A critical compilation of Henry's law constant temperature dependence relations for organic compounds in dilute aqueous solutions. *Chemosphere* 44, 561–576

Steele, W.V., Chirico, R.D., Nguyen, A., Knipmeyer, S.E. (1995) Vapor pressure, high-temperature heat capacities, critical properties, derived thermodynamic functions, and barriers to methyl-group rotation, for the six dimethylpyridines. *J. Chem. Thermodyn.* 27, 311–334.

Steen, W.C. (1991) *Microbial Transformation Rate Constants of Structurally Diverse Man-made Chemicals.* EPA 600/3–91/016. PB91–181958. Environmental Research Lab., Office of Research and Development, US Environmental Protection Agency, Athens, GA.

Steen, W.C., Karickhoff, S.W. (1981) Biosorption of hydrophobic organic pollutants by mixed microbial populations. *Chemosphere* 10, 27–32.

Stegeman, M.H.L., Peijnenburg, W.J.G.M., Verboom, H. (1993) A quantitative structure-activity relationship for the direct photohydrolysis of meta-substituted halobenzene directives in water. *Chemosphere* 26(5), 837–849.

Stephen, H., Stephen, Y. (1963) *Solubilities of Inorganic and Organic Compounds.* Vol. 1 and 2, Pergamon Press, Oxford, U.K.

Stephenson, R.M. (1993a) Mutual solubility of water and pyridine derivatives. *J. Chem. Eng. Data* 38, 428–431.

Stephenson, R.M. (1993b) Mutual solubility of water and aliphatic amines. *J. Chem. Eng. Data* 38, 625–629.

Stephenson, R.M. (1993c) Mutual solubilities: water + cyclic amines, water + alkanolamines, and water + polyamines. *J. Chem. Eng. Data* 38, 634–637.

Stephenson, R.M. (1994) Mutual solubility of water and nitriles. *J. Chem. Eng. Data* 39, 255–227.

Stephenson, R.M., Malanowski, S. (1987) *Handbook of Thermodynamics of Organic Compounds.* Elsevier Science Publishing Co. Inc., New York.

Stull, D.R. (1947) Vapor pressure of pure substances: Organic compounds. *Ind. Eng. Chem.* 39(4), 517–560.

Subba-Rao, R.V., Rubbin, H.E., Alexander, M. (1982) Kinetics and extent of mineralization of organic chemicals in trace levels in freshwater and sewage. *Appl. Environ. Microbiol.* 43, 1139–1150.

Sverdrup, L.E., Jensen, J., Kelley, A.E., Krogh, P.J., Stenersen, J. (2002) Effects of eight polycyclic aromatic compounds on the survival and reproduction on *Enchytraeus crypticus* (Oligochaeta, Clitellata). *Environ. Toxicol. Chem.* 21, 109–114.

Swan, T.H., Mack, Jr., E. (1925) Vapor pressures of organic crystals by an effusion method. *J. Am. Chem. Soc*. 47, 2112–2116.

Swift, Jr., E., Hochanadel, H.P. (1945) The vapor pressure of trimethylamine from 0 to 40°C. *J. Am. Chem. Soc*. 67, 880–881.

Szabo, G., Guczi, J., Bulman, R.A. (1995) Examination of silica-salicylic acid and silica-8-hydroxyquinoline HPLC stationary phases for estimation of the adsorption coefficient of soil for some aromatic hydrocarbons. *Chemosphere* 30, 1717–1727.

Szabo, G., Guczi, J., Kordel, W., Zsolnay, A., Major, V., Keresztes, P. (1999) Comparison of different HPLC stationary phases for determination of soil-water distribution coefficient, K_{OC} values of organic chemicals in RP-HPLC system. *Chemosphere* 39, 431–442.

Tabak, H.H., Govind, R. (1993) Prediction of biodegradation kinetics using a nonlinear group contribution method. *Environ. Toxicol. Chem.* 12, 251–260.

Taft, R.W., Abraham, M.H., Famini, G.R., Doherty, R.M., Abboud, J.-L.M., Kamlet, M.J. (1985) Solubility properties in polymers and biological media. 5: An analysis of the physicochemical properties which influence octanol-water partition coefficients of aliphatic and aromatic solutes. *J. Pharm. Sci.* 74(8), 807–814.

Takagishi, T., Katayama, A., Konishi, K., Kuroki, N. (1968) The solubilities of azobenzene derivatives in water. *Kolloid-Zeitschrift Zeit. Polym.* 232(1), 693–699.

Takahashi, K., Tamagawa, S., Katagi, T., Rytting, J.H., Mishibata, T., Mizuno, N. (1993) Percutaneous permeation of basic compounds through shed snakeskin as model membrane. *J. Phar. Pharmacol*. 45, 882–886.

Takayama, C., Akamatsu, M., Fujita, T. (1985) Effects of structure on 1-octanol/water partitioning behaviour of aliphatic amines and ammonium ions. *Quant. Struct.-Act. Relat*. 4, 149–160.

Tanii, H., Hashimoto, K. (1984) Studies on the mechanism of acute toxicity of nitriles in mice. *Arch. Toxicol.* 55, 47–54.

Tate, R.L., III, Alexander, M. (1975) Stability of nitrosoamines in samples of lake water, soil and sewage. *J. Nat′l Cancer Inst.* 54(2), 327–330.

Tate, R.L., III, Alexander, M. (1976) Microbial formation and degradation of dimethylamine. *Appl. Environ. Microbiol.* 31, 399–403.

Taylor, C.A., Rinkenbach, W.H. (1923) The solubility of trinitrotoluene in organic solvents. *J. Am. Chem. Soc.* 45, 44–49.

Tewari, Y.B., Miller, M.M., Wasik, S.P., Martire, D.E. (1982) Aqueous solubility and octanol/water partition coefficient of organic compounds at 25°C. *J. Chem. Eng. Data* 27, 451–454.

Thomsen, A.B., Henriksen, K., Grøn, C., Møldrup, P. (1999) Sorption, transport, and degradation of quinoline in unsaturated soil. *Environ. Sci. Technol*. 33. 2891–2898.

Toräng, L., Reuschenbach, P., Müller, B., Nyholm, N. (2002) Laboratory shake flask batch test can predict field biodegradation of aniline in the Rhine. *Chemosphere* 49, 1257–1265.

Tsai, R.S., El Tayar, N., Testa, B. (1991) Toroidal coil centrifugal partition chromatography, a method for measuring partition coefficients. *J. Chromatogr.* 538(1), 119–123.

Tsonopoulos, C., Prausnitz, J.M. (1971) Activity coefficients of aromatic solutes in dilute aqueous solutions. *Ind. Eng. Chem. Fundam.* 10, 593–600. Supplement Materials.

Tsuda, T., Aoki, M., Kojima, M., Fujita, T. (1993) Accumulation and excretion of chloroanilines by carp. *Chemosphere* 26, 2301–2306.

Tuazon, E.C., Winer, A.M., Pitts, J.N., Jr. (1978) Fourier transform infrared detection of nitroamines in irradiated amine-NO_x systems. *Environ. Sci. Technol.* 12, 954–958.

Tuazon, E.C., Carter, W.P.L., Atkinson, R., Winer, A.M., Pitts, Jr., J.N. (1984) Atmospheric reactions of *N*-nitrosodimethylamine and dimethylnitramine. *Environ. Sci. Technol*. 18, 49–54.

Umeyama, H., Nagai, T., Nogami, H. (1971) Mechanism of adsorption of phenols by carbon black from aqueous solution. *Chem. Pharm. Bull.* 19(8), 1714–1721.

Unger, S.H., Chiang, G.H. (1981) Octanol-physiological buffer distribution coefficients of lipophilic amines by reversed-phase high-performance liquid chromatography and their correlation with biological activity. *J. Med. Chem.* 24(3), 262–270.

Unger, S.H., Cook, J.R., Hollenberg, J.S. (1978) Simple procedure for determining octanol-aqueous partition, distribution, and ionization coefficients by reversed-phase high-pressure liquid chromatography. *J. Pharm. Sci.* 67(10), 1664–1667.

Urano, K., Kato, Z. (1986) Evaluation of biodegradation ranks of priority organic compounds. *J. Haz. Mat.* 13, 135–145.

Urbanski, S.P., Stickel, R.E., Wine, P.H. (1998) Mechanistic and kinetic study of the gas-phase reaction of hydroxyl radical with dimethyl sulfoxide. *J. Phys. Chem*. A, 102, 10,522–10,529.

USEPA (1979) *Status Assessment of Toxic Chemicals: Benzidine.* U.S. EPA-600/2–79–210.

USEPA (1980) *Ambient Water Quality Criteria for Benzidine.* pp. B1 to B6.

USEPA (1986) EXAMS II Computer Modeling System.

USEPA (1987) *EXAMS II Computer Modeling System.*

Vallat, P., El Tayar, N., Testa, B., Slacanin, I., Marston, A., Hostettmann., K. (1990) Centrifugal counter-current chromatography, a promising means of measuring partition coefficients. *J. Chromatogr.* 504, 411–419.

Valvani, S.C., Yalkowsky, S.H., Roseman, T.J. (1981) Solubility and partitioning. IV. Aqueous solubility and octanol-water partition coefficient of liquid nonelectrolytes. *J. Pharm. Sci.* 70, 502–507.

Van Bladel, R., Moreale, A. (1977) Adsorption of herbicide-derived *p*-chloroaniline residues in soils: A predictive equation. *J. Soil Sci.* 28, 93–102.

Van De Rostyne, C., Prausnitz, J.M. (1980) Vapor pressure of some nitrogen-containing, coal-derived liquids. *J. Chem. Eng. Data* 25, 1–3.

Veith, G.D., Austin, N.M., Morris, R.T. (1979a) A rapid method for estimating log *p* for organic chemicals. *Water Res.* 13, 43–47.

Veith, G.D., DeFoe, D.L., Bergstedt, B.V. (1979b) Measuring and estimating the bioconcentration factor of chemicals in fish. *J. Fish Res. Board Can.* 36, 1040–1048.

Veith, G.D., Macek, K.J., Petrocelli, S.R., Carroll, J. (1980) An evaluation of using partition coefficients and water solubility to estimate bioconcentration factors for organic chemicals in fish. In: *Aquatic Toxicology. ASTM STP* 707, American Society for Testing and Materials. Eaton, J.G., Parrish, P., Hendricks, A.C., Editors. pp. 116–129.

Vera, A., Montes, M., Usero, J.L., Casado, J. (1992) Quantitative structure-activity relationship study of the biophysicochemical behavior of nitrosamine. *J. Pharm. Sci.* 61, 791–796.

Vermillion, H.E., Werbel, B., Saylor, J.H., Gross, P.M. (1941) Solubility studies. VI. The solubility of nitrobenzene in deuterium water and in ordinary water. *J. Am. Chem. Soc.* 63, 1345–1347.

Verschueren, K. (1977) *Handbook of Environmental Data on Organic Chemicals*. Van Nostrand Reinhold, New York, NY.

Verschueren, K. (1983) *Handbook of Environmental Data on Organic Chemicals*. 2nd. Edition, Van Nostrand Reinhold, New York, NY.

Vitenberg, A.G., Ioffe, B.V., St. Dimitrova, Z., Butaeva, I.L. (1975) Determination of gas-liquid partition coefficients by means of gas chromatographic analysis. *J. Chromatogr.* 112, 319–327.

von Oepen, B., Kördel, W., Klein, W. (1991) Sorption of nonpolar and polar compounds in soils: Processes, measurements and experience with the applicability of the modified OECD-guideline 106. *Chemosphere* 22, 285–304.

Vonterres, E., et al. (1955) *Brennstoff. Chem.* 36, 272.-reference in Boublik et al. 1984.

Waddington, G., Smith, J.C., Williamson, K.D., Scott, D.W. (1962) Carbon disulfide as a reference substance for vapor-flow calorimetry; the chemical thermodynamic properties. *J. Am. Chem. Soc.* 66, 1074–1077.

Wahner, A., Zetzsch, C. (1983) Rate constants for the addition of hydroxyl radicals to aromatics (benzene, *p*-chloroaniline, and *o-, m-* and *p*-dichlorobenzene) and the unimolecular decay of the adduct. Kinetics into a quasi-equilibrium. *J. Phys. Chem.* 87, 4945–4951.

Wakita, K., Yoshimoto, M., Miyamoto, S. (1986) A method for calculation of the aqueous solubility of organic compounds by using new fragment solubility constants. *Chem. Pharm. Bull.* 34, 4663–4681.

Waddington, G., Knowlton, J.W., Scott, D.W., Oliver, G.D., Todd, S.S., Jubbar, W.M., Smith, J.C., Juffman, H.M. (1949) Thermodynamic properties of thiophene. *J. Am. Chem. Soc.* 71, 797–808.

Wallington, T.J. (1986) Kinetics of the gas phase reaction of OH radicals with pyrrole and thiophene. *Int. J. Chem. Kinet.* 18, 487–496.

Wallington, T.J., Atkinson, R., Tuazon, E.C., Aschmann, S.M. (1986a) The reaction of OH radicals with dimethyl sulfide. *Int. J. Chem. Kinet.* 18, 837–846.

Wallington, T.J., Atkinson, R., Winer, A.M., Pitts, Jr., J.N. (1986b) Absolute rate constants for the gas-phase reactions of the NO_3 radical with CH_3SH, CH_3SCH_3, CH_3SSCH_3, H_2S, SO_2 and CH_3OCH_3 over the temperature range 280–350 K. *J. Phys. Chem.* 90, 5393–5396.

Wallington, T.J., Dagaut, P., Kurylo, M.J. (1988) Correlation between gas-phase and solution-phase reactivities of hydroxyl radicals toward saturated organic compounds. *J. Phys. Chem.* 92, 5024–5028.

Walton, B.T., Hendricks, M.S., Anderson, T.A., Griest, W.H., Merriweather, R., Beauchamp, J.J., Francis, C.W. (1992) Soil sorption of volatile and semivolatile organic compounds in a mixture. *J. Environ. Quality* 21, 552–558.

Wang, L., Xu, L., Xu, O., Tian, L., Zhang, Z. (1989) Determination of partition coefficients of organic acids and bases and the correlation of partition coefficients in different systems. *Huanjing Kexue Xuebao* 9(4), 418–424.

Wang, S., Arnold, W.A. (2003) Abiotic reduction of dinitroaniline herbicides. *Water Res.* 37, 4191–4201.

Wang, X., Harada, S., Watanabe, M., Koshikawa, H., Geyer, P.R. (1996) Modelling the bioconcentration of hydrophobic organic organisms. *Chemosphere* 32, 1783–1793.

Wasik, S.P., Tewari, Y.B., Miller, M.M., Martire, D.E. (1981) *Octanol/Water Partition Coefficients and Water Solubilities of Organic Compounds.* NBSIR No.81–2406. U.S. Dept. of Commerce, Washington, D.C.

Weast, R.C., Ed. (1972–73) *Handbook of Chemistry and Physics*. 53rd Edition, CRC Press, Cleveland, OH.

Weast, R.C., Editor (1982–83) *Handbook of Chemistry and Physics.* 63rd edition, CRC Press, Boca Raton, FL.

Wilson, J.T., Enfield, C.G., Dunlap, W.J. (1981) Transport and fate of selected organic pollutants in a sandy soil. *J. Environ. Qual.* 10, 501–506.

Windholz, M., Editor (1976) *The Merck Index.* Volume 9, Merck & Co., Rahway, NJ.

Windholz, M., Editor (1983) *The Merck Index.* Volume 10, Merck & Co., Rahway, NJ.

Wine, P.H., Kreutter, N.M., Gump, C.A., Ravishankara, A.R. (1981) Kinetics of OH reactions with the atmospheric sulfur compounds H_2S, CH_3SH, CH_3SCH_3, and CH_3SSCH_3. *J. Phys. Chem.* 85, 2660–2665.

Wine, P.H., Thompson, R.J. (1984) Kinetics of OH reactions with furan, thiophene, and tetrahydrothiophene. *Int. J. Chem. Kinet.* 16, 867–878.

Winer, A.M., Atkinson, R., Pitts, Jr., J.N. (1984) Gaseous nitrate radical: possible nighttime atmospheric sink for biogenic organic compounds. *Science* 224, 156–158.

Witte, F., Urbanik, E., Zetzsch, C. (1986) Temperature dependence of the rate constants for the addition of hydroxyl radical to benzene and to some monosubstituted aromatics (aniline, bromobenzene, and nitrobenzene) and the unimolecular decay of the adducts. Part 2. Kinetics into a quasi-equilibrium. *J. Phys. Chem.* 90, 3251–3259.

Wolfenden, R.V. (1978) Interaction of the peptide bond with solvent water: A vapor phase analysis. *Biochemistry* 17(1), 201–204.

Wolff, C.J.M., Crossland, N.O. (1985) Fate and effects of 3,4-dichloroaniline in the laboratory and in outdoor ponds. 1. Fate. *Environ. Toxicol. Chem.* 4, 481–487.

Wong, P.K., Wang, Y.H. (1997) Determination of the Henry's law constant for dimethyl sulfide in seawater. *Chemosphere* 35, 535–544.

Yaguzhinskii, L.S., Smirnova, E.G., Ratnikova, L.A., Kolesova, G.M., Krasinskaya, I.P. (1973) Hydrophobic sites of the mitochondrial electron transfer system. *J. Bioenerg.* 5(3), 163–174.

Yalkowsky, S.H., Morozowich, W. (1980) Chapter 3, A physical chemical basis for the design of orally active prodrugs. In: *Drug Design.* Vol. IX. Academic Press, Inc., New York.

Yalkowsky, S.H., Valvani, S.C. (1980) Solubility and partitioning I: Solubility of nonelectrolytes in water. *J. Pharm. Sci.* 69(8), 912–922.

Yalkowsky, S.H., Valvani, S.C., Kun, W.-Y., Dannenfelser, R.M., Editors (1987) *Arizona Database of Aqueous Solubility for Organic Compounds.* College of Pharmacy, University of Arizona, Tucson, AZ.

Yamagami, C., Takao, N. (1992) Hydrophobicity parameters determined by reversed-phase liquid chromatography. V. Relationship between capacity factor and the octanol-water partition coefficient for simple heteroaromatic compounds and their ester derivatives. *Chem. Pharm. Bull.* 40(4), 925–929.

Yamagami, C., Takao, N., Fujita, T. (1990) Hydrophobicity parameter of diazines. 1. Analysis and prediction of partition coefficients of monosubstituted diazines. *Quant. Struct.-Act. Relat.* 9(4), 313–320.

Yaws, C.L. (1994) *Handbook of Vapor Pressure*, Vol. 1 C_1 to C_4 Compounds, Vol. 2. C_5 to C_7 Compounds, Vol. 3, C_8 to C_{28} Compounds. Gulf Publishing Co., Houston, TX.

Yao, C.C.D., Haag, W.R. (1991) Rate constants for direct reactions of ozone with several drinking water contaminants. *Water Res.* 25, 761–773.

Yaws, C.L., Yang, H.-C., Hopper, J.R., Hansen, K.C. (1990) Organic chemicals: water solubility data. *Chem. Eng.* July, 115–118.

Yaws, C., Yang, H.C., Pan, X. (1991) Henry's law constants for 362 organic compounds in water. *Chem. Eng.* 98(11), 179–185.

Yeh, K.C., Higuchi, W.I. (1976) Oil-water distribution of *p*-alkylpyridines. *J. Pharm. Sci.* 65, 80–86.

Yoshida, K., Shigeoka, T., Yamauchi, F. (1983) Non-steady state equilibrium model for the preliminary prediction of the fate of chemicals in the environment. *Ecotoxicol. Environ. Saf.* 7, 179–190.

Yu, G., Xu, X. (1992) Investigation of aqueous solubilities of nitro-PAH by dynamic couple-column HPLC. *Chemosphere* 24(12), 1699–1705.

Zachara, J.M., Ainsworth, C.C., Cowan, C.E., Thomas, B.L. (1987) Sorption of binary mixtures of aromatic nitrogen heterocyclic compounds on subsurface materials. *Environ. Sci. Technol.* 21, 397–402.

Zepp, R.G., Schlotzhauer, P.F., Simmons, M.F., Miller, G.C., Baughman, G.L., Wolfe, N.L. (1984) Dynamics of pollutant photoreactions in the hydrosphere. *Fresenius Z. Anal. Chem.* 319, 119–125.

Zepp, R.G., Baughman, G.L., Schlotzhauer, P.F. (1981) Comparison of photochemical behavior of various humic substances in water: I. Sunlight induced reactions of aquatic pollutants photosensitized by humic substances. *Chemosphere* 109-118.

Zetzsch, C. (1982) *Predicting the rate of OH-addition to aromatics using* σ^+*-electrophilic substituent constants for mono- and polysubstituted benzene.* 15th Informal Conference on Photochemistry, June 27-July 1, 1982, Stanford, CA.

Zoeteman, B.C.F., Harmsen, K.M., Linders, J.B.H.J., Morra, C.F.H., Slooff, W. (1980) Persistent organic pollutants in river water and groundwater of the Netherlands. *Chemosphere* 9, 231–249.

Zok, S., Görge, G., Kalsch, W., Nagel, R. (1991) Bioconcentration, metabolism and toxicity of substituted anilines in the zebrafish *(Brachydanio rerio). Sci. Total Environ.* 109/110, 411–421.

Zwolinski, B.J., Wilhoit, R.C. (1971) *Handbook of Vapor Pressures and Heats of Vaporization of Hydrocarbons and Related Compounds.* API 44, TRC Publication No. 101, Texas A & M University, College Station, TX.

17 Herbicides

CONTENTS

Triazines:

Uracils:

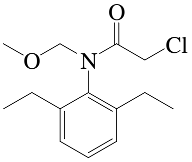
Ureas:

Miscellaneous:

17.1 LIST OF CHEMICALS AND DATA COMPILATIONS (By Functional Group)

17.1.1 HERBICIDES

17.1.1.1 Alachlor



Common Name: Alachlor

Synonym: alachlore, alochlor, Alanex, Bronco, Bullet, Cannon, Lasso, Lazo, metachlor, Pillarzo

Chemical Name: 2-chloro-2,6-diethyl-*N*-methoxymethylacetanilide; 2-chloro-*N*-(2,6-diethylphenyl)-*N*-(methoxymethyl)acetamide

Uses: pre-emergence, early post-emergence or soil-incorporated herbicide to control most annual grasses and many annual broadleaf weeds in beans, corn, cotton, milo, peanuts, peas, soybeans, sunflower, and certain woody ornamentals.

CAS Registry No: 15972-60-8

Molecular Formula: $C_{14}H_{20}ClNO_2$

Molecular Weight: 269.768

Melting Point (°C):

40 (Lide 2003)

Boiling Point (°C):

100 (at 0.02 mmHg, Ashton & Crafts 1981; Herbicide Handbook 1989; Worthing & Hance 1991; Montgomery 1993; Tomlin 1994; Milne 1995)

135 (at 0.30 mmHg, Herbicide Handbook 1989; Milne 1995)

Density (g/cm^3 at 20°C):

1.133 (25°C, Hartley & Kidd 1987; Montgomery 1993; Tomlin 1994)

Molar Volume (cm^3/mol):

240.7 (calculated-Le Bas method at normal boiling point)

Dissociation Constant pK$_a$:

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

29.288 (DSC method, Plato 1972)

Entropy of Fusion, ΔS_{fus} (J/mol K):

Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F: 0.713 (mp at 40°C)

Water Solubility (g/m^3 or mg/L at 25°C or as indicated):

242 (20°C, Weber 1972; Weber et al. 1980)

200 (Bailey & White 1965)

242 (Herbicide Handbook 1974, 1978, 1983, 1989; Martin & Worthing 1977)

240 (Hartley & Graham-Bryce 1980; Beste & Humburg 1983)

148 (Khan 1980)

242 (Ashton & Crafts 1981; Worthing & Walker 1987, Worthing & Hance 1991)

242 (Hartley & Kidd 1983, 1987; Tomlin 1994)

130 (20°C, selected, Suntio et al. 1988; quoted, Majewski & Capel 1995)

148, 242 (literature data variability, Heller et al. 1989)

140 (23°C, Budavari 1989)

240 (Wauchope 1989)

240 (20–25°C, selected, Wauchope et al. 1992; Hornsby et al. 1996)

23.5 (calculated-group contribution fragmentation method, Kühne et al. 1995)

140 (23°C, Milne 1995)

512 (predicted-AQUAFAC, Lee et al. 1996)

532, 785 (supercooled liquid S_L: literature derived value LDV, final adjust value FAV, Muir et al. 2004)

Vapor Pressure (Pa at 25°C or as indicated):

0.00293	(20°C, Weber 1972; Worthing & Walker 1987, Worthing & Hance 1991)
0.00293	(Herbicide Handbook 1974, 1983, 1989)
0.00293	(20–25°C, Weber et al. 1980)
0.00293	(Ashton & Crafts 1981; Schnoor & McAvoy 1981; Schnoor 1992)
0.00290	(Beste & Humburg 1983)
0.00290	(Hartley & Kidd 1987; Worthing & Hance 1991; Tomlin 1994)
0.00300	(20°C, selected, Suntio et al. 1988; quoted, Majewski & Capel 1995)
0.00187	(20–25°C, selected, Wauchope et al. 1992; Hornsby et al. 1996)
0.00413	(Montgomery 1993)
0.0064. 0.0044	(supercooled liquid P$_L$: literature derived value LDV, final adjust value FAV, Muir et al. 2004)

Henry's Law Constant (Pa·m^3/mol at 25°C or as indicated. Additional data at other temperatures designated * are compiled at the end of this section):

6.20×10^{-3}	(20°C, calculated-P/C, Suntio et al. 1988)
8.43×10^{-4}	(wetted-wall-GC/ECD, Fendinger & Glotfelty 1988)
3.26×10^{-3}	(calculated-P/C, Taylor & Glotfelty 1988)
1.12×10^{-3}	(fog chamber-GC/ECD, Fendinger et al. 1989)
8.38×10^{-4}	(23°C, known LWAPC of Fendinger et al. 1989, Meylan & Howard 1991)
1.21×10^{-5}	(bond-estimated LWAPC, Meylan & Howard 1991)
3.26×10^{-3}	(20°C, calculated-P/C, Muir 1991)
6.20×10^{-3}	(calculated-P/C, Montgomery 1993)
3.22×10^{-3}	(Gish et al. 1995)
7.24×10^{-3}*	(Gas stripping-GC/MS, measured range 10–25°C, Gautier et al. 2003)
$\ln [H'/(M\ atm^{-1})] = -20.946 + 9200/(T/K)$; temp range 2830298 K	(gas stripping-GC/MS, Gautier et al. 2003)
0.00101. 1.49	(literature derived value LDV, final adjust value FAV, Muir et al. 2004)

Octanol/Water Partition Coefficient, log K$_{OW}$:

2.92	(Leo et al. 1971)
2.30	(Kenaga 1980)
2.64	(Rao & Davidson 1980)
3.087	(shake flask, Dubelman & Bremer 1983)
3.52	(shake flask, Log P Database, Hansch & Leo 1987)
3.27	(RP-HPLC-RT correlation, Sicbaldi & Finizio 1993)
3.52	(recommended, Sangster 1993)
3.52	(recommended, Hansch et al. 1995)
3.27	(RP-HPLC-RT correlation, Finizio et al. 1997)
3.09	(literature derived value LDV, Muir et al. 2004)

Octanol/Air Partition Coefficient, log K$_{OA}$:

9.31	(final adjust value FAV, Muir et al. 2004)

Bioconcentration Factor, log BCF:

1.45	(calculated-solubility, Kenaga 1980)
0.954	(calculated-K$_{OC}$, Kenaga 1980)
1.88	(Schnoor & McAvoy 1981, Schnoor 1992)
0.778	(freshwater fish, Call et al. 1984)
1.70	(Pait et al. 1992)

Sorption Partition Coefficient, log K$_{OC}$:

2.28	(soil, Beestman & Demming 1976)
2.32	(soil, calculated, Kenaga & Goring 1980)
2.30	(soil, Kenaga 1980)
1.70	(sediment/water, Schnoor & McAvoy 1981)

1.91 (soil, average for soils 2–7, Weber & Peter 1982)
2.08 (soil, screening model calculations, Jury et al. 1987b)
2.28 (Carsel 1989)
2.18, 2.23, 2.28, 2.53 (soil, lit. values, Bottoni & Funari 1992)
2.23 (soil, 20–25°C, selected, Wauchope et al. 1992; Hornsby et al. 1996)
1.63–2.28 (quoted values, Montgomery 1993)
2.21 (selected, Wienhold & Gish 1994)
2.28 (soil, calculated-MCI $^1\chi$, Sabljic et al. 1995)
2.28; 2.53 (soil, quoted exptl.; estimated-general model using molecular descriptors, Gramatica et al. 2000)
2.22, 2.22, 2.20 (soils: organic carbon OC $\geq$ 0.1%, OC $\geq$ 0.5%, 0.1 $\leq$ OC < 0.5%, average, Delle Site 2001)

Environmental Fate Rate Constants, k, or Half-Lives, $t_{1/2}$:

Volatilization: k(measured) = 9000 d^{-1} and k(estimated) = 49000 d^{-1} (Glotfelty et al. 1989);
  estimated $t_{1/2}$ = 2444 d from 1-m depth of water at 20°C (Muir 1991)
  Volatilization rate k = 4.4×10^{-4} d^{-1}, 2.8×10^{-3} d^{-1}, 4.3×10^{-3} d^{-1} at 15, 25, 35°C, respectively, for commercial formulation; k = 5.8×10^{-5} d^{-1}, 8.7×10^{-3} d^{-1}, 1.4×10^{-2} d^{-1} at 15, 25, 35°C, respectively, for starch encapsulated formulation after application (Weinhold et al. 1993)

Photolysis: $t_{1/2}$ = 2.25 h in distilled water (Tanaka et al. 1981; quoted, Cessna & Muir 1991); 640 ppb contaminated water in the presence of TiO_2 and H_2O_2 photodegraded to 3.5 ppb by 15 h solar irradiation with complete degradation after 75 h (Muszkat et al. 1992).

Oxidation: rate constant k, for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO3} with NO_3 radical and k_{O3} with O_3 or as indicated, *data at other temperatures see reference:
  k(aq.) = (3.8 ± 0.4) M^{-1} s^{-1} for direct reaction with ozone in water at pH 2–6.0 and 21°C, with a half-life of 2.4 h at pH 7 (Yao & Haag 1991).
  k(calc) = 7×10^9 M^{-1} s^{-1} for the reaction with hydroxyl radical in aqueous solutions at 24 ± 1°C (Haag & Yao 1992) k_{OH} = 2.3×10^{-11} $cm^3 \cdot molecule^{-1}$ s^{-1} with calculated tropospheric lifetime about 0.5 d at 298 K assuming an average OH concn of 1×10^6 molecule/cm^3 (Gautier et al. 2003)

Hydrolysis: alkaline chemical hydrolysis $t_{1/2}$ > 365 d (Schnoor & McAvoy 1981; quoted, Schnoor 1992).

Biodegradation: $t_{1/2}$ < 6 months for 0.07 µg/mL to biodegrade in ground water, $t_{1/2}$ > 15 months for 10.0 µg/mL to biodegrade in groundwater both at 25°C and $t_{1/2}$ < 12 wk for 3.2 µg/mL to biodegrade in soil-water suspension at 35°C (Weidner 1974; quoted, Muir 1991);
  $t_{1/2}$ = 23 d for 0.244 µg/mL to biodegrade in river water at 23°C with biodegradation rate k = 0.030 d^{-1} (Schnoor et al. 1982; quoted, Muir 1991);
  $t_{1/2}$ = 18 d from screening model calculations (Jury et al. 1987b);
  $t_{1/2}$ > 6 wk for 0.01–1.0 µg/mL to biodegrade in sewage effluent lake water at 28°C (Novick & Alexander 1985; quoted, Muir 1991);
  overall degradation rate constant k = 0.0403 h^{-1} with $t_{1/2}$ = 17.2 h in sewage sludge and rate constant k = 0.1601 d^{-1} with $t_{1/2}$ = 4.3 d in garden soil (Müller & Buser 1995).

Biotransformation:

Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants:

Half-Lives in the Environment:

Air: tropospheric lifetime of 0.5 d for gas phase reaction with OH radicals; wet deposition lifetime estimated to be 2.8 d in the atmosphere by rainfall (Gautier et al. 2003)

Surface water: $t_{1/2}$ = 23 d for 0.244 µg/mL to biodegrade in river water at 23°C with biodegradation rate k = 0.030 d^{-1} (Schnoor et al. 1982; quoted, Muir 1991);
  $t_{1/2}$ > 6 wk for 0.01–1.0 µg/ml to biodegrade in sewage effluent lake water at 28°C (Novick & Alexander 1985; quoted, Muir 1991);
  k(measured) = (3.8 ± 0.4) M^{-1} s^{-1} for direct reaction with ozone in water at pH 2–6 and 21°C, with $t_{1/2}$ = 2.4 h at pH 7 (Yao & Haag 1991).

Ground water: $t_{1/2}$ < 6 months for 0.07 µg/mL to biodegrade in groundwater, and $t_{1/2}$ > 15 months for 10.0 µg/mL to biodegrade in groundwater both at 25°C (Weidner 1974; quoted, Muir 1991) reported $t_{1/2}$ = 7, 4–21 and 38 d (Bottoni & Funari 1992)

Sediment:

Soil: dissipation $t_{1/2}$ = 7.8 d in soil (Beestman & Demming 1974); measured dissipation rate k = 0.077 d^{-1} (Zimdahl & Clark 1982);
$t_{1/2}$ = 23 and 5.7 d in soil containing 6 and 15% moisture, respectively (Walker & Brown 1985);
$t_{1/2}$ = 18 d from screening model calculations (Jury et al. 1987b);
estimated dissipation rate k = 0.020 and 0.036 d^{-1} (Nash 1988);
field $t_{1/2}$ < 1.5 wk by using field lysimeters (Bowman 1990);
degradation rate constant k = (4.52 ± 0.192) × 10^{-2} d^{-1} with $t_{1/2}$ = 15.3 d in control soil and k = (7.27 ± 0.772 × 10^{-2} d^{-1} with $t_{1/2}$ = 9.53 d in pretreated soil in the field; k = (2.77 ± 0.226) × 10^{-2} d^{-1} with $t_{1/2}$ = 25 d in control soil and k = (14.1 ± 1.75) × 10^{-2} d^{-1} with $t_{1/2}$ = 4.93 d in pretreated soil once only in the laboratory (Walker & Welch 1991);
selected field $t_{1/2}$ = 15 d (Wauchope et al. 1992; Hornsby et al. 1996; quoted, Richards & Baker 1993);
soil $t_{1/2}$ = 30 d (quoted, Pait et al. 1992);
reported $t_{1/2}$ = 7, 4–21 and 38 d (Bottoni & Funari 1992);
soil $t_{1/2}$ = 14–28 d (Di Guardo et al. 1994);
dissipation $t_{1/2}$ = 42 d from soil surface (Gish et al. 1995);
degradation $t_{1/2}$ = 4.3 d in garden soil (Müller & Buser 1995);
$t_{1/2}$ = 15 d (selected, Halfon et al. 1996);
dissipation $t_{1/2}$(calc) = 5 and 5.3 d in soil in model ecosystem, $t_{1/2}$ = 3.3 and 3.4 d in water in model ecosystem (Ramesh & Maheswari 2004).

Biota: biochemical $t_{1/2}$ = 18 d from screening model calculations (Jury et al. 1987b).

TABLE 17.1.1.1.1
Reported Henry's law constants of alachlor at various temperatures

Gautier et al. 2003			
gas stripping-GC/MS			
t/°C	H/(Pa m^3/mol)	t/°C	H/(Pa m^3/mol)
10	$1.097\times10^{+3}$	23	$3.46\times10^{+3}$
10	$1.26\times10^{+3}$	25	$6.33\times10^{+3}$
10	$1.30\times10^{+3}$	25	$8.44\times10^{+3}$
11	$9.76\times10^{+4}$	25.0	$7.24\times10^{+3}$
12	$2.115\times10^{+3}$		
15	$1.68\times10^{+3}$	Arrhenius expression:	
17	$2.58\times10^{+3}$	ln H'/(M atm^{+1}) = –A + B/(T/K)	
18	$3.13\times10^{+3}$	A	20.946
20	$4.24\times10^{+3}$	B	9200
23	$3.07\times10^{+3}$		

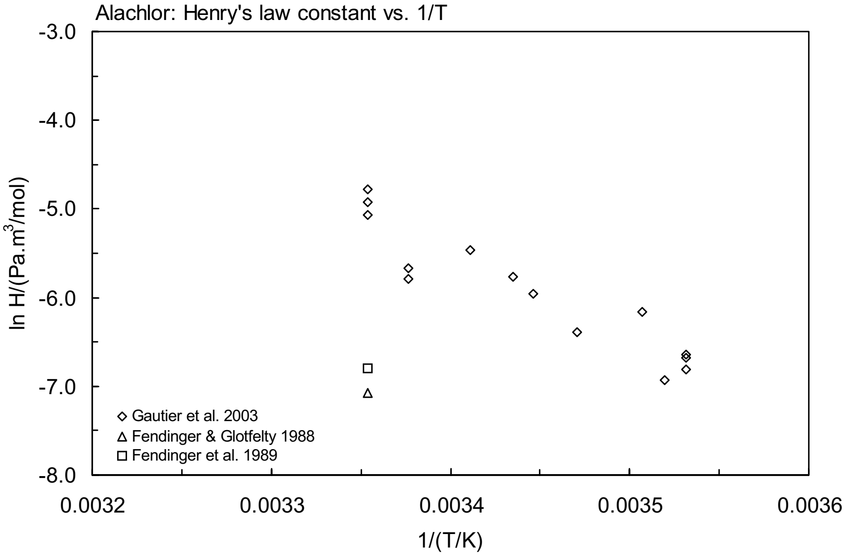
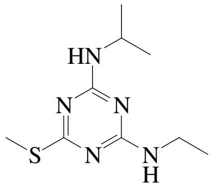


FIGURE 17.1.1.1.1 Logarithm of Henry's law constant versus reciprocal temperature for alachlor.

17.1.1.2 Ametryn



Common Name: Ametryn
Synonym: Amephyt, Ametrex, Evik, Gesapax
Chemical Name: 6-methylthio-2-(ethylamino)-4-(isopropylamino)-1,3,5-triazine; N-ethyl-N′-(1-methylethyl)-6-(methyl-thio)-1,3,5-triazine-2,4-diamine
Uses: herbicide to control broadleaf and grass weeds in corn, sugarcane, some citrus fruits, and in noncropland; also used as pre-harvest and post-harvest dessicant in potatoes to control crop and weeds.
CAS Registry No: 834-12-8
Molecular Formula: $C_9H_{17}N_5S$
Molecular Weight: 227.330
Melting Point (°C):
88 (Lide 2003)
Boiling Point (°C): 328.78 (Rordorf 1989)
Density (g/cm^3 at 20°C):
1.19 (Hartley & Kidd 1987; Worthing & Hance 1991; Montgomery 1993; Tomlin 1994)
Molar Volume (cm^3/mol):
277.5 (calculated-Le Bas method at normal boiling point)
Dissociation Constant:
4.00 (pK_a, Weber 1970; quoted, Bintein & Devillers 1994)
4.10 (pK_a, Worthing & Hance 1991; Montgomery 1993)
10.07 (pK_b, Wauchope et al. 1992; Hornsby et al. 1996)
9.90 (pK_b, Tomlin 1994)
Enthalpy of Vaporization, ΔH_V (kJ/mol):
91.96 (Rordorf 1989)
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
19.8 (Rordorf 1989)
Entropy of Fusion, ΔS_{fus} (J/mol K):
55 (Rordorf 1989)
Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F: 0.241 (mp at 88°C)

Water Solubility (g/m^3 or mg/L at 25°C or as indicated):
700 (Woodford & Evans 1963)
405, 195, 192 (26°C, shake flask-UV at pH 3.0, 7.0, 10.0, Ward & Weber 1968)
185 (Martin & Worthing 1977; Herbicide Handbook 1978)
185 (20°C, Khan 1980; Ashton & Crafts 1981; Verschueren 1983)
194 (Weber et al. 1980)
185 (20°C, Hartley & Kidd 1987; Herbicide Handbook 1989; Worthing & Hance 1991; Montgomery 1993; Milne 1995)
185 (20–25°C, selected, Wauchope et al. 1992; Hornsby et al. 1996)
200 (Tomlin 1994)
134 (calculated-group contribution fragmentation method, Kühne et al. 1995)

Vapor Pressure (Pa at 25°C or as indicated and reported temperature dependence equations):
1.12×10^{-4} (20°C, extrapolated-Antoine eq. from gas saturation-GC measurements, measured range 50–130°C, Friedrich & Stammbach 1964) (See figure at the end of this section.)
log (P/mmHg) = 11.911 – 4933/(T/K), temp range 50–130°C (gas saturation-GC, data presented in Antoine eq., Friedrich & Stammbach 1964) (See figure at the end of this section.)

1.12×10^{-4} (20°C, Khan 1980; Ashton & Crafts 1981; Verschueren 1983)
1.12×10^{-4} (20°C, Hartley & Kidd 1987; Worthing & Hance 1991; Montgomery 1993)
$\log (P_S/kPa) = 11.036 - 5270/(T/K)$, temp range 323–403 K, (solid, Antoine eq., Stephenson & Malanowski 1987)
1.00×10^{-4} (20°C, selected, Suntio et al. 1988)
1.12×10^{-4}, 4.40×10^{-4} (20°C, 30°C, Herbicide Handbook 1989)
3.74×10^{-4}, 1.40×10^{-2}, 0.30, 4.40, 46 (25, 50, 70, 100, 125°C, gas saturation-GC, Rordorf 1989)
$\log (P_S/Pa) = 16.85 - 6048.6/(T/K)$; measured range 49.5–85°C (gas saturation-GC, Rordorf 1989)
$\log (P_L/Pa) = 13.396 - 4803.6/(T/K)$; measured range 49.5–140°C (gas saturation-GC, Rordorf 1989)
3.65×10^{-4} (20–25°C, selected, Wauchope et al. 1992; Hornsby et al. 1996)
3.65×10^{-4} (Tomlin 1994)

Henry's Law Constant (Pa·m^3/mol at 25°C or as indicated):
1.20×10^{-4} (20°C, calculated, Suntio et al. 1988)
1.38×10^{-4} (calculated-P/C, Montgomery 1993)
1.23×10^{-4} (calculated-P/C, this work)

Octanol/Water Partition Coefficient, log K_{OW}:
2.69 (Kenaga & Goring 1980)
2.58 (Gerstl & Helling 1987)
2.98 (shake flask, Log P Database, Hansch & Leo 1987)
2.82 (Worthing & Hance 1991)
2.98 (shake flask, Biagi et al. 1991)
3.07 (RP-HPLC-RT correlation, Finizio et al. 1991)
2.88 (RP-HPLC-RT correlation, Sicbaldi & Finizio 1993)
2.98 (recommended, Sangster 1993)
2.63 (Tomlin 1994)
2.61 (shake flask-UV, Liu & Qian 1995)
2.58 (calculated-RP-HPLC-k′ correlation, Liu & Qian 1995)
2.83 (Milne 1995)
2.98 (recommended, Hansch et al. 1995)
2.88 (RP-HPLC-RT correlation, Finizio et al. 1997)

Bioconcentration Factor, log BCF:
1.52 (calculated-S, Kenaga 1980)
1.32 (calculated-K_{OC}, Kenaga 1980)

Sorption Partition Coefficient, log K_{OC}:
2.59 (soil, Hamaker & Thompson 1972;)
2.40 (soil, calculated, Kenaga & Goring 1980)
2.59 (soil, Kenaga & Goring 1980)
2.59 (Rao & Davidson 1980)
2.59, 2.86 (quoted, calculated-MCI χ, Gerstl & Helling 1987)
2.59, 2.51 (reported as log K_{OM}, estimated as log K_{OM}, Magee 1991)
2.40–2.59, 2.58 (soil, quoted values, Bottoni & Funari 1992)
2.48 (soil, 20–25°C, selected, Wauchope et al. 1992; Hornsby et al. 1996)
2.23–2.44 (Montgomery 1993)
2.48 (Tomlin 1994)
2.42 (calculated-K_{OW}, Liu & Qian 1995)
2.59 (soil, calculated-MCI $^1\chi$, Sabljic et al. 1995)
2.70, 2.59 (soil, estimated-class-specific model, estimated-general model using molecular descriptors, Gramatica et al. 2000)
2.52, 2.63, 2.60, 2.35 (soils with organic carbon OC $\geq$ 0.5% at: pH 4.5–9.0, pH 4.5–5.4, pH 5.5–6.0, pH-6.1, average, Delle Site 2001)
1.84, 2.23 (Kishon river sediments, sorption isotherm, Chefetz et al. 2004)

Environmental Fate Rate Constants, k, or Half-Lives, $t_{½}$:

Volatilization:

Photolysis: $t_{½}$ = 10 h for 10 μg mL^{-1} to degrade in distilled water under > 290 nm light and $t_{½}$ = 3.3 h in 1% acetone solution (Burkhard & Guth 1976; quoted, Cessna & Muir 1991);

$t_{½}$ = 2.25 h for 17% of 33 μg mL^{-1} to degrade in 0.2% aqueous solutions of the surfactant Triton X-100 and for 8% of 33 μg/mL to degrade in distilled water both under 300 nm light (Tanaka et al. 1981; quoted, Cessna & Muir 1991).

Oxidation:

Hydrolysis: $t_{½}$ = 32 d at pH 1 and $t_{½}$ > 200 d at pH 13 (Montgomery 1993).

Biodegradation:

Biotransformation:

Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants:

Half-Lives in the Environment:

Air:

Surface water:

Groundwater: reported half-lives or persistence, $t_{½}$ = 7–120 d (Bottoni & Funari 1992)

Sediment:

Soil: $t_{½}$ = 6.0 months at 15°C and $t_{½}$ = 4.5 months at 30°C in soils (Freed & Haque 1973);

$t_{½}$ = 70–120 d (Bottoni & Funari 1992);

selected $t_{½}$ = 60 d (Wauchope et al. 1992; Hornsby et al. 1996);

$t_{½}$ = 70–129 d in soil (Tomlin 1994).

Biota:

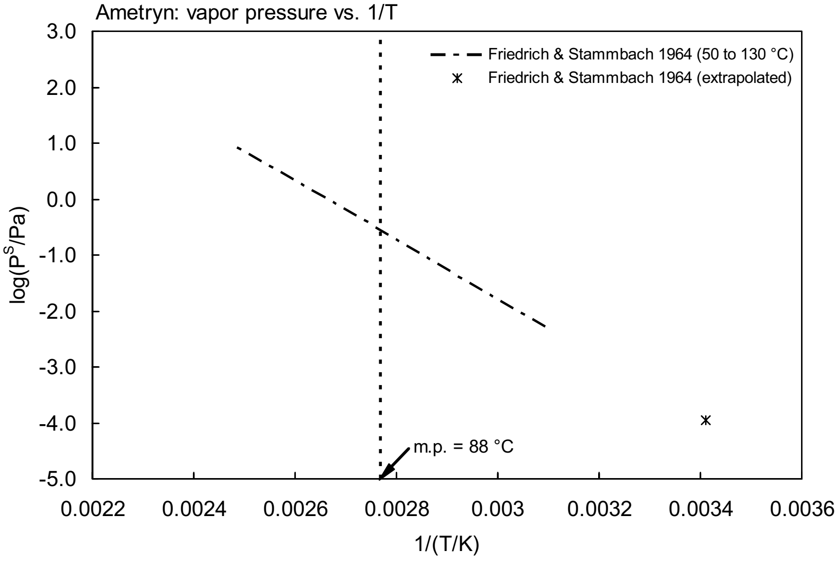
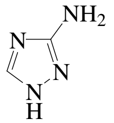


FIGURE 17.1.1.2.1 Logarithm of vapor pressure versus reciprocal temperature for ametryn.

17.1.1.3 Amitrole



Common Name: Amitrole
Synonym: Amazole, Amitrol, Amizole, aminotriazole, Azolan, Azole, cytrol, Diurol
Chemical Name: 3-amino-1,2,4-triazole; 3-amino-*s*-triazole; 1H-1,2,4-triazol-3-amine
Uses: nonselective, foliage-applied herbicide in uncropped land and orchards to control perennial weeds in certain grasses.
CAS Registry No: 61-82-5
Molecular Formula: $C_2H_4N_4$
Molecular Weight: 84.080
Melting Point (°C):

159	(Khan 1980; Herbicide Handbook 1989; Lide 2003)

Boiling Point (°C):
Density (g/cm^3 at 20°C):

1.138	(Hartley & Kidd 1987; Herbicide Handbook 1989; Montgomery 1993; Tomlin 1994)

Molar Volume (cm^3/mol):

85.1	(calculated-Le Bas method at normal boiling point)

Dissociation Constant:

9.83	(pK_b, Wauchope et al. 1992; Hornsby et al. 1996)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

24.69	(DSC method, Plato 1972)

Entropy of Fusion, ΔS_{fus} (J/mol K):
Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F: 0.0484 (mp at 159°C)

Water Solubility (g/m^3 or mg/L at 25°C or as indicated):

252000	(Freed & Burschel 1957)
280000	(Martin 1961; Spencer 1981)
280000	(Bailey & White 1965; Khan 1980; Weber et al. 1980; Ashton & Crafts 1981; Willis & McDowell 1982)
soluble	(Wauchope 1978)
280000	(Worthing 1983, Worthing & Hance 1991)
280000	(Hartley & Kidd 1987; Herbicide Handbook 1989; Reinert 1989)
360000	(20–25°C, selected, Wauchope et al. 1992; Lohninger 1994; Hornsby et al. 1996)
280000	(20°C at pH 7, quoted, Montgomery 1993)
280000	(23°C, Tomlin 1994)

Vapor Pressure (Pa at 25°C or as indicated):

< 0.001	(Agrochemicals Handbook 1983; quoted, Howard 1991)
< 0.001	(Hartley & Kidd 1987)
5.50×10^{-8}	(20°C, Worthing & Hance 1991; Tomlin 1994)
5.87×10^{-5}	(20–25°C, selected, Wauchope et al. 1992; Hornsby et al. 1996)
5.51×10^{-7}	(20°C, quoted, Montgomery 1993)

Henry's Law Constant (Pa·m^3/mol at 25°C or as indicated):

$< 3.04 \times 10^{-7}$	(calculated-P/C, Howard 1991)
1.650×10^{-10}	(20°C, calculated-P/C, Montgomery 1993)
1.650×10^{-10}	(calculated-P/C, this work)

Octanol/Water Partition Coefficient, log K_{OW}:

–0.85	(shake flask, pH 7, Lichtner 1983)
0.52	(selected, Dao et al. 1983; Gerstl & Helling 1987)
–0.15	(Reinert 1989; quoted, Howard 1991; Montgomery 1993)
–0.87, –0.84	(pH 7) (Hansch et al. 1995)
–0.87	(LOGPSTAR or CLOGP data, Sabljic et al. 1995)

Bioconcentration Factor, log BCF:

–0.301	(estimated-S, Lyman et al. 1982; quoted, Howard 1991)
–0.347	(estimated-log K_{OW}, Lyman et al. 1982; quoted, Howard 1991)

Sorption Partition Coefficient, log K_{OC}:

2.04	(soil, estimated-molecular topology & QSAR, Sabljic 1984)
0.23	(calculated-MCI χ, Gerstl & & Helling 1987)
1.26	(Reinert 1989)
2.00	(soil, 20–25°C, selected, Wauchope et al. 1992; Hornsby et al. 1996)
1.73–2.31	(quoted, Montgomery 1993)
2.00	(estimated-chemical structure, Lohninger 1994)
1.25	(soil, calculated-MCI $^1\chi$, Sabljic et al. 1995)

Environmental Fate Rate Constants, k, or Half-Lives, $t_{1/2}$:

Volatilization:

Photolysis:

Oxidation: photooxidation $t_{1/2}$ = 3.2–32 h in air, based on estimated rate constant for the vapor-phase reaction with hydroxyl radicals in air (Atkinson 1987; quoted, Howard et al. 1991).

Hydrolysis:

Biodegradation: aqueous aerobic $t_{1/2}$ = 672–4032 h, based on reported half-lives in soil and water (Freed & Haque 1973; Reinert & Rogers 1987; quoted, Howard et al. 1991); aqueous anaerobic $t_{1/2}$ = 2688–16128 h, based on estimated aqueous aerobic biodegradation half-life (Howard et al. 1991).

Biotransformation:

Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants:

Half-Lives in the Environment:

Air: $t_{1/2}$ = 3.8 d, based on a theoretical calculation for the vapor-phase reaction with hydroxyl radicals in the atmosphere at 25°C (GEMS 1986; quoted, Howard 1989);
$t_{1/2}$ = 3.2–32 h, based on estimated rate constant for the vapor-phase reaction with hydroxyl radicals in air (Atkinson 1987; quoted, Howard et al. 1991).

Surface water: $t_{1/2}$ = 672–4320 h, based on estimated aqueous aerobic biodegradation half-life (Howard et al. 1991).

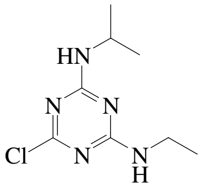
Groundwater: $t_{1/2}$ = 1344–8640 h, based on estimated aqueous aerobic biodegradation half-life (Howard et al. 1991).‘

Sediment:

Soil: $t_{1/2}$ = 1.4, 1.6, 1.3, 92, 36, and 56 d with disappearance rates: k = 0.495, 0.433, 0.533, 0.0075, 0.0193, and 0.124 d^{-1} at pH 6.0, 7.0, 8.0, 5.3, 6.5, and 7.5 (Hamaker 1972; quoted, Nash 1988);
$t_{1/2}$ = 1.5 month at 15°C and $t_{1/2}$ = 1.0 month at 30°C in soils (Freed & Haque 1973);
persistence of one month in soil (Wauchope 1978);
persistence in soil for ca. 2–4 wk (Herbicide Handbook 1989; Tomlin 1994);
$t_{1/2}$ = 672–4320 h, based on estimated aqueous aerobic biodegradation half-life (Howard et al. 1991);
selected field $t_{1/2}$ = 14 d (Wauchope et al. 1992; Hornsby et al. 1996).

Biota:

17.1.1.4 Atrazine



Common Name: Atrazine
Synonym: Aatrex, Akikon, Aktikon, Aktinit, Atratol, Atred, Atrex, Candex, Fenamine, Gesaprim, Hungazin, Inakor, Primatol, Primaze, Radazine, Strazine, Triazine A, Vectal, Weedex A, Wonuk, Zeazine
Chemical Name: 2-chloro-4-(ethylamino)-6-(isopropylamino)-1,3,5-triazine; 6-chloro-*N*-ethyl-*N'*-(1-methylethyl)-1,3,5-triazine-diamine
Uses: pre-emergence and post-emergence herbicide to control some annual grasses and broadleaf weeds in corn, fallow land, rangeland, sorghum, noncropland, certain tropical plantations, evergreen nurseries, fruit crops, and lawns.
CAS Registry No: 1912-24-9
Molecular Formula: $C_8H_{14}ClN_5$
Molecular Weight: 215.684
Melting Point (°C):
173 (Lide 2003)
Boiling Point (C):
Density (g/cm^3 at 20°C):
1.187 (Worthing & Hance 1991; Montgomery 1993; Tomlin 1994)
Molar Volume (cm^3/mol):
250.6 (calculated-Le Bas method at normal boiling point)
Dissociation Constant:
1.68 (pK_a, Weber 1970; Somasundaram et al. 1991; Bintein & Devillers 1994)
1.70 (pK_a, Weber et al. 1980; Willis & McDowell 1982; Worthing & Hance 1991; Francioso et al. 1992; Montgomery 1993; Tomlin 1994)
1.60 (pK_a, Yao & Haag 1991; Haag & Yao 1992)
12.32 (pK_b, Wauchope et al. 1992; Hornsby et al. 1996)
1.62 (pK_a, 20°C, Montgomery 1993)
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
40.585 (DSC method, Plato 1972)
Entropy of Fusion, ΔS_{fus} (J/mol K):
Fugacity Ratio at 20°C (assuming ΔS_{fus} = 56 J/mol K),
F: 0.0353 (mp at 173°C)

Water Solubility (g/m^3 or mg/L at 25°C or as indicated):
70.0 (26°C, Bailey & White 1965)
50.0 (Günther et al. 1968)
31.1, 34.9, 36.8 (26°C, shake flask-UV at pH 3.0, 7.0. 10.0, Ward & Weber 1968)
98.0 (50°C, Getzen & Ward 1971)
33.0 (shake flask-GC, Hörmann & Eberle 1972)
29.9 (shake flask-UV, Hurle & Freed 1972)
30.0 (20°C, Weber 1972; Worthing & Walker 1987; Worthing & Hance 1991; Burkhard & Guth 1981)
33.0 (27°C, Ashton & Crafts 1973, 1981; Khan 1980; Herbicide Handbook 1989; Pait et al. 1992)
32.0 (Freed 1976; Beste & Humburg 1983; Jury et al. 1983)
31.5 (Spencer 1976)
33.0 (Wauchope 1978; Kenaga 1980; Kenaga & Goring 1980)
35.0 (Weber et al. 1980)
30.0 (shake flask-HPLC, Ellgehausen et al. 1981)
24.0 (Thomas 1982)
70.0 (Windholz 1983)

28.0 (20°C, Hartley & Kidd 1987)
29.9, 33, 70 (literature data variability, Heller et al. 1989)
33.0 (20–25°C, selected, Wauchope et al. 1992; Hornsby et al. 1996)
28.0, 33.0 (20°C, 27°C, Montgomery 1993)
33.0 (20°C, Tomlin 1994)
28.0 (Milne 1995)
4012, 4012 (supercooled liquid S_L: literature derived value LDV, final adjust value FAV, Muir et al. 2004)

Vapor Pressure (Pa at 25°C or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):
44.0×10^{-5}* (20°C, extrapolated-Antoine eq. from gas saturation-GC measurements, measured range 50–130°C, Friedrich & Stammbach 1964)
$\log (P/\text{mmHg}) = 13.766 - 5945/(T/K)$, temp range 50–130°C (gas saturation-GC, data presented in graph and Antoine eq., Friedrich & Stammbach 1964)
4.00×10^{-5} (20°C, Weber 1972; Worthing 1979; Worthing & Walker 1987, Worthing & Hance 1991; quoted, Khan 1980; Dobbs et al. 1984; Muir 1991)
3.99×10^{-5} (20°C, gas saturation, extrapolated from Friedrich & Stammbach 1964, Spencer 1976)
4.00×10^{-5} (20°C, Hartley & Graham-Bryce 1980; Beste & Humburg 1983)
4.00×10^{-5} (20–25°C, Weber et al. 1980)
4.00×10^{-5} (20°C, Ashton & Crafts 1981)
1.33×10^{-4} (selected, Schnoor & McAvoy 1981)
3.70×10^{-5}* (20°C, extrapolated from gas saturation measurement, Grayson & Fosbracey 1982)
$\ln (P/\text{Pa}) = 36.8 - 13778/(T/K)$, for temp range 51–81.5°C, (Antoine eq., gas saturation, Grayson & Fosbracey 1982)
1.13×10^{-4} (Thomas 1982)
4.00×10^{-5} (20°C, Hartley & Kidd 1987)
$\log (P_S/\text{kPa}) = 12.8909 - 5945/(/K)$, temp range 323–403 K, (solid, Antoine eq., Stephenson & Malanowski 1987)
8.70×10^{-5} (selected, Nash 1989)
3.99×10^{-5}, 18.6×10^{-5} (20°C, 30°C, Herbicide Handbook 1989)
3.90×10^{-5}* (gas saturation-GC, measured range 40.5–125°C, Rordorf 1989)
$\log (P_S/\text{Pa}) = 13.27071 - 6558.5/(T/K)$; measured range 40.5–125°C (gas saturation-GC, Rordorf 1989)
$\log (P_L/\text{Pa}) = 13.396 - 4803.6/(T/K)$; measured range not specified (gas saturation-GC, Rordorf 1989)
4.05×10^{-5} (Riederer 1990)
3.85×10^{-5} (20–25°C, selected, Wauchope et al. 1992; Hornsby et al. 1996)
4.00×10^{-5} (20°C, Montgomery 1993)
2.00×10^{-5} (selected, Sieber et al. 1994)
3.90×10^{-5} (Tomlin 1994; quoted, Halfon et al. 1996)
6.70×10^{-4}* (40°C, Knudsen effusion method, measured range 40–80°C, Goodman 1997)
$\log (P/\text{Pa}) = 16.08 - 6040/(T/K)$; temp range 40–80°C, Goodman 1997)
0.0096, 0.0096 (supercooled liquid P_L: literature derived value LDV, final adjust value FAV, Muir et al. 2004)

Henry's Law Constant ($\text{Pa·m}^3/\text{mol}$ at 25°C or as indicated):
6.20×10^{-4} (calculated-P/C, Jury et al. 1983, 1984, 1987a; Jury & Ghodrati 1989)
2.90×10^{-4} (20°C, calculated-P/C, Suntio et al. 1988)
6.19×10^{-4} (calculated-P/C, Taylor & Glotfelty 1988)
5.70×10^{-4} (calculated-P/C, Nash 1989)
3.04×10^{-4} (Riederer 1990)
2.66×10^{-4} (calculated-P/C, Howard 1991)
2.89×10^{-4} (20°C, calculated-P/C, Muir 1991)
3.08×10^{-4} (20°C, calculated-P/C, Montgomery 1993)
1.00×10^{-3} (calculated-P/C, Sieber et al. 1994)
6.20×10^{-4} (Gish et al. 1995)
2.88×10^{-4} (calculated-P/C, this work)
0.518 (final adjust value FAV, Muir et al. 2004)

Octanol/Water Partition Coefficient, log K_{OW}:

2.75 (shake flask-GC, Erkell & Walum 1979)
2.63 (HPLC-RT correlation, Veith et al. 1979, 1980; Veith & Kosian 1982)
2.35 (Rao & Davidson 1980)
2.71 (shake flask-both phases analyzed by GC and UV spec., Brown & Flagg 1981)
2.40, 2.21 (HPLC-k′ correlation, McDuffie 1981)
2.75 (shake flask, Ellgehausen et al. 1981)
2.80 (Elgar 1983)
2.05 (RP-HPLC-k′ correlation, Braumann et al. 1983)
2.64 (shake flask-GC, Geyer et al. 1984)
2.75 (Hansch & Leo 1985)
2.64 (OECD method 1981, Kerler & Schönherr 1988)
2.68 (Lopez-Avila et al. 1989)
2.61, 2.61 (RP-HPLC-RT correlation, calculated, Finizio et al. 1991)
2.34 (Worthing & Hance 1991; Milne 1995)
2.10 (shake flask, pH 7, Baker et al. 1992)
2.33–2.80 (quoted values, Montgomery 1993)
2.75 (recommended, Sangster 1993)
2.42 (RP-HPLC-RT correlation, Sicbaldi & Finizio 1993)
2.50 (Tomlin 1994)
2.27 (shake flask-UV, Liu & Qian 1995)
2.61 (selected, Hansch et al. 1995)
2.43 (RP-HPLC-RT correlation, Finizio et al. 1997)
2.00 (RP-HPLC-RT correlation using short ODP column, Donovan & Pescatore 2002)
2.63 ± 0.07, 2.47 ± 0.15, 2.46 ± 0.09 (shake flask, isocratic RP-HPLC-k′ correlation, gradient RP-HPLC-k′ correlation, Paschke et al. 2004)
2.40 (literature derived value LDV, Muir et al. 2004)

Octanol/Air Partition Coefficient, log K_{OA}:

9.08 (final adjust value FAV, Muir et al. 2004)

Bioconcentration Factor, log BCF:

–2.00 (vegetation, correlated-K_{OW}, Beynon et al. 1972; quoted, Travis & Arms 1988)
1.04 (Metcalf & Sanborn 1975; quoted, Kenaga & Goring 1980; Isensee 1991)
1.00 (Isensee 1976)
0.50 (whitefish, Burkhard & Guth 1976)
0.90 (fathead minnow, Veith et al. 1979)
0.30 (catfish, Ellgehausen et al. 1980; quoted, Howard 1991)
0.26 (*Daphnia magna*, wet wt. basis, Ellgehausen et al. 1980)
0.48 (*Corygonus fera.* at 12°C, Gunkel & Streit 1980)
1.93, 0.845 (calculated-S, K_{OC}, Kenaga 1980)
< 0.90 (Veith et al. 1980)
1.90 (selected, Schnoor & McAvoy 1981)
1.93, 1.77 (estimated-S, estimated-K_{OW}, Bysshe 1982)
0.90 (fathead minnow, Veith & Kosian 1982)
2.00 (mottled sculpin, Lynch et al. 1982)
1.60 (activated sludge, Freitag et al. 1984)
1.00 (golden ide, Freitag et al. 1985)
0.477, 0.954, 0.845, 0.778 (zebrafish: egg, embryo, yolk sac fry, juvenile; Görge & Nagel 1990)
0.78 (*Brachydanio rerio*, Görge & Nagel 1990)
0.983 (*Hydrilla*, Hinman & Klaine 1992)
1.98, 0.748, 0.230 (algae *Scenedesmus acutus*, catfish *Ictalurus melas*, *Daphnia magna*, wet wt basis, Wang et al. 1996)

Bioaccumulation Factor, log BAF:

1.710 (algae, Ellgehausen et al. 1980;)
0.329 (catfish, Ellgehausen et al. 1980)
0.261 (daphnids, Ellgehausen et al. 1980)
1.72, 0.477, 1.60 (algae, fish, sludge, Klein et al. 1984)
1.70, < 1.00, 1.60 (algae, fish, sludge, Freitag et al. 1985)

Sorption Partition Coefficient, log K_{OC} at 25°C or as indicated:

2.17 (soil, Hamaker & Thompson 1972)
2.09 (average of 4 soils, Rao & Davidson 1979; Davidson et al. 1980)
2.81 (calculated, Kenaga & Goring 1980; Kenaga 1980)
2.20 (average of soils/sediments, Rao & Davidson 1980)
2.21 (average of 56 soils from lit. review, Rao & Davidson 1980)
2.33 (a Georgia pond sediment, sorption isotherms by shake flask-GC/ECD, Brown & Flagg 1981)
1.59 (a Swiss soil, Burkhard & Guth 1981)
3.11, 2.31; 1.94, 2.42 (estimated-S, calculated-S and mp; estimated-K_{OW}, Karickhoff 1981)
0.7–1.48 (selected, sediment/water, Schnoor & McAvoy 1981)
2.18 (soil, Thomas 1982)
2.29–3.18 (Wolf & Jackson 1982)
3.23–4.13 (Means & Wijayaratne 1982)
2.21 (soil average, Jury et al. 1983)
1.63–3.29 (Wauchope & Myers 1985; 1991)
2.46 (calculated-MCI χ, Gerstl & Helling 1987)
2.20 (soil, screening model calculations, Jury et al. 1987a,b; Jury & Ghodrati 1989)
1.92 (RP-HPLC-k′ correlation, cyanopropyl column, Hodson & Williams 1988)
2.21 (estimated as log K_{OM}, Magee 1991)
2.0, 2.18, 2.17–2.81, 2.26 (soil, literature values, Bottoni & Funari 1992)
2.27, 2.41, 2.59, 2.16 (soils, no. 1, 2, 3, 4; Francioso et al. 1992)
1.81 (soil, HPLC-screening method, mean value from different stationary and mobile phases, Kördel et al. 1993, 1995a,b)
2.00 (soil, 20–25°C, selected, Wauchope et al. 1992; quoted, Dowd et al. 1993; Richards & Baker 1993; Wienhold & Gish 1994; Hornsby et al. 1996)
1.95–2.71 (quoted values, Montgomery 1993)
2,60 (soil with 9.23% organic carbon, Donati et al. 1994)
2.04 (agricultural soil, Dousset et al. 1994)
2.40 (estimated-chemical structure, Lohninger 1994)
2.05 (soil with low organic carbon 0.18%, Roy & Krapac 1994)
1.95–2.19 (Tomlin 1994)
2.23 (calculated-K_{OW}, Liu & Qian 1995)
2.24 (soil, calculated-MCI $^1\chi$, Sabljic et al. 1995)
1.81; 2.36 (HPLC-screening method; calculated-PCKOC fragment method, Müller & Kördel 1996)
1.00 (sediment/water, Chung et al. 1996)
2.64 (Levy wetland soil, sorption equilibrium technique, 24°C, Mersie & Seybold 1996)
2.14–2.21; 2.03–2.12 (Teufelsweiher pond sediment: field measurement; exptl laboratory data, Gao et al. 1997)
2.19 (sediment from Teufelsweiher pond, batch equilibrium isotherm, Gao et al. 1998)
1.93, 1.80–1.85, 1.81 (soil, liquid sewage sludge amended soil, sludge, pH 7.2, batch equilibrium-sorption isotherm, Celis et al. 1998)
1.93, 1.83, 1.79 (soil + $CaCl_2$ at pH 7.2, soil + liquid sewage sludge and dissolved organic matter at pH 7.5, soil + liquid sewage sludge at pH 7.2, batch equilibrium-sorption isotherm, Celis et al. 1998)
2.566, 1.72, 1.75, 1.505, 2.40 (first generation Eurosoils ES-1, ES-2, ES-3, ES-4, ES-5, shake flask/batch equilibrium-HPLC/UV, Gawlik et al. 1998, 1999)
2.24, 2.45; 2.82., 1.81, 2.81, 1.98, 1.99 (quoted lit., calculated-K_{OW}; HPLC-screening method with different LC-columns, Szabo et al. 1999)
2.154, 1.97, 1.77, 1.61, 2.496 (second generation Eurosoils ES-1, ES-2, ES-3, ES-4, ES-5, shake flask/batch equilibrium-HPLC/UV, Gawlik et al. 1999)

1.69 (sandy loam soil, column equilibrium method, 20°C, Xu et al. 1999)

2.154, 1.969, 1.769, 1,610, 2.486 (second generation Eurosoils ES-1, ES-2, ES-3, ES-4, ES-5, shake flask/batch equilibrium-HPLC/UV and HPLC-k′ correlation, Gawlik et al. 2000)

2.24; 2.27, 2.47 (soil, quoted obs.; estimated-class-specific model, estimated-general model using molecular descriptors, Gramatica et al. 2000)

2.59, 2.16 (average values for sediments, soils, Delle Site 2001)

2.31, 2.17, 2.56 (soils: organic carbon OC ≥ 0.1%, OC ≥ 0.5%, 0.1 ≤ OC < 0.5%, and pH 3.2–8.2, average, Delle Site 2001)

2.34, 2.24, 2.06, 2.59 (soils with organic carbon OC ≥ 0.5% at: pH 3.2–5.0, pH 5.1–5.9, pH-6.0, pH 4.4–7.7, average, Delle Site 2001)

1.77, 2.10 (Kishon river sediments, sorption isotherm, Chefetz et al. 2004)

Environmental Fate Rate Constants, k, or Half-Lives, $t_{1/2}$:

Volatilization: initial rate constant $k = 6.4 \times 10^{-4}$ h^{-1} and predicted rate constant $k = 4.2 \times 10^{-4}$ h^{-1} from soil with $t_{1/2}$ = 1650 h (Thomas 1982);

$t_{1/2}$ = 97 d (Jury et al. 1983; quoted, Grover 1991);

rate constants k(measured) = 1100 d^{-1} and k(est.) = 6000 d^{-1} (Glotfelty et al. 1989);

Half-lives from soil surfaces: $t_{1/2}$ = 655 to > 1000 d in peat soil and $t_{1/2}$ = 143–939 d in sandy soil; half-lives from plant surfaces: $t_{1/2}$ = 25.6 d in bean, $t_{1/2}$ = 24.3 d in turnips and $t_{1/2}$ = 14.6 d in oats at 20 ± 1°C (Dörfler et al. 1991)

Volatilization rate $k = 1.4 \times 10^{-4}$ d^{-1}, 2.6×10^{-3} d^{-1}, 4.4×10^{-3} d^{-1} at 15, 25, 35°C, respectively, for commercial formulation; $k = 1.2 \times 10^{-5}$ d^{-1}, 4.8×10^{-4} d^{-1}, 8.1×10^{-4} d^{-1} at 15, 25, 35°C, respectively, for starch-encapsulated formulation after application (Weinhold et al. 1993)

Photolysis: $t_{1/2}$ = (19 ± 9) h under summer sunlight of 9.1 h d^{-1} exposure and $t_{1/2}$ = 61 ± 29 h under spring sunlight of 3.7 h d^{-1} exposure in 10 ppm aqueous solutions: (Burkhard et al. 1975);

$t_{1/2}$ = 4.9 h for 10 µg/mL to degrade in 1% acetone solution and $t_{1/2}$ = 25 h for 10 µg/mL to degrade in distilled water both under > 290 nm light (Burkhard & Guth 1976);

nearsurface direct sunlight photolysis rate constant $k = 9 \times 10^{-6}$ d^{-1} with $t_{1/2}$ = 81,000 d (Schnoor & McAvoy 1981; quoted, Schnoor 1992);

$t_{1/2}$ = 2.25 h for 17–27% of 100 µg/mL to degrade in distilled water under 300 nm light (Tanaka et al. 1981; quoted, Cessna & Muir 1991);

rate of photolytic degradation was slightly higher in water ($t_{1/2}$ = 3–12 d) than in sediments ($t_{1/2}$ = 1–4 wk) (Jones et al. 1982; quoted, Montgomery 1993);

40 ppb contaminated water in presence of TiO_2 and H_2O_2 degraded to 4 ppb after 15 h by solar irradiation with complete degradation after 75 h (Muszkat et al. 1992)

$t_{1/2}$(aq.) = 335 d at pH 7 under natural light; $t_{1/2}$ = 17.5 h at pH 7 using mercury lamp in aqueous solution; soil photolysis $t_{1/2}$= 12 d under natural light, $t_{1/2}$ = 5 d using mercury lamp and $t_{1/2}$ = 45 d using xenon lamp (Solomon et al. 1996);

Oxidation: rate constant k, for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO3} with NO_3 radical and k_{O3} with O_3 or as indicated, *data at other temperatures see reference:

$k_{OH} = 147.2 \times 10^{-12}$ cm^3 molecule^{-1} s^{-1} with n half-life of 2.6 h at 25°C for the vapor-phase reaction with hydroxyl radical in air (Atkinson 1987; quoted, Howard et al. 1991);

k(aq.) = 5.9×10^9 M^{-1} s^{-1} for the reaction (photo-Fenton with reference to acetophenone) with OH radical in aqueous solutions at pH 3.6 and 24 ± 1°C (Buxton et al. 1988; quoted, Faust & Hoigné 1990; Haag & Yao 1992)

k(aq.) = (24 ± 4) M^{-1} s^{-1} for direct reaction with ozone at pH 4 and 26°C; k = (13 ± 1) M^{-1} s^{-1} at pH 4.2 and 21°C and k = (24 ± 4) M^{-1} s^{-1} at pH 4.1 and 19°C in water, with a half-life of 1.5 h at pH 7 (Yao & Haag 1991)

k(aq.) = $(2.6 \pm 0.4) \times 10^9$ M^{-1} s^{-1} for the reaction (photo-Fenton with reference to acetophenone) with hydroxyl radical in aqueous solutions at pH 3.6 and 24 ± 1°C (Haag & Yao 1992)

k(aq.) = 0.82×10^9 M^{-1} s^{-1} for reaction with hydroxyl radical in irradiated field water (Mabury & Crosby 1996)

Hydrolysis: $t_{1/2}$ ~ 70 d at pH 3.1 of citrate buffer; $t_{1/2}$ ~ 75 d at pH 11.1 of carbonate buffer and $t_{1/2}$ ~ 2 d at 3.9 of phosphate buffer + sterile lake sediment in aqueous solutions at 25°C (Armstrong et al. 1967; quoted, Muir 1991)

Over all rate constant $k = 7.6 \times 10^{-5}\ s^{-1}$ with $t_{1/2}$ = 2.5 h at 25°C and pH 7 (Mabey & Mill 1978)

$t_{1/2}$ = 3.3, 14, 58, 240, 100, 12.5, and 1.5 d at pH 1, 2, 3, 4, 11, 12, and 13, respectively, in aqueous buffered solutions in soil at 25°C (Armstrong et al. 1967; quoted, Montgomery 1993);

$t_{1/2}$ = 244 d without humic materials, $t_{1/2}$ = 1.37 d with the presence of 2% humic acid at pH 4 and 25°C (Li & Felbeck 1972; quoted, Howard 1991; Montgomery 1993)

$k = 3.9 \times 10^{-5}\ M^{-1}\ s^{-1}$ and $k = 7.6 \times 10^{-5}\ M^{-1}\ s^{-1}$ with $t_{1/2}$ = 66 and 81 d in aqueous solutions of pH 3.1 and 11.1, respectively (Wolfe et al. 1976; quoted, Muir 1991)

k(aq.) = 19.9 d^{-1} at pH 2.9, k = 3.99 d^{-1} at pH 4.5, k = 1.74 d^{-1} at pH 6.0, and k = 0.934 d^{-1} at pH 7.0 with corresponding $t_{1/2}$ = 34.8, 174, 398, and 742 d all at 25°C in 0.5 mg mL^{-1} concn. of aqueous fulvic acid (Khan 1978; quoted, Howard 1991; Montgomery 1993)

k(aq.) = 28.4 d^{-1} at pH 2.8, k = 12.6 d^{-1} at pH 4.5, k = 3.16 d^{-1} at pH 6.0, and k = 1.23 d^{-1} at pH 7.0 with corresponding $t_{1/2}$ = 24.4, 55.0, 219, and 563 d all at 25°C in 1.0 mg mL^{-1} concn. of aqueous fulvic acid (Khan 1978)

k(aq.) = 151 d^{-1} at pH 2.4, k = 43.7 d^{-1} at pH 4.5, k = 13.2 d^{-1} at pH 6.0, and k = 7.93 d^{-1} at pH 7.0 with corresponding $t_{1/2}$ = 4.60, 15.9, 52.5 and 87.3 d all at 25°C in 5.0 mg mL^{-1} concn. of aqueous fulvic acid (Khan 1978)

k(aq.) = $9.30 \times 10^{-6}\ s^{-1}$ with $t_{1/2}$ = 86 d at 20°C in a buffer at pH 5 (Burkhard & Guth 1981; quoted, Muir 1991)

$t_{1/2}$ > 3 months (in sterile buffer solution at pH 7.2) and $t_{1/2}$ > 14 d (in sterile mineral salt solution at pH 7.2) for 20 μg mL^{-1} to hydrolyze at 23°C (Geller 1980; quoted, Muir 1991)

k(alkaline) = $1 \times 10^{-16}\ M^{-1}\ s^{-1}$ with $t_{1/2}$ = 742 d (Schnoor & McAvoy 1981; quoted, Schnoor 1992)

$t_{1/2}$ = 1771 yr at pH 7 and 25°C (Montgomery 1993)

Biodegradation:

$t_{1/2}$ = 64 d in soil (Armstrong et al. 1967; Dao et al. 1979; quoted, Means et al. 1983)

$t_{1/2}$ = 3.21 d in aqueous solution from river die-away tests (Furmidge & Osgerby 1967; quoted, Scow 1982)

$t_{1/2}$(aerobic) > 90 d for 10–20 μg mL^{-1} to degrade in soil-water suspension (Goswami & Green 1971; quoted, Muir 1991)

k(aq.) = 0.019 d^{-1} by soil incubation die-away studies (Rao & Davidson 1980; quoted, Scow 1982);

$t_{1/2}$(aerobic) > 35 d for 0.1–1.0 μg mL^{-1} to slowly biodegrade in sediment/water at 25°C (Wolf & Jackson 1982; quoted, Muir 1991)

$t_{1/2}$ = 36 and 110 d in soil (Jones et al. 1982; quoted, Means et al. 1983)

$t_{1/2}$ = 71 d for a 100 d leaching and screening test in 0–10 cm depth of soil (Jury et al. 1983, 1984, 1987a; Jury & Ghodrati 1989; quoted, Grover 1991)

k = 0.22 d^{-1} of aerobic degradation rate observed in incubations of river water samples (Lyman et al. 1990; quoted, Hemond & Fechner 1994)

$t_{1/2}$ = 201 d with 12 mM methanol, for aqueous atrazine using first-order decay rate, $t_{1/2}$ = 289 d with 6 mM sodium acetate, $t_{1/2}$ = 164 d with 6 mM acetic acid and $t_{1/2}$ = 200 d with 2 mM glucose; however $t_{1/2}$ = 224 d in the sample reactors without any organic amendments (Chung et al. 1996)

degradation $t_{1/2}$ = 39 h and 43 h by soil micro *Rhodococcus*. sp. NI86/21 with atrazine concn 4 μg/mL and 8 μg/mL respectively (Van Zwieten & Kennedy 1995)

first order removal of atrazine from sediment organic carbon: k = –0.0054 d^{-1} with $t_{1/2}$ = 128 d in surface sediment 0–6 cm depth, k = –0.0016 d^{-1} with $t_{1/2}$ = 433 d in sub-surface sediment 24–34 cm depth from Blue Heron Pond; k = –0.007 d^{-1} with $t_{1/2}$ = 99 d in surface sediment 0–6 cm depth, k = –0.0022 d^{-1} with $t_{1/2}$ = 630 d in sub-surface sediment 24–34 cm depth rom Oyster Rake Pond; k = –0.0142 d^{-1} with $t_{1/2}$ = 49 d in surface sediment 0–6 cm depth, k = –0.0009 d^{-1} with $t_{1/2}$ = 770 d in sub-surface sediment 24–34 cm depth from Trumpet Creeper East Pond, and k = –0.0149 d^{-1} with $t_{1/2}$ = 47 d in surface sediment 0–6 cm depth, k = –0.0000 d^{-1} with $t_{1/2}$ = 70 d in sub-surface sediment 24–34 cm depth from Trumpet Creeper North, Kiawah island (Smalling & Aelion 2004)

50–60% degradation in 35–100 d by anaerobic mixed culture microorganisms with atrazine as sole carbon source (Ghosh & Philip 2004)

Biotransformation:

Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants:

k_2 = 0.0248, 1.26 h^{-1} (algae, daphnids, Ellgehausen et al. 1980)
k_2 = 27.2 d^{-1} (catfish, Ellgehausen et al. 1980)
k_1 = 2.4, 30, 19.0 h^{-1} (zebrafish: egg, yolk sac fry, juvenile; Görge & Nagel 1990)
k_1 = 227.0 h^{-1}; k_2 = 2.354 h^{-1} (algae *Scenedesmus acutus*, Wang et al. 1996)
k_1 = 0.412 h^{-1}; k_2 = 0.073 h^{-1} (catfish *Ictalurus melas*, Wang et al. 1996)
k_1 = 2.027 h^{-1}; k_2 = 1.161 h^{-1} (water flea *Daphnia magna*, Wang et al. 1996)

Half-Lives in the Environment:

Air: $t_{1/2}$ = 2.6 h, based on estimated rate constant k = 147.2 × 10^{-12} cm^3 $molecule^{-1}$ s^{-1} at 25°C for the vapor-phase reaction with hydroxyl radical in air (Atkinson 1987; quoted, Howard 1991).

Surface water: estimated $t_{1/2}$ ~ 3.21 d in aqueous solution from river die-away tests (Furmidge & Osgerby 1967; quoted, Scow 1982);
$t_{1/2}$ = 1–4 wk in estuarine systems (Jones et al. 1982; quoted, Meakins et al. 1994);
under laboratory conditions in distilled water and river water was completely degraded after 21.3 and 7.3 h, respectively (Mansour et al. 1989; quoted, Montgomery 1993);
$t_{1/2}$ = 3.2 d to 7–8 months in aquatic environments (Eisler 1985; quoted, Day 1991);
measured rate constant k = (24 ± 4) M^{-1} s^{-1} at pH 4.0, k = (13 ± 1) M^{-1} s^{-1} at pH 4.2, for direct reaction with ozone in water at 26 and 21°C, respectively, with $t_{1/2}$ = 1.5 h at pH 7 (Yao & Haag 1991);.
$t_{1/2}$ = 35.6–168 h in surface water system of a small stream in Iowa by water quality analyses (Kolpin & Kalkhoff 1993);
$t_{1/2}$ = 235 d at 6°C, $t_{1/2}$ = 164 d at 22°C in darkness, $t_{1/2}$ = 59 d under sunlight conditions for river water at pH 17.3; $t_{1/2}$ = 130 d at 22°C in darkness for filtered river water at pH 7.3 and $t_{1/2}$ = 200 d at 22°C in darkness, $t_{1/2}$ = 169 d under sunlight conditions for seawater, pH 8.1 (Lartiges & Garrigues 1995)

Groundwater: $t_{1/2}$ = 6–15 months for 0.72–10 μg mL^{-1} to biodegrade slowly at 25°C (Weidener 1974; quoted, Muir 1991)
reported half-lives or persistence, $t_{1/2}$ = 60–150, 71, 74, and 130 d (Bottoni & Funari 1992)

Sediment: $t_{1/2}$ = 145 d in a Wisconsin Lake sediment (Armstrong et al. 1967; quoted, Jones et al. 1982; Means et al. 1983) and $t_{1/2}$ ~ 30 d for Chesapeake Bay sediment (Ballantine et al. 1978; quoted, Jones et al. 1982);
$t_{1/2}$ = 7–28 d for 0.1 μg mL^{-1} to rapid degrade in both aerobic and low oxygen systems in estuarine sediment/water at 12–35°C (Jones et al. 1982, quoted, Muir 1991);
$t_{1/2}$(aerobic) > 35 d for 0.1–1.0 μg mL^{-1} to slowly biodegrade in sediment/water at 25°C (Wolf & Jackson 1982; quoted, Muir 1991)
$t_{1/2}$ = 60–120 d in surface sediment, $t_{1/2}$ = 60–223 d in subsurface sediment
biodegradation $t_{1/2}$ = 47–128 d in the surface and $t_{1/2}$ = 70–770 in subsurface sediment (Smalling & Aelion 2004)

Soil: half-lives in aqueous buffered solutions in soil at 25°C and pH 1, 2, 3, 4, 11, 12, and 13 were reported to be 3.3, 14, 58, 240, 100, 12.5, and 1.5 d, respectively (Armstrong et al. 1967; quoted, Montgomery 1993);
$t_{1/2}$ = 3–5 yr in agricultural soils (Armstrong et al. 1967; quoted, Jones et al. 1982);
estimated persistence of 10 months in soil (Kearney et al. 1969; quoted, Jury et al. 1987a);
$t_{1/2}$ = 1.73, and 244 d at 25°C and pH 4 with and without fulvic acid (2%) (Li & Felbeck 1972; quoted, Montgomery 1993);
persistence of 10 months in soil (Edwards 1973; quoted, Morrill et al. 1982);
$t_{1/2}$ = 6.0 months at 15°C and $t_{1/2}$ = 2.0 months at 30°C in soils (Freed & Haque 1973);
persistence of 12 months (Wauchope 1978);
correlated $t_{1/2}$ = 37 d at pH 5.1–7.0, and $t_{1/2}$ = 28 d at pH 7.7–8.2 (Boddington Barn soil, Hance 1979),
$t_{1/2}$ ~ 30 d at pH 4.6–5.3 and $t_{1/2}$ = 40 d at pH 6.3–8.0 (Triangle soil, Hance 1979);
$t_{1/2}$ = 37 d in agricultural soils (Dao et al. 1979; quoted, Jones et al. 1982);
estimated first-order $t_{1/2}$ = 36.5 d from biodegradation rate constant k = 0.019 d^{-1} by soil incubation die-away studies (Rao & Davidson 1980; quoted, Scow 1982);
$t_{1/2}$ = 53 and 113 d at pH 6.5 at 22°C in a Hatzenbühl soil at pH 4.8 and Neuhofen soil, respectively (Burkhard & Guth 1981; quoted, Montgomery 1993);
$t_{1/2}$ = 1–6 months (Jones et al. 1982; quoted, Meakins et al. 1994);
moderately persistent in soils with $t_{1/2}$ = 20–100 d (Willis & McDowell 1982);
biodegradation $t_{1/2}$ = 71 d from screening model calculations (Jury et al. 1984; 1987a,b; Jury & Ghodrati 1989);

$t_{1/2}$ ~ 6–10 wk (Hartley & Kidd 1987; quoted, Montgomery 1993);
field $t_{1/2}$ = 4 wk by using lysimeters (Bowman 1990);
half-lives from soil surfaces: $t_{1/2}$ = 655 to > 1000 d in peat soil and $t_{1/2}$ = 143–939 d in sandy soil at 20 ± 1°C (Dörfler et al. 1991);
degradation rate constant k = (1.20 ± 0.097) × 10^{-2} d^{-1} with $t_{1/2}$ = 57.8 d in control soil and k = (1.01 ± 0.034) × 10^{-2} d^{-1} with $t_{1/2}$ = 68.6 d in pretreated soil once only in the laboratory (Walker & Welch 1991);
$t_{1/2}$ ~ 21 d based on extractable residues in microcosm studies, compared to $t_{1/2}$ = 14 d in surface field soil (Winkelmann & Klaine 1991);
selected field $t_{1/2}$ = 60 d (Wauchope et al. 1992; quoted, Dowd et al. 1993; Richards & Baker 1993; Hornsby et al. 1996);
soil $t_{1/2}$ = 130 d (quoted, Pait et al. 1992);
field $t_{1/2}$ = 35–50 d in soil and water but may be longer under cold or dry conditions; $t_{1/2}$ = 105 to > 200 d under groundwater conditions, depending on test system (Wood et al. 1991; quoted, Tomlin 1994);
reported $t_{1/2}$ = 60–150 d, 71 d, 74 d and 130 d (Bottoni & Funari 1992);
first-order k = –0.017 to –0.003 d^{-1} with corresponding $t_{1/2}$ = 41 d in the 0- to 30-cm soil to $t_{1/2}$ = 231 d in the 90 to 120-cm soil in Ames, Iowa (Kruger et al. 1993);
dissipation $t_{1/2}$ = 71 d from soil surface (Gish et al. 1995);
$t_{1/2}$ = 60 d (selected, Halfon et al. 1996).
$t_{1/2}$ = 60 d (Gao et al. 1997)

Biota: $t_{1/2}$ = 0.03 h in algae, $t_{1/2}$ = 1.52 d in catfish and $t_{1/2}$ = 9.5 h in daphnids (Ellgehausen et al. 1980);
biochemical $t_{1/2}$ = 64 d from screening model calculations (Jury et al. 1987b);
$t_{1/2}$ = 25.6 d in bean, $t_{1/2}$ = 24.3 d in turnips and $t_{1/2}$ = 14.6 d in oats at 20 ± 1°C from plant surfaces (Dörfler et al. 1991).

TABLE 17.1.1.4.1
Reported vapor pressures of atrazine at various temperatures and the coefficients for the vapor pressure equations

$\log P = A - B/(T/K)$ (1)
$\log P = A - B/(C + t/°C)$ (2)
$\log P = A - B/(C + T/K)$ (3)
$\log P = A - B/(T/K) - C\cdot\log(T/K)$ (4)
$\ln P = A - B/(T/K)$ (1a)
$\ln P = A - B/(C + t/°C)$ (2a)

Friedrich & Stammbach 1964		**Grayson & Fosbracey 1982**		**Rordorf 1989**		**Goodman 1997**	
gas saturation-GC		**gas saturation-GC**		**gas saturation-GC**		**Knudsen effusion method**	
t/°C	**P/Pa**	**t/°C**	**P/Pa**	**t/°C**	**P/Pa**	**t/°C**	**P/Pa**
20	4.0×10^{-5}	51.0	0.0040	25	3.9×10^{-5}	40	6.7×10^{-4}
	extrapolated	55.5	0.0048	50	1.9×10^{-3}	50	2.2×10^{-3}
measured range 50–130°C		63.0	0.0095	75	0.056	60	9.5×10^{-3}
Antoine eq.		66.0	0.0337	100	1.0	70	0.030
eq. 1	P/mmHg	66.7	0.023	125	13.0	80	0.098
A	13.766	76.5	0.0713				
B	5945	81.5	0.117	eq. 1	P_S/Pa	eq. 1	P/Pa
		20	3.7×10^{-5}	A	17.583	A	16.08
				B	6558.5	B	6040
		eq. 1a	P/Pa	for temp range 40–125°C			
		A	36.80				
		B	13.778		liquid		
				eq. 1	P_L/Pa		
				A	13.2701		
				B	4626.79		

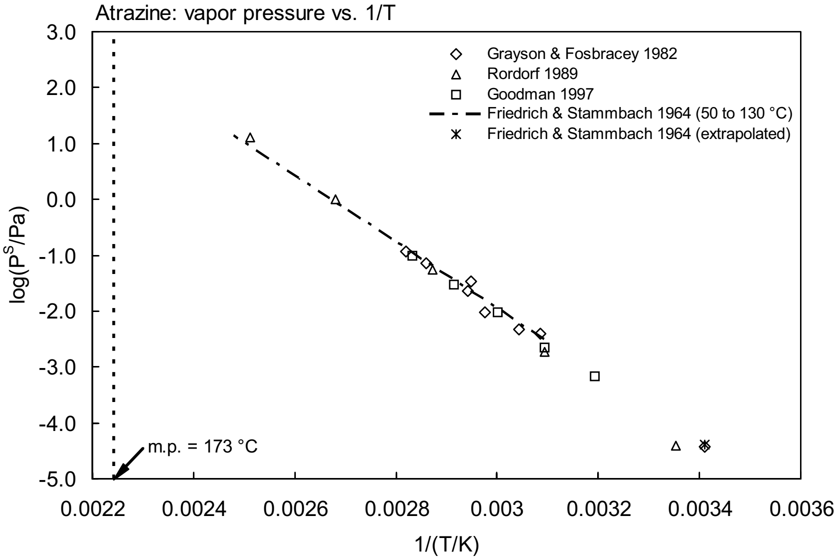
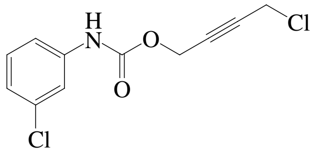


FIGURE 17.1.1.4.1 Logarithm of vapor pressure versus reciprocal temperature for atrazine.

17.1.1.5 Barban



Common Name: Barban
Synonym: Barbamate, Barbane, Carbine, Carbyne, CBN, Chlorinat
Chemical Name: carbamic acid, (3-chlorophenyl)-, 4-chloro-2-butynyl ester; 4-chlorobut-2-ynyl 3-chloro-carbanilate; 4-chloro-2-butynyl 3-chlorophenylcarbamate
Uses: herbicide for post-emergence control of wild oats in wheat, barley, broad beans, field beans, soybeans, peas, sugar beet, flax, lucerne, lentils, mustard, oilseed rape, sunflowers, etc.
CAS Registry No: 101-27-9
Molecular Formula: $C_{11}H_9Cl_2NO_2$
Molecular Weight: 258.101
Melting Point (°C):
75 (Khan 1980; Herbicide Handbook 1989; Lide 2003)
Boiling Point (°C):
Density (g/cm^3 at 20°C):
1.403 (25°C, Hartley & Kidd 1987)
Molar Volume (cm^3/mol):
262.8 (calculated-Le Bas method at normal boiling point, this work)
Dissociation Constant pK_a:
Enthalpy of Vaporization, ΔH_V (kJ/mol):
109.1 (Rordorf 1989)
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
26.8 (Rordorf 1989)
Entropy of Fusion, ΔS_{fus} (J/mol K):
Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F: 0.323 (mp at 75°C)

Water Solubility (g/m^3 or mg/L at 25°C or as indicated):
15.0 (Swezey & Nex 1961)
11.0 (20°C, Weber 1972; Worthing & Walker 1987)
11.0 (Martin & Worthing 1977; Ashton & Crafts 1981; Hartley & Kidd 1987; Worthing & Walker 1987; Herbicide Handbook 1989, Budavari 1989; Milne 1995)
11.0 (20–25°C, selected, Augustijn-Beckers et al. 1994; Hornsby et al. 1996)

Vapor Pressure (Pa at 25°C or as indicated and reported temperature dependence equations):
1.33×10^{-3} (20°C, Weber 1972; Worthing & Walker 1987)
5.00×10^{-5} (Hartley & Kidd 1987)
1.60×10^{-4} (Worthing & Walker 1987)
5.05×10^{-5} (Herbicide Handbook 1989)
3.50×10^{-5}, 1.0×10^{-3}, 0.019, 0.240, 2.20 (25, 50, 70, 100, 125°C, gas saturation-GC, Rordorf 1989)
$\log (P_L/Pa) = 14.669 - 5703.8/(T/K)$; measured range 72–150°C (gas saturation-GC, Rordorf 1989)
5.07×10^{-5} (20–25°C, selected, Augustijn-Beckers et al. 1994; Hornsby et al. 1996)

Henry's Law Constant (Pa·m^3/mol at 25°C or as indicated):
0.00117 (20°C, calculated-P/C, Muir 1991)
1.17 (calculated-P/C as per Worthing & Walker 1987, Majewski & Capel 1995)
0.00117 (calculated-P/C, this work)

Octanol/Water Partition Coefficient, log K_{OW}:

2.68	(selected, Gerstl & Helling 1987)

Bioconcentration Factor, log BCF:

2.20	(calculated-S, Kenaga 1980)

Sorption Partition Coefficient, log K_{OC} at 25°C or as indicated:

3.06	(soil, calculated-S, Kenaga 1980)
2.66	(calculated-MCI χ, Gerstl & Helling 1987)
3.00	(20–25°C, estimated, Augustijn-Beckers et al. 1994; Hornsby et al. 1996)

Environmental Fate Rate Constants, k, or Half-Lives, $t_{½}$:

Volatilization: estimated $t_{½}$ = 6690 d from 1 m depth of water at 20°C (Muir 1991).

Photolysis: $t_{½}$ = 2.25 h for 22–99% of 10 μg/ml to degrade in distilled water under 300 nm light (Tanaka et al. 1981; quoted, Cessna & Muir 1991).

Oxidation:

Hydrolysis:

Biodegradation:

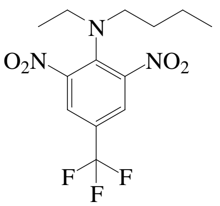
Biotransformation:

Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants:

Half-Lives in the Environment:

Soil: estimated persistence of 2 months (Kearney et al. 1969; quoted, Jury et al. 1987);
persistence of 2 weeks in soil (Edwards 1973; quoted, Morrill et al. 1982);
persistence of about 3 weeks in soil (Herbicide Handbook 1989);
selected field $t_{½}$ = 5 d (Augustijn-Beckers et al. 1994; Hornsby et al. 1996).

17.1.1.6 Benefin



Common Name: Benefin
Synonym: Balan, Bonalan, benfluralin
Chemical Name: *N*-butyl-*N*-ethyl-α,α,α-trifluoro-2,6-dinitro-*p*-toluidine
Uses: as pre-emergence herbicide for the control of annual grasses and broadleaf weeds in chicory, cucumbers, endive, groundnuts, lettuce, lucerne, and other foliage crops.
CAS Registry No: 1861-40-1
Molecular Formula: $C_{13}H_{16}F_3N_3O_4$
Molecular Weight: 335.279
Melting Point (°C):
66 (Lide 2003)
Boiling Point (°C):
121–122 (0.5 mmHg), 148–149 at 7 mmHg (Tomlin 1994)
Density (g/cm^3 at 20°C):
1.28 (tech., Tomlin 1994)
Molar Volume (cm^3/mol):
295.9 (calculated-Le Bas method at normal boiling point)
Dissociation Constant pK_a:
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
38.70 (DSC method, Plato & Glasgow 1969)
Entropy of Fusion, ΔS_{fus} (J/mol K):
Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F: 0.396 (mp at 66°C)

Water Solubility (g/m^3 or mg/L at 25°C or as indicated):
< 1.0 (Ashton & Crafts 1973)
0.50 (Weber et al. 1980)
1.0 (20°C, selected, Suntio et al. 1988)
0.10 (Herbicide Handbook 1983; Tomlin 1994)
0.10 (20–25°C, selected, Hornsby et al. 1996)

Vapor Pressure (Pa at 25°C or as indicated):
0.00519 (30°C, Ashton & Crafts 1973)
0.0104 (Herbicide Handbook 1983)
0.0040 (20°C, estimated, Suntio et al. 1988)
0.0087 (Tomlin 1994)
0.0088 (20–25°C, selected, Hornsby et al. 1996)

Henry's Law Constant (Pa·m^3/mol at 25°C or as indicated):
1.34 (20°C, calculated-P/C, Suntio et al. 1988)

Octanol/Water Partition Coefficient, log K_{OW}:
5.34 (selected, Magee 1991)
5.29 (20°C, pH 7, Tomlin 1994)
5.29 (pH 7, selected, Hansch et al. 1995)

Bioconcentration Factor, log BCF:
3.36 (calculated-S per Kenaga 1980, this work)

Sorption Partition Coefficient, log K_{OC}:

4.03	(quoted exptl., Sabljic 1987)
4.03, 3.75	(quoted, estimated; Magee 1991)
3.95	(soil, Hornsby et al. 1996)
2.96 (2.59–3.33)	(soil: organic carbon OC ≥ 0.5%, average, Delle Site 2001)

Environmental Fate Rate Constants, k, or Half-Lives, $t_{1/2}$:

Volatilization:

Photolysis: atmospheric and aqueous photolysis half-lives were estimated to be 288–864 h (Howard et al. 1991).

Oxidation: photooxidation $t_{1/2}$ ~ 0.782–7.82 h based on reaction with OH radicals in air (Howard et al. 1991).

Hydrolysis: no hydrolyzable group (Howard et al. 1991).

Biodegradation: aerobic $t_{1/2}$ ~ 504–2880 h in soil, and anaerobic soil $t_{1/2}$ = 144–480 h (Howard et al. 1991).

Biotransformation:

Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants:

Half-Lives in the Environment:

Air: $t_{1/2}$ = 0.782–7.82 h based on estimated reaction with OH radicals in the gas-phase (Howard et al. 1991).

Surface water: $t_{1/2}$ = 288–864 h based on observed photolysis by sunlight (Howard et al. 1991).

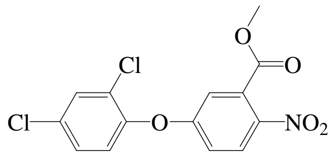
Groundwater: $t_{1/2}$ = 144–5760 h based on unacclimated aqueous aerobic and anaerobic biodegradation half-lives (Howard et al. 1991).

Sediment:

Soil: $t_{1/2}$ = 504–2880 h based on aerobic solid die-away test data (Howard et al. 1991);
field $t_{1/2}$ = 40 d (Hornsby et al. 1996).

Biota:

17.1.1.7 Bifenox



Common Name: Bifenox
Synonym: MC-4379, Modown
Chemical Name: benzoic acid, 5-(2,4-dichlorophenoxy)-2-nitro-, methyl ester; methyl-5-(2,4-dichlorophenoxy)-2-nitrobenzoate
Uses: selective pre-emergence and post-emergence herbicide to effectively control a wide variety of broadleaf weeds in corn, grain, sorghum, maize, rice, and soybeans.
CAS Registry No: 42576-02-3
Molecular Formula: $C_{14}H_9Cl_2NO_5$
Molecular Weight: 342.131
Melting Point (°C):
85 (Lide 2003)
Boiling Point (°C):
Density (g/cm^3 at 20°C):
1.155 (Ashton & Crafts 1981; Herbicide Handbook 1989; Montgomery 1993)
Molar Volume (cm^3/mol):
305.5 (calculated-Le Bas method at normal boiling point)
Dissociation Constant pK_a:
Enthalpy of Vaporization, ΔH_V (kJ/mol):
90.5 (Rordorf 1989)
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
26.4 (Rordorf 1989)
Entropy of Fusion, ΔS_{fus} (J/mol K):
74.0 (Rordorf 1989)
Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F: 0.258 (mp at 85°C)

Water Solubility (g/m^3 or mg/L at 25°C or as indicated):
0.35 (20°C, Weber 1972; Worthing & Walker 1987)
0.35 (Martin & Worthing 1977; Herbicide Handbook 1978)
0.35 (Ashton & Crafts 1981; Herbicide Handbook 1989; Budavari 1989)
0.35 (30°C, Worthing & Walker 1987)
0.35 (Hartley & Kidd 1987; Worthing & Hance 1991; Montgomery 1993; Tomlin 1994; Milne 1995)
0.398 (20–25°C, selected, Wauchope et al. 1992; Lohninger 1994; Hornsby et al. 1996)

Vapor Pressure (Pa at 25°C or as indicated and reported temperature dependence equations):
0.00032 (20°C, Weber 1972; Worthing & Walker 1987)
0.00032 (30°C, Ashton & Crafts 1981; Worthing & Hance 1991; Tomlin 1994)
0.00032 (30°C, Hartley & KIdd 1987; Budavari 1989; Montgomery 1993)
5.40×10^{-6}, 2.0×10^{-4}, 4.40×10^{-3}, 0.064, 0.67 (25, 50, 70, 100, 125°C, gas saturation-GC, Rordorf 1989)
$\log (P_S/Pa) = 14.996 - 6040.4/(T/K)$; measured range 36.9–85.5°C (solid, gas saturation-GC, Rordorf 1989)
$\log (P_L/Pa) = 13.815 - 5582.5/(T/K)$; measured range 90.5–175°C (liquid, gas saturation-GC, Rordorf 1989)
0.00032 (20–25°C, selected, Wauchope et al. 1992; Hornsby et al. 1996)

Henry's Law Constant ($Pa \cdot m^3/mol$ at 25°C or as indicated):
0.321 (20°C, calculated-P/C, Muir 1991)
0.011 (calculated-P/C, Montgomery 1993)
0.313 (calculated-P/C, this work)

Octanol/Water Partition Coefficient, log K_{OW}:

5.63	(selected, Dao et al. 1983)
4.50	(Worthing & Hance 1991)
4.48	(Montgomery 1993; Tomlin 1994)
4.48	(selected, Hansch et al. 1995)
5.24	(RP-HPLC-RT correlation using short ODP column, Donovan & Pescatore 2002)

Bioconcentration Factor, log BCF:

2.30	(static water, Metcalf & Sanborn 1975; quoted, Kenaga & Goring 1980; Isensee 1991)
3.05	(calculated-S, Kenaga 1980; quoted, Isensee 1991)

Sorption Partition Coefficient, log K_{OC}:

3.89	(soil, calculated per Kenaga & Goring, Kenaga 1980)
4.0	(soil, 20–25°C, estimated, Wauchope et al. 1992; Hornsby et al. 1996)
2.24–4.39	(Montgomery 1993)
4.0	(estimated-chemical structure, Lohninger 1994)
2.70–4.36	(Tomlin 1994)

Environmental Fate Rate Constants, k, or Half-Lives, $t_{1/2}$:

Volatilization: estimated $t_{1/2}$ = 29.8 d from 1 m depth of water at 30°C (Muir 1991).

Photolysis: with < 5% degradation by UV light of 290–400 nm in 48 h (Worthing & Hance 1991).

Oxidation:

Hydrolysis: stable in aqueous solution at pH 5.0–7.3 but rapidly hydrolyzed at pH 9.0 both at 22°C (Worthing & Hance 1991).

Biodegradation: $t_{1/2}$ = 2–5 d for 10 μg/mL to biodegrade in flooded soil at 30°C (Ohyama & Kuwatsuka 1978; quoted, Muir 1991).

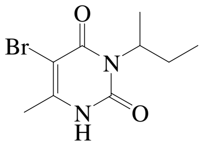
Biotransformation:

Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants:

Half-Lives in the Environment:

Soil: $t_{1/2}$ = 2–5 d for 10 μg/ml to biodegrade in flooded soil at 30°C (Ohyama & Kuwatsuka 1978; quoted, Muir 1991);
average $t_{1/2}$ = 7–14 d in soils (Hartley & Kidd 1987; Herbicide Handbook 1989; quoted, Montgomery 1993);
selected field $t_{1/2}$ = 7.0 d (Wauchope et al. 1992; Hornsby et al. 1996);
average $t_{1/2}$ = 7–14 d (Herbicide Handbook 1989);
$t_{1/2}$ ~ 5–7 d in soil (Tomlin 1994).

17.1.1.8 Bromacil



Common Name: Bromacil
Synonym: Borea, Bromax, Bromazil, Cynogan, Hyvar, Hyvarex, Krovar I or II, Nalkil, Uragan, Urox B, Uron HX, Weed Blast
Chemical Name: 5-bromo-3-*sec*-butyl-6-methyluracil; 5-bromo-6-methyl-3-(1-methylpropyl)-2,4-(1*H*,3*H*)pyrimidinedione
Uses: Herbicide applied to soil to control annual and perennial grasses, broadleaf weeds, and general vegetation on uncropped land; also used for selective weed control in apple, asparagus, cane fruit, hops, and citrus crops.
CAS Registry No: 314-40-9
Molecular Formula: $C_9H_{13}BrN_2O_2$
Molecular Weight: 261.115
Melting Point (°C):
158 (Lide 2003)
Boiling Point (°C):
Density (g/cm^3 at 20°C):
1.55 (25°C, Hartley & Kidd 1987; Herbicide Handbook 1989; Worthing & Hance 1991; Montgomery 1993)
1.59 (23°C, Tomlin 1994)
1.55 (Milne 1995)
Molar Volume (cm^3/mol):
193.1 (calculated-Le Bas method at normal boiling point)
Dissociation Constant pK_a:
9.10 (Wauchope et al. 1992; Hornsby et al. 1996)
< 7.0 (Montgomery 1993)
9.27 (Tomlin 1994)
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
Entropy of Fusion, ΔS_{fus} (J/mol K):
Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F: 0.0496 (mp at 158°C)

Water Solubility (g/m^3 or mg/L at 25°C or as indicated):
815 (Bailey & White 1965; Khan 1980; Hartley & Kidd 1987; Montgomery 1993; Milne 1995)
815 (Melnikov 1971; Spencer 1973; Herbicide Handbook 1978; Herbicide Handbook 1989)
815 (20°C, Weber 1972; Worthing & Walker 1987, Worthing & Hance 1991)
820 (Beste & Humburg 1983; Jury et al. 1983)
1064 (shake flask-GC or LSC, Gerstl & Mingelgrin 1984; Gerstl & Helling 1987)
626, 775, 1043 (4, 25, 40°C, shake flask-LSS, Madhun et al. 1986)
700 (20–25°C, selected, Wauchope et al. 1992; Lohninger 1994; Hornsby et al. 1996)
700, 807, 1287 (at pH 7, 5, 9, Tomlin 1994)

Vapor Pressure (Pa at 25°C or as indicated):
5×10^{-5} (20°C, Weber 1972; Worthing & Walker 1987)
3×10^{-5} (estimated, USEPA 1975)
0.107 (100°C, Khan 1980)
2.9×10^{-5} (Jury et al. 1983)
0.00033 (Hartley & Kidd 1987; Worthing & Hance 1991)
4×10^{-5} (20–25°C, selected, Wauchope et al. 1992)
3.3×10^{-5} (Montgomery 1993)

Henry's Law Constant (Pa·m^3/mol at 25°C at 25°C or as indicated):
9.17×10^{-6} (Beste & Humburg 1983; Jury et al. 1983)
9.17×10^{-5} (calculated-P/C, Jury et al. 1984, 1987a; Jury & Ghodrati 1989)
0.0019 (20°C, selected, Suntio et al. 1988)
1.06×10^{-5} (20°C, calculated-P/C, Muir 1991)
1.06×10^{-5} (calculated-P/C, Montgomery 1993)

Octanol/Water Partition Coefficient, log K_{OW}:
2.02 (Rao & Davidson 1980)
1.33 (selected, Dao et al. 1983)
1.84 (shake flask-GC or LSC, Gerstl & Mingelgrin 1984)
1.84, 1.87, 1.90 (4, 25, 40°C, shake flask-LSS, Madhun et al. 1986)
1.85 (selected, Gerstl & Helling 1987)
2.11 selected, Magee 1991; Devillers et al. 1996)
1.84–2.04 (Montgomery 1993)
2.11 (selected, Sangster 1993)
1.87, 1.88, 1.63 (at pH 7, 5, 9, Tomlin 1994)
2.11 (recommended, Hansch et al. 1995)

Bioconcentration Factor, log BCF:
0.505 (measured, Kenaga 1980)
2.27 (calculated-S, Kenaga 1980)
0.477 (calculated-K_{OC}, Kenaga 1980)
0.51 (*Pimephales promelas*, Call et al. 1987)

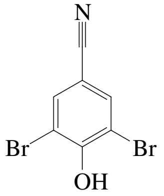
Sorption Partition Coefficient, log K_{OC} at 25°C or as indicated:
1.86 (soil, Hamaker & Thompson 1972)
3.13 (soil, calculated as per Kenaga & Goring 1980, Kenaga 1980)
1.86 (Rao & Davidson 1980)
2.33, 1.34, 1.63 (estimated-S, calculated-S and mp, calculated-K_{OW}, Karickhoff 1981)
1.61 (sediments average-Freundlich adsorption, Corwin & Farmer 1984)
1.41–2.46 (California lake sediments, Corwin & Farmer 1984)
1.98, 1.88 (4, 25°C, Semiahmoo soil, in μmol/kg OC, batch equilibrium method-LSS, Madhun et al. 1986)
2.11, 1.88 (4, 25°C, Adkins soil, in μmol/kg OC, Madhun et al. 1986)
1.90, 1.66, 1.75; 1.86, 1.89, 1.34 (estimated-K_{OW}; S, Madhum et al. 1986)
1.53, 2.73 (quoted, calculated-MCI χ, Gerstl & Helling 1987)
1.86 (soil, screening model calculations, Jury et al. 1987a,b; Jury & Ghodrati 1989; Carsel 1989)
2.56 (calculated-MCI χ, Bahnick & Doucette 1988)
1.86, 1.80 (reported, estimated as log K_{OM}, Magee 1991)
1.53, 1.86, 3.13 (soil, quoted values, Bottoni & Funari 1992)
1.51 (soil, 20–25°C, selected, Wauchope et al. 1992; Hornsby et al. 1996)
1.51 (Montgomery 1993)
2.09 (estimated-chemical structure, Lohninger 1994)
1.60 (quoted or calculated-QSAR MCI $^1\chi$, Sabljic et al. 1995)
1.43, 1.72 (average values for sediments, soils, Delle Site 2001)
1.48, 1.46, 1.53 (soils: organic carbon OC $\geq$ 0.1%, OC $\geq$ 0.5%, 0.1 $\leq$ OC < 0.5%, and pH 6.3–7.9, average, Delle Site 2001)
1.80, 1.72 (soils: organic carbon OC $\geq$ 0.1%, OC $\geq$ 0.5%, and pH $\leq$ 7.3 undissociated, average, Delle Site 2001)

Environmental Fate Rate Constants, k, or Half-Lives, $t_{1/2}$:
Volatilization: estimated $t_{1/2}$ ~ 10,000 d from 1 m depth of water at 20°C (Muir 1991).
Photolysis: 115 ppb contaminated water in the presence of TiO_2 and H_2O_2 photodegraded to 6 ppb by 15 h solar irradiation with complete degradation after 75 h (Muszkat et al. 1992).
Oxidation:
Hydrolysis:

Biodegradation: $t_{1/2}$ = 350 d for 100 d leaching and screening test in 0–10 cm depth of soil (Rao & Davidson 1980; quoted, Jury et al. 1983, 1984, 1987a).
Biotransformation:
Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants:

Half-Lives in the Environment:
Air:
Surface water:
Ground water: reported $t_{1/2}$ = 150–158 and 350 d (Bottoni & Funari 1992)
Sediment:
Soil: $t_{1/2}$ = 7.0 months at 15°C and $t_{1/2}$ = 4.5 months at 30°C in soils (Freed & Haque 1973);
rate constant k = 0.0038 d^{-1} with biodegradation $t_{1/2}$ = 350 d under field conditions (Rao & Davidson 1980; quoted, Jury et al. 1984);
$t_{1/2}$ = 350 d from screening model calculations (Jury et al. 1987a,b; Jury & Ghodrati 1989);
$t_{1/2}$ > 100 d (Willis & McDowell 1982)
$t_{1/2}$ ~ 5429–46200 d in loamy sand and peat at 25–35°C as follows (Madhum & Freed 1987):
$t_{1/2}$ = 46200, 12391, and 5856 d at 25, 30, and 35°C, respectively, at herbicide concn at 5 μg/kg, while $t_{1/2}$ = 18851, 9925, and 7588 d at 25, 30, and 35°C, respectively, at herbicide concn at 100 μg/kg in an Adkins loamy sand; however, the half-lives in peat. $t_{1/2}$ = 5429, 6789, and 8044 d at 25, 30, and 35°C, respectively, at herbicide concn at 5 μg/kg while $t_{1/2}$ = 6293, 5986, and 6784 d at 25, 30, and 35°C, respectively, at herbicide concn at 100 μg/kg in a Semiahoo mucky peat (Madhun & Freed 1987)
selected field $t_{1/2}$ = 60 d (Wauchope et al. 1992; Hornsby et al. 1996);
$t_{1/2}$ = 150–180d and 350 d (Bottoni & Funari 1992).
Biota: biochemical $t_{1/2}$ = 350 d from screening model calculations (Jury et al. 1987a,b; Jury & Ghodrati 1989).

17.1.1.9 Bromoxynil



Common Name: Bromoxynil

Synonym: Brittox, Brominal, Brominex, Brominil, Broxynil, Buctril, Chipco crab-kleen, ENT 20852, Nu-lawn weeder, Oxytril M, Partner

Chemical Name: 3,5-dibromo-4-hydroxybenzonitrile; 4-cyano-2,6-dibromophenol

Uses: herbicide for post-emergence control of annual broadleaf weeds and it is often used in combination with other herbicides to extend the spectrum of control.

CAS Registry No: 1689-84-5

Molecular Formula: $C_7H_3Br_2NO$

Molecular Weight: 276.913

Melting Point (°C):

190	(Khan 1980; Herbicide Handbook 1989; Montgomery 1993; Lide 2003)

Boiling Point (°C):

Density (g/cm^3 at 20°C):

Molar Volume (cm^3/mol):

176.7	(calculated-Le Bas method at normal boiling point, this work)

Dissociation Constant pK_a:

4.20	(radiometer/pH meter, Cessna & Grover 1978)
4.06	(Herbicide Handbook 1989; Montgomery 1993)
4.06	(Budavari 1989; Worthing & Hance 1991)
3.86	(Tomlin 1994)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

31.80	(DSC method, Plato 1972)

Entropy of Fusion, ΔS_{fus} (J/mol K):

Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F: 0.0241 (mp at 190°C)

Water Solubility (g/m^3 or mg/L at 25°C or as indicated):

130	(20–25°C, Spencer 1973)
131	(Kenaga 1980)
< 200	(Khan 1980)
130	(20–25°C, Ashton & Crafts 1981)
130	(Hartley & Kidd 1987; Montgomery 1993; Tomlin 1994; Milne 1995)
130	(Worthing & Walker 1987, Worthing & Hance 1991)
130	(20–25°C, Herbicide Handbook 1989)

Vapor Pressure (Pa at 25°C or as indicated):

< 0.0010	(20°C, Hartley & Kidd 1987; Tomlin 1994)
0.00064	(Herbicide Handbook 1989)
0.00064	(Montgomery 1993)

Henry's Law Constant (Pa·m^3/mol at 25°C or as indicated):

0.14180	(20–25°C, calculated-P/C, Montgomery 1993)
1.36×10^{-3}	(calculated-P/C, this work)

Octanol/Water Partition Coefficient, log K_{OW}:

2.60	(selected, Dao et al. 1983)

< 2.00	(Herbicide Handbook 1989)
< 2.00	(Montgomery 1993)

Bioconcentration Factor, log BCF:

1.60	(calculated, Kenaga 1980)

Sorption Partition Coefficient, log K_{OC}:

2.48	(soil, quoted from Kenaga 1980, Bottoni & Funari 1992)
2.48	(calculated, Montgomery 1993)
2.86, 3.06	(soil, quoted exptl.; estimated-general model using molecular descriptors, Gramatica et al. 2000)

Environmental Fate Rate Constants, k or Half-Lives, $t_{½}$:

Volatilization:

Photolysis: rate constant of degradation in water, $k = 1.04 \times 10^{-3}\ s^{-1}$ at pH 8.3 and $k = 1.08 \times 10^{-3}\ s^{-1}$ at pH 11.6 (Kochany 1992).

Oxidation:

Hydrolysis:

Biodegradation: $t_{½}$ ~ 24 h for 0.03 µg/mL to biodegrade in runoff water at 20–25°C (Brown et al. 1984; quoted, Muir 1991).

Biotransformation:

Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants:

Half-Lives in the Environment:

Air:

Surface water: $t_{½}$ ~ 24 h for 0.03 µg mL^{-1} to biodegrade in runoff water at 20–25°C (Brown et al. 1984; quoted, Muir 1991).

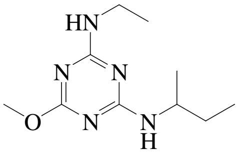
Ground water: reported $t_{½}$ = 10 d (Bottoni & Funari 1992)

Sediment:

Soil: $t_{½}$ ~ 10 d in soil (Hartley & Kidd 1987; Worthing & Hance 1991; quoted, Bottoni & Funari 1992; Montgomery 1993; Tomlin 1994);.

Biota:

17.1.1.10 *sec*-Bumeton



Common Name: *sec*-Bumeton
Synonym: etazine, GS14254, secbumeton
Chemical Name: *N*-ethyl-6-methoxy-*N′*-(1-methylpropyl)-1,3,5-triazine-2,4-diamine
CAS Registry No: 26259-45-0
Uses: herbicide
Molecular Formula: $C_{10}H_{19}N_5O$
Molecular Weight: 225.291
Melting Point (°C):

87	(Lide 2003)

Boiling Point (°C):
Density (g/cm^3 at 20°C):

1.105	(Hartley & Kidd 1987; Worthing & Walker 1987)

Molar Volume (cm^3/mol):
Dissociation Constant pK_a:

4.4	(Worthing 1987)
4.4, 4.36	(Augustijn-Beckers et al. 1994; Hornsby et al. 1996)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
Entropy of Fusion, ΔS_{fus} (J/mol K):
Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F: 0.246 (mp at 87°C)

Water Solubility (g/m^3 or mg/L at 25°C or as indicated):

620	(quoted, Kenaga & Goring 1980)
620	(Ashton & Crafts 1981)
600	(20°C, Hartley & Kidd 1987; Worthing & Walker 1987)
600	(20–25°C, selected, Augustijn-Beckers et al. 1994; Hornsby et al. 1996)

Vapor Pressure (Pa at 25°C or as indicated):

9.7×10^{-4}	(20°C, Ashton & Crafts 1981; Worthing & Walker 1987)
9.71×10^{-4}	(20°C, Hartley & Kidd 1987)
9.7×10^{-4}	(20–25°C, selected, Augustijn-Beckers et al. 1994; Hornsby et al. 1996)

Henry's Law Constant ($Pa \cdot m^3/mol$):

Octanol/Water Partition Coefficient, log K_{OW}:

3.20	(LOGPSTAR or CLOGP data, Sabljic et al. 1995)

Octanol/Air Partition Coefficient, log K_{OA}:

Bioconcentration Factor, log BCF or log K_B:

1.20	(fish, Kenaga 1980b)

Sorption Partition Coefficient, log K_{OC}:

2.54	(soil, calculated, Kenaga & Goring 1980)
2.11	(soil, calculated, Kenaga 1980b)
2.18	(soil, pH 7, Augustijn-Beckers et al. 1994; Hornsby et al. 1996)
2.78; 2.29	(soil: quoted, calculated-MCI χ, Meylan et al. 1992)
2.78	(soil, calculated-MCI χ, Sabljic et al. 1995)

2.78; 2.78, 2.55 (soil, estimated-class-specific model, estimated-general model using molecular descriptors, Gramatica et al. 2000)

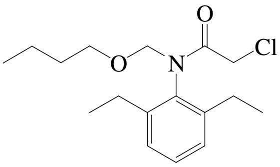
Environmental Fate Rate Constants, k, or Half-Lives, $t_{1/2}$:

Hydrolysis: on hydrolysis at 20°C, $t_{1/2}$ ~ 30 d at pH 1, $t_{1/2}$ = 75 d at pH 13 (Worthing & Walker 1987).

Half-Lives in the Environment:

Air:
Surface water: on hydrolysis at 20°C, $t_{1/2}$ ~ 30 d at pH 1, $t_{1/2}$ = 75 d at pH 13 (Worthing & Walker 1987).
Ground water:
Sediment:
Soil: field $t_{1/2}$ ~ 60 d (estimated, Augustijn-Beckers et al. 1994; Hornsby et al. 1996).
Biota:

17.1.1.11 Butachlor



Common Name: Butachlor
Synonym: Butanex, Butanox, CP 53619, Lambast, Machete, Pillarsete
Chemical Name: N-butoxymethyl-2-chloro-2′6′-diethylacetanilide; N-(butoxymethyl)-2-chloro-N-(2,6-diethylphenyl)-acetamide
Uses: herbicide for pre-emergence control of most annual grasses, some broadleaf weeds, and many aquatic weeds in both seeded and transplanted rice.
CAS Registry No: 23184-66-9
Molecular Formula: $C_{17}H_{26}ClNO_2$
Molecular Weight: 311.847
Melting Point (°C):

< –5.0	(Hartley & Kidd 1987; Worthing & Hance 1991; Tomlin 1994; Milne 1995; Lide 2003)

Boiling Point (°C):

156	(at 0.5 mmHg, Ashton & Crafts 1981; Herbicide Handbook 1989; Tomlin 1994; Milne 1995)

Density (g/cm^3 at 20°C):

1.07	(25°C, Ashton & Crafts 1981; Hartley & Kidd 1987; Herbicide Handbook 1989; Tomlin 1994; Milne 1995)

Molar Volume (cm^3/mol):

387.8	(calculated-Le Bas method at normal boiling point)

Dissociation Constant pK_a:
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
Entropy of Fusion, ΔS_{fus} (J/mol K):
Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F: 1.0

Water Solubility (g/m^3 or mg/L at 25°C or as indicated):

23	(20°C, Weber 1972; Worthing 1987)
20	(Martin & Worthing 1977)
23	(24°C, Ashton & Crafts 1981; Herbicide Handbook 1989)
20	(20°C, Hartley & Kidd 1987; Tomlin 1994; Milne 1995)
23	(24°C, Worthing & Walker 1987, Worthing & Hance 1991)
23	(20–25°C, selected, Augustijn-Beckers et al. 1994; Hornsby et al. 1996)

Vapor Pressure (Pa at 25°C or as indicated):

0.0007	(20°C, Weber 1972; Worthing & Walker 1987)
0.0006	(Ashton & Crafts 1981; Herbicide Handbook 1989)
0.0006	(Hartley & Kidd 1987; Worthing & Hance 1991; Tomlin 1994)
0.0006	(20–25°C, selected, Augustijn-Beckers et al. 1994; Hornsby et al. 1996)

Henry's Law Constant (Pa·m^3/mol at 25°C or as indicated):

0.00817	(20°C, calculated-P/C, Muir 1991)
0.00814	(calculated-P/C, this work)

Octanol/Water Partition Coefficient, log K_{OW}:

4.50	(quoted and recommended, Hansch et al. 1995; quoted, Sabljic et al. 1995)

Bioconcentration Factor, log BCF:

2.06	(calculated-S, Kenaga 1980)
1.03, 0.756	(18, 9 μg/L concn in water; carp, 3–5 d exposure, Wang et al. 1992)

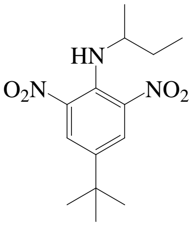
0.38, 0.845 (10, 1 μg/L concn in water; tilapia, 3–5 d exposure, Wang et al. 1992)
0.447, 0.845 (10, 1 μg/L concn in water; loach, 3–5 d exposure, Wang et al. 1992)
1.76, 2.02 (2.5, 1.25 μg/L concn in water; grass carp, 3–5 d exposure, Wang et al. 1992)
1.71, 1.90 (5, 2.5 μg/L concn in water; eel, 3–5 d exposure, Wang et al. 1992)
1.99, 2.34 (2.4, 0.4 μg/L concn in water; black silver carp, 3–5 d exposure, Wang et al. 1992)
0.041, 0.778 (100, 10 μg/L concn in water; freshwater clam, 3–5 d exposure, Wang et al. 1992)

Sorption Partition Coefficient, log K_{OC}:
2.92 (calculated-solubility, Kenaga 1980)
2.85 (20–25°C, selected, Augustijn-Beckers et al. 1994; Hornsby et al. 1996)
2.86 (soil, calculated-MCI $^1\chi$, Sabljic et al. 1995)

Environmental Fate Rate Constants, k, or Half-Lives, $t_{½}$:
Volatilization: estimated $t_{½}$ ~ 1049 d from 1 m depth of water at 20°C (Muir 1991).
Photolysis: $t_{½}$ = 0.8–5.4 h in distilled water (Chen et al. 1982; quoted, Cessna & Muir 1991).
Oxidation:
Hydrolysis: $t_{½}$ > 2.5 months for 2 μg/mL to hydrolyze in phosphate buffer at pH 6 and borate buffer at pH 9 both at 25°C (Chen & Chen 1979; quoted, Muir 1991).
Biodegradation:
Biotransformation:
Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants:

Half-Lives in the Environment:
Soil: persists for 6–10 wk in soil (Hartley & Kidd 1987; Tomlin 1994);
$t_{½}$ = 4 to 8 d depending upon soil type (Herbicide Handbook 1989);
persists in soil 42–70 d (Worthing & Hance 1991);
selected field $t_{½}$ = 12 d (Augustijn-Beckers et al. 1994; Hornsby et al. 1996).

17.1.1.12 Butralin



Common Name: Butralin
Synonym: Amex, Butalin, Rutralin, Sector, Tamex
Chemical Name: N-*sec*-butyl-4-*tert*-butyl-2,6-dinitroaniline; 4-(1,1-dimethylethyl)-N-(1-methylpropyl)-2,6-dinitrobenzenamine
Uses: herbicide for pre-emergence control of annual broadleaf weeds and grasses in cotton, beans, barley, rice, soybeans, alliums, vines, ornamentals and orchards of fruit and nut trees; also to control suckers on tobacco.
CAS Registry No: 33629-47-9e
Molecular Formula: $C_{14}H_{21}N_3O_4$
Molecular Weight: 295.335
Melting Point (°C):

60	(Lide 2003)

Boiling Point (°C):

134–136	(at 0.5 mmHg, Hartley & Kidd 1987; Worthing & Hance 1991; Tomlin 1994; Milne 1995)

Density (g/cm^3 at 20°C):
Molar Volume (cm^3/mol):

313.6	(calculated-Le Bas method at normal boiling point)

Dissociation Constant pK_a:
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
Entropy of Fusion, ΔS_{fus} (J/mol K):
Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F: 0.454 (mp at 60°C)

Water Solubility (g/m^3 or mg/L at 25°C or as indicated):

1.0	(Herbicide Handbook 1978)
1.0	(Khan 1980)
10	(24°C, Ashton & Crafts 1981)
1.0	(24°C, Hartley & Kidd 1987; Tomlin 1994; Milne 1995)
1.0	(24–26°C, Worthing & Walker 1987, Worthing & Hance 1991)
1.0	(Budavari 1989)

Vapor Pressure (Pa at 25°C):

0.002	(Ashton & Crafts 1981)
0.0017	(Hartley & Kidd 1987; Worthing & Hance 1991; Tomlin 1994)
0.0017	(Budavari 1989)

Henry's Law Constant (Pa·m^3/mol at 25°C):

0.502	(calculated-P/C, this work)

Octanol/Water Partition Coefficient, log K_{OW}:

4.54	(selected, Dao et al. 1983)
5.16	(quoted LOGPSTAR or CLOGP data, Sabljic et al. 1995)

Bioconcentration Factor, log BCF:

2.79	(calculated-S, Kenaga 1980; quoted, Isensee 1991)
2.80	(calculated-K_{OC}, Kenaga 1980)

Sorption Partition Coefficient, log K_{OC}:

3.64	(calculated, Kenaga & Goring 1980; quoted, Kenaga 1980)
3.91	(soil, Kenaga & Goring 1980; quoted, Sabljic 1987; Bahnick & Doucette 1988)
3.75	(calculated-MCI χ, Bahnick & Doucette 1988)
3.98	(soil, calculated-MCI $^1\chi$, Sabljic et al. 1995)
3.98; 3.38	(soil, quoted exptl.; estimated-general model using molecular descriptors, Gramatica et al. 2000)

Environmental Fate Rate Constants, k, or Half-Lives, $t_{1/2}$:

Volatilization:

Photolysis: $t_{1/2}$ = 8 h for 25% of 2000 μg/mL to degrade in methanol under sunlight (Plimmer & Klingebiel 1974; quoted, Cessna & Muir 1991).

Oxidation:

Hydrolysis:

Biodegradation: $t_{1/2}$ = 24 d for 0.5 μg/mL to biodegrade in soil at 20–42°C (Savage 1978; quoted, Muir 1991).

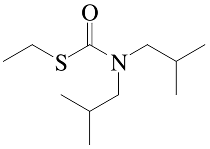
Biotransformation:

Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants:

Half-Lives in the Environment:

Soil: $t_{1/2}$ = 24 d for 0.5 μg/mL to biodegrade in soil at 20–42°C (Savage 1978; quoted, Muir 1991).

17.1.1.13 Butylate



Common Name: Butylate
Synonym: Butilate, diisocarb, Genate, R 1910, Sutan
Chemical Name: *S*-ethyldiisobutylthiocarbamate; *S*-ethyl-bis(2-methylpropylcarbamothioate
Uses: herbicide to control annual grass weeds in maize, by pre-plant soil incorporation; also to control some broadleaf weeds.
CAS Registry No: 2008-41-5
Molecular Formula: $C_{11}H_{23}NOS$
Molecular Weight: 217.372
Melting Point (°C): liquid
Boiling Point (°C):
  137.5–138 (at 21 mmHg, Hartley & Kidd 1987; Worthing & Hance 1991; Tomlin 1994; Milne 1995)
  71.0 (at 10 mmHg, Herbicide Handbook 1989)
Density (g/cm^3 at 20°C):
  0.9402 (25°C, Hartley & Kidd 1987; Herbicide Handbook 1989; Worthing & Hance 1991; Tomlin 1994)
  0.9417 (Milne 1995)
Molar Volume (cm^3/mol):
  280.9 (calculated-Le Bas method at normal boiling point, Suntio et al. 1988)
Dissociation Constant pK_a:
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
Entropy of Fusion, ΔS_{fus} (J/mol K):
Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F: 1.0

Water Solubility (g/m^3 or mg/L at 25°C or as indicated):
  45.0 (Kenaga 1980; Weber et al. 1980)
  45.0 (22°C, Ashton & Crafts 1981; Hartley & Kidd 1987; Herbicide Handbook 1989)
  46.0 (20°C, Worthing & Walker 1987, Worthing & Hance 1991)
  44.0 (20–25°C, selected, Wauchope et al. 1992; Hornsby et al. 1996)
  36.0 (20°C, Tomlin 1994)
  45.0 (22°C, Milne 1995)

Vapor Pressure (Pa at 25°C or as indicated):
  1.73 (Ashton & Crafts 1973)
  0.096 (20°C, Hartley & Graham-Bryce 1980)
  1.733 (Herbicide Handbook 1983, 1989)
  0.287 (20°C, GC-RT correlation, Kim 1985)
  0.10 (20°C, selected, Suntio et al. 1988)
  0.17 (Worthing & Hance 1991)
  1.733 (20–25°C, selected, Wauchope et al. 1992; Hornsby et al. 1996)
  1.73 (Tomlin 1994)

Henry's Law Constant (Pa·m^3/mol at 25°C or as indicated):
  0.560 (20°C, calculated-P/C, Suntio et al. 1988)

Octanol/Water Partition Coefficient, log K_{OW}:
  4.15 (Worthing & Hance 1991; Tomlin 1994; Milne 1995)
  4.15 (recommended, Hansch et al. 1995)
  4.17, 4.01, 3.45 (RP-HPLC-RT correlation, CLOGP, calculated-S, Finizio et al. 1997)

Bioconcentration Factor, log BCF:

1.86	(calculated-S, Kenaga 1980)
3.06	(calculated-K_{OW} as per Kenaga 1980, this work)

Sorption Partition Coefficient, log K_{OC}:

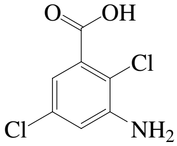
2.73	(soil, Kenaga 1980)
2.73, 4.09	(quoted values, Bottoni & Funari 1992)
2.60	(soil, 20–25°C, selected, Wauchope et al. 1992)
2.60	(estimated-chemical structure, Lohninger 1994)
2.11	(soil, calculated-MCI $^1\chi$, Sabljic et al. 1995)
2.39, 2.13	(soil, estimated-class specific model, estimated-general model using molecular descriptors, Gramatica et al. 2000)

Environmental Fate Rate Constants, k, or Half-Lives, $t_{½}$:

Half-Lives in the Environment:

Air:
Surface water:
Ground water: reported half-lives or persistence, $t_{½}$ = 11–21 d (Bottoni & Funari 1992)
Sediment:
Soil: measured dissipation rate k = 3.6 d^{-1} (Nash 1983; quoted, Nash 1988);
  estimated dissipation rate k = 23 and 0.61 d^{-1} (Nash 1988);
  $t_{½}$ = 1.5–3.0 wk in several soils under crop growing conditions (Herbicide Handbook 1989);
  selected field $t_{½}$ = 13 d (Wauchope et al. 1992; quoted, Richards & Baker 1993; Hornsby et al. 1996)
  reported $t_{½}$ = 11–21 d (Bottoni & Funari 1992);
  soil $t_{½}$ = 12 d (quoted, Pait et al. 1992);
  $t_{½}$ = 1.5–10 wk in soil and water (Tomlin 1994);
  soil $t_{½}$ = 13 d (selected, Halfon et al. 1996).
Biota: disappear from the stems and leaves of corn plants 7 to 14 d after application (Herbicide Handbook 1989).

17.1.1.14 Chloramben



Common Name: Chloramben

Synonym: ACP-M-728, Amiben, Amoben, Chlorambed, Chlorambene, M-728, NCI-C00055, Ornamental weeder, Vegaben, Vegiben

Chemical Name: 3-amino-2,5-dichlorobenzoic acid

Uses: pre-emergence or pre-plant herbicide used in many vegetable and field crops to control annual broadleaf weeds and grasses.

CAS Registry No: 133-90-4

Molecular Formula: $C_7H_5Cl_2NO_2$

Molecular Weight: 206.027

Melting Point (C):

200 (Lide 2003)

Boiling Point (°C):

Density (g/cm^3 at 20°C):

Molar Volume (cm^3/mol):

190.8 (calculated-Le Bas method at normal boiling point)

Dissociation Constant pK_a:

3.40 (Hornsby et al. 1996)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

38.91 (DSC method, Plato 1972)

Entropy of Fusion, ΔS_{fus} (J/mol K):

Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F: 0.0192 (mp at 200°C)

Water Solubility (g/m^3 or mg/L at 25°C):

700 (Spencer 1973; Ashton & Crafts 1981)
700 (Martin & Worthing 1977; Herbicide Handbook 1978; 1989)
700 (Hartley & Kidd 1987; Budavari 1989; Montgomery 1993; Milne 1995)
700 (Worthing & Walker 1987, Worthing & Hance 1991; Tomlin 1994; Majewski & Capel 1995)

Vapor Pressure (Pa at 25°C or as indicated):

0.933 (100°C, Segal & Sutherland 1967; Spencer 1976)
0.93 (100°C, Hartley & Kidd 1987; Worthing & Hance 1991; Tomlin 1994)
52.7 (Worthing & Walker 1987)

Henry's Law Constant (Pa·m^3/mol at 25°C):

0.274 (calculated-P/C as per Worthing 1987)

Octanol/Water Partition Coefficient, log K_{OW}:

1.11 (quoted, Rao & Davidson 1980)
1.46 (selected, Dao et al. 1983)
–2.64 (selected, Gerstl & Helling 1987)
1.11 (Magee 1991)
1.11 (Montgomery 1993)
1.11 (Log P database of Hansch & Leo 1987, Sangster 1993)
1.90 (CLOGPSTAR or CLOGP data, Sabljic et al. 1995)

Bioconcentration Factor, log BCF:

1.18 (calculated-S, Kenaga 1980)

–0.097 (calculated-K_{OC}, Kenaga 1980)

Sorption Partition Coefficient, log K_{OC}:

1.32	(soil, Harris & Warren 1964; Farmer 1976)
2.08	(soil, calculated as per Kenaga & Goring 1980, Kenaga 1980)
1.78	(calculated-MCI χ, Gerstl & Helling 1987)
1.32	(reported as log K_{OM}, Magee 1991)
2.28	(Montgomery 1993)
1.56	(selected, Lohninger 1994)
1.48	(soil, calculated-MCI $^1\chi$, Sabljic et al. 1995)

Environmental Fate Rate Constants, k, or Half-Lives, $t_{½}$:

Volatilization:

Photolysis: $t_{½}$ = 6 h for 206 μg/mL to degrade in distilled water under sunlight (Sheets 1963; quoted, Cessna & Muir 1991);

$t_{½}$ < 2 d for 16 μg/mL to degrade in distilled water under sunlight (Hahn et al. 1969; quoted, Cessna & Muir 1991).

Oxidation:

Hydrolysis:

Biodegradation: $t_{½}$ > 70 d for 50 μg/mL to degrade in incubated soil with nutrient medium of 3 g/L (Schliebe et al. 1965; quoted, Muir 1991).

Biotransformation:

Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants:

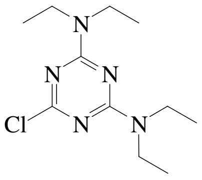
Half-Lives in the Environment:

Soil: estimated persistence of 3 months (Kearney et al. 1969; quoted, Jury et al. 1987);

$t_{½}$ = 36, 38, 41, and 20 d with disappearance rates: k = 0.0193, 0.0182, 0.0169 and 0.0347 d^{-1} at pH 4.3, 5.3, 6.5 and 7.5 (Hamaker 1972; quoted, Nash 1988);

persistence in soil is of 6–8 wk (Hartley & Kidd 1987; Herbicide Handbook 1989; quoted, Montgomery 1993).

17.1.1.15 Chlorazine



Common Name: Chlorazine
Synonym:
Chemical Name: 6-chloro-*N,N,N′,N′*-tetraethyl-1,3,5-triazine-2,4-diamine
Uses: herbicide
CAS Registry No: 580-48-3
Molecular Formula: $C_{11}H_{20}ClN_5$
Molecular Weight: 257.764
Melting Point (°C):
27 (Howard 1991; Lide 2003)
Boiling Point (°C):
154–156/4.0 mmHg (Howard 1991)
Density (g/cm^3):
Acid Dissociation Constants, pK$_a$:
1.74 (pK$_a$ of conjugate acid, Howard 1991)
Molar Volume (cm^3/mol):
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
Entropy of Fusion, ΔS_{fus} (J/mol K):
Fugacity Ratio at 25°C, (assuming ΔS_{fus} = 56 J/mol K), F: 0.956 (mp at 27°C)

Water Solubility (g/m^3 or mg/L at 25°C or as indicated):
23.7, 22.2, 21.4 (26°C, shake flask-UV at pH 3.0, 7.0, 10.0, Ward & Weber 1968)

Vapor Pressure (Pa at 25°C):

Henry's Law Constant (Pa·m^3/mol at 25°C):

Octanol/Water Partition Coefficient, log K_{OW}:
3.236 (estimated, Howard 1991)

Octanol/Air Partition Coefficient, log K_{OA}:

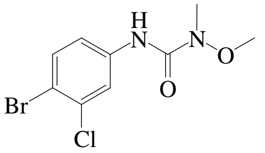
Bioconcentration Factor, log BCF or log K_B:
2.033 (estimated-S, Howard 1991)

Sorption Partition Coefficient, log K_{OC}:
2.90 (calculated-S, Howard 1991)

Environmental Fate Rate Constants, k, and Half-Lives, $t_{½}$:
Hydrolysis: may be more important at low pH (Howard 1991).

Half-Lives in the Environment:
Air: $t_{½}$ = 2.5 h for the vapor phase reaction with OH radicals (estimated, Howard 1991).

17.1.1.16 Chlorbromuron



Common Name: Chlorbromuron
Synonym: Maloran
Chemical Name: 3-(4-bromo-3-chlorophenyl)-1-methoxy-1-methylurea
Uses: herbicide
CAS Registry No: 13360-45-7
Molecular Formula: $C_9H_{10}BrClN_2O_2$
Molecular Weight: 293.544
Melting Point (°C):
 96 (Lide 2003)
Boiling Point (°C):
Density (g/cm^3): 1.69 (Tomlin 1994)
Acid Dissociation Constants, pK_a:
Molar Volume (cm^3/mol):
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
Entropy of Fusion, ΔS_{fus} (J/mol K):
Fugacity Ratio at 25°C, (assuming ΔS_{fus} = 56 J/mol K) F: 0.201 (mp at 96°C)

Water Solubility (g/m^3 or mg/L at 25°C or as indicated):
 50 (Kenaga & Goring 1980, Kenaga 1980a; Ashton & Crafts 1981
 35 (20°C, Spencer 1982; Worthing 1983; Hartley & Kidd 1987; Tomlin 1994)
 35; 27.4 (quoted; calculated-MCI χ, Patil 1994)
 35 (selected, 20–25°C, Augustjin-Beckers 1994; Hornsby et al. 1996)

Vapor Pressure (Pa at 25°C or as indicated):
 5.33×10^{-5} (20°C, Ashton & Crafts 1981)
 5.3×10^{-5} (Spencer 1982; Worthing 1983; Hartley & Kidd 1987; Tomlin 1994)
 5.33×10^{-5} (selected, 20–25°C, Augustijn-Beckers et al. 1994; Hornsby et al. 1996)

Henry's Law Constant (Pa·m^3/mol):

Octanol/Water Partition Coefficient, log K_{OW}:
 3.06 (quoted, Rao & Davidson 1980)
 3.09 (shake flask, Brigg 1981)
 3.09; 3.26 (quoted lit.; calculated-MCI χ, Patil 1994)
 3.09 (recommended, Hansch et al. 1995)
 2.86, 2.99, 3.45 (RP-HPLC-RT correlation, CLOGP, HPLC-k′ correlation, Finizio et al. 1997)

Octanol/Air Partition Coefficient, log K_{OA}:

Bioconcentration Factor, log BCF or log K_B:
 1.83, 1.40 (quoted, calculated, Kenaga 1980b)

Sorption Partition Coefficient, log K_{OC}:
 2.66 (soil, Kenaga & Goring 1980)
 2.66, 2.71 (quoted, calculated-K_{OW}, Kenaga 1980b)
 3.00 (mean value of 5 soils, Rao & Davidson 1980)
 2.34, 2.94 (quoted, calculated-MCI χ, Gerstl & Helling 1987)
 2.19–3.61 (range of reported data, Augustijn-Beckers et al. 1994)

2.70	(estimated and recommended, soil, Augustjin-Beckers et al. 1994; Hornsby et al. 1996)
2.70	(soil, calculated-MCI $^1\chi$, Sabljic et al. 1995)
2.70, 2.97	(soil, estimated-class-specific model, estimated-general model using molecular descriptors, Gramatica et al. 2000)
2.54, 2.55	(soils: organic carbon OC ≥ 0.1%, OC ≥ 0.5%, average, Delle Site 2001)

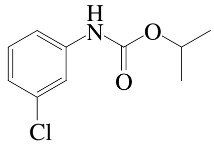
Environmental Fate Rate Constants, k, and Half-Lives, $t_{1/2}$:

Hydrolysis: slowly hydrolyzed in neutral, slightly acidic, and slightly alkaline media (Hartley & Kidd 1987; Tomlin 1994).

Half-Lives in the Environment:

Soil: persists in soil > 56 d (Worthing 1983);
$t_{1/2}$ = 45 d (Hartley & Kidd 1987);
$t_{1/2}$ = 45–120 d (Tomlin 1994);
$t_{1/2}$ = 21–45 d and 40 d (range of reported values and recommended field half-life, Augustjin-Beckers et al. 1994; Hornsby et al. 1996)

17.1.1.17 Chlorpropham



Common Name: Chlorpropham
Synonym: Beet-Kleen, Bud-nip, Chlor-IFC, Chloro-IPC, CIPC, Ebanil, ENT 18060, Fasco Wy-hoe, Furloe, Nexoval, Prevenol, Preweed, Sprout-nip, Taterpex
Chemical Name: isopropyl N-(3-chlorophenyl) carbamate; isopropyl 3-chlorocarbanilate
Uses: pre-emergent and post-emergent herbicide used to regulate plant growth and control weeds in carrot, onion, garlic, and other crops.
CAS Registry No: 101-21-3
Molecular Formula: $C_{10}H_{12}ClNO_2$
Molecular Weight: 213.661
Melting Point (°C):
41 (Lide 2003)
Boiling Point (°C):
149 (at 2 mmHg, Budavari 1989)
Density (g/cm^3 at 20°C):
1.180 (30°C, Hartley & Kidd 1987; Herbicide Handbook 1989; Worthing & Hance 1991; Montgomery 1993; Tomlin 1994)
1.5388 (Budavari 1989)
Molar Volume (cm^3/mol):
232.4 (calculated-Le Bas method at normal boiling point)
Enthalpy of Vaporization, ΔH_V (kJ/mol):
88.67 (Rordorf 1989)
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
20.50 (DSC method, Plato & Glasgow 1969)
16 (Rordorf 1989)
Entropy of Fusion, ΔS_{fus} (J/mol K):
Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F: 0.697 (mp at 41°C)

Water Solubility (g/m^3 or mg/L at 25°C or as indicated):
0.470 (Brust 1966)
102.3 (shake flask-GC, Freed et al. 1967)
108 (20°C, Günther et al. 1968)
89 (20°C, Weber 1972; Martin & Worthing 1977; Worthing & Walker 1987)
2.0 (Spencer 1973; quoted, Shiu et al. 1990)
88 (Martin & Worthing 1977; Herbicide Handbook 1978, 1989)
0.70 (19°C, shake flask-GC, Bowman & Sans 1979)
0.73 (20°C, shake flask-GC, Bowman & Sans 1983a,b)
88 (Khan 1980; Ashton & Crafts 1981)
80–102 (Weber et al. 1980)
89 (Hartley & Kidd 1987; Worthing & Hance 1991; Tomlin 1994)
89 (selected, Gerstl & Helling 1987; Montgomery 1993; Lohninger 1994)
2.0 (20°C, Worthing & Walker 1987)

Vapor Pressure (Pa at 25°C or as indicated and reported temperature dependence equations):
0.00050 (20°C, Weber 1972; Worthing & Walker 1987)
0.00133 (extrapolated, Spencer 1976)
0.00133 (Khan 1980)
0.00133 (Ashton & Crafts 1981; Herbicide Handbook 1989)
0.00100 (20°C, selected, Suntio et al. 1988)

0.012, 0.30, 5.0, 56, 470 (25, 50, 70, 100, 125°C, gas saturation-GC, Rordorf 1989)
log (P_S/Pa) = 16.402 – 5467.7/(T/K); measured range 44.9–140°C (solid, gas saturation-GC, Rordorf 1989)
log (P_L/Pa) = 13.753 – 4631.9/(T/K); measured range 44.9–140°C (liquid, gas saturation-GC, Rordorf 1989)

0.00130	(selected, Taylor & Spencer 1990)
0.00107	(20–25°C, selected, Wauchope et al. 1992; Hornsby et al. 1996)
0.00133	(estimated, Montgomery 1993)

Henry's Law Constant (Pa m^3/mol at 25°C or as indicated):

0.0021	(20°C, calculated-P/C, Suntio et al. 1988)
0.0032	(20°C, calculated-P/C, Muir 1991)
0.0021	(20–25°C, calculated-P/C, Montgomery 1993)

Octanol/Water Partition Coefficient, log K_{OW}:

3.06	(Rao & Davidson 1980; Karickhoff 1981)
3.42	(selected, Dao et al. 1983; Gerstl & Helling 1987)
3.51	(shake flask, Mitsutake et al. 1986)
3.10	(selected, Suntio et al. 1988)
3.51	(recommended, Sangster 1993)
3.09	(calculated, Patil 1994)
3.51	(recommended, Hansch et al. 1995)

Bioconcentration Factor, log BCF:

1.70	(calculated-S, Kenaga 1980)
1.52	(calculated-K_{OC}, Kenaga 1980)

Sorption Partition Coefficient, log K_{OC}:

2.77	(soil, Hamaker & Thompson 1972)
2.57	(soil, calculated-S as per Kenaga & Goring 1980, Kenaga 1980)
2.85, 2.80	(estimated-S, Karickhoff 1981)
3.17, 3.08	(estimated-S and mp, Karickhoff 1981)
2.67	(estimated-K_{OW}, Karickhoff 1981)
2.31	(calculated-MCI χ, Gerstl & Helling 1987)
2.32	(calculated-MCI χ and fragment contribution method, Meylan et al. 1992)
2.60	(soil, 20–25°C, estimated, Wauchope et al. 1992; Hornsby et al. 1996)
2.77, 2.91	(Montgomery 1993)
2.60	(estimated-chemical structure, Lohninger 1994)
2.53	(soil, calculated-MCI $^1\chi$, Sabljic et al. 1995)
2.40, 2.05	(soil, estimated-class-specific model, estimated-general model using molecular descriptors, Gramatica et al. 2000)
2.62 (2.37–2.87)	(soil: organic carbon OC ≥ 0.5%, average, Delle Site 2001)

Environmental Fate Rate Constants, k, or Half-Lives, $t_{1/2}$:

Volatilization: $t_{1/2}$ = 2220 d from 1-m depth of water at 20°C (estimated, Muir 1991).

Photolysis: $t_{1/2}$ = 130 h for 4 μg/mL to degrade in distilled water under > 280 nm light (Guzik 1978; quoted, Cessna & Muir 1991)

direct photolysis $t_{1/2}$ = 121 d in distilled water pH 5–7 for a mid-summer day at latitude of 40° (Wolfe et al. 1978)

$t_{1/2}$= 2.25 h for 21–76% of 80 μg/mL to degrade in distilled water under 300 nm light (Tanaka et al. 1981; quoted, Cessna & Muir 1991).

Oxidation:

Hydrolysis: $t_{1/2}$ > 4 months for 4274 μg/mL to hydrolyze in phosphate buffer at pH 5–9 and 20°C (El-Dib & Aly 1976; quoted, Muir 1991)

k(alkaline) = 2.0×10^{-5} M^{-1} s^{-1} at 27°C, 1.9×10^{-4} M^{-1} s^{-1} at 50°C, 6.4×10^{-4} M^{-1} s^{-1} at 70°C; with $t_{1/2} > 1 \times 10^4$ d at pH 5, 7 and 9 (Wolfe et al. 1978)

$t_{1/2}$ > 1 wk for 2.10 μg/mL to hydrolyze in natural waters at 67°C (Schnoor et al. 1982; quoted, Muir 1991).

Biodegradation:

$t_{1/2}$(aerobic) = 10–75 d for 0.1–5.4 μg/mL to biodegrade in activated sludge (Schwartz 1967; quoted, Muir 1991)

k = (3.6–6.7) × 10^{-10} mL $cell^{-1}$ d^{-1} of different river water samples (Paris et al. 1978; quoted, Scow 1982)

$t_{1/2}$ = 120 d by fungi *Aspergillus fumigatus* and $t_{1/2}$ = 2.9 d by bacteria at 28°C (Wolfe et al. 1978)

k = 2.5 × 10^{-4} L (mg M)$^{-1}$ h^{-1} with $t_{1/2}$ = 120 d for 2–25 μg/mL fungus *Aspergillus fumigatus*; k = 0.1 L (mg M)$^{-1}$ h^{-1} with $t_{1/2}$ = 2.9 d for bacteria *Pseudomonas striata* to biodegrade in stream water at pH 7 and 28°C (Wolfe et al. 1978; quoted, Muir 1991)

k = (1.6–1.8) × 10^{-8} mL $cell^{-1}$ d^{-1} of different river water samples (Steen et al. 1979; quoted, Scow 1982)

k = (2.6 ± 0.72) × 10^{-14} L $cell^{-1}$ h^{-1} in North American waters (Paris et al. 1981; quoted, Battersby 1990)

k = (1.3–4.9) × 10^{-4} L org^{-1} h^{-1} with $t_{1/2}$(aerobic) = 190 h for 0.1–1.0 μg/mL to biodegrade in lake water at 22°C (Schnoor et al. 1982; quoted, Muir 1991)

k = (1.4–4.2) × 10^{-13} L org^{-1} h^{-1} for 75 μg/mL to biodegrade at 28°C in natural and sediment waters (Steen et al. 1982; quoted, Muir 1991);

$t_{1/2}$(aerobic) > 4 months for 6–7 μg/mL to biodegrade in river water at 25°C (Stepp et al. 1985; quoted, Muir 1991).

Biotransformation:

Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants:

Half-Lives in the Environment:

Air:

Surface water: rate constant k = 3.6–6.7 × 10^{-10} mL $cell^{-1}$ d^{-1} from measurements of different river water samples (Paris et al. 1978; quoted, Scow 1982);

hydrolysis $t_{1/2}$ > 1 × 10^4 d based on neutral and alkaline hydrolysis assuming pseudo-first order kinetics; direct photolysis $t_{1/2}$ = 121 d assuming a quantum efficiency of 1 and for a mid-summer day at altitude 40°, and biolysis $t_{1/2}$ = 120 d for 1mg/L of fungus and $t_{1/2}$ = 2.9 d for bacteria at 28°C (Wolfe et al. 1978);

k = (1.6–1.8) × 10^{-8} mL $cell^{-1}$ d^{-1} from measurements of different river water samples (Steen et al. 1979; quoted, Scow 1982);

aerobic $t_{1/2}$ = 190 h for 0.1–1.0 μg/mL to biodegrade in lake water with biodegradation rate of (1.3–4.9) × 10^{-4} L org^{-1} h^{-1} at 22°C (Schnoor et al. 1982; quoted, Muir 1991);

aerobic $t_{1/2}$ > 4 months for 6–7 μg mL^{-1} to biodegrade in river water at 25°C (Stepp et al. 1985; quoted, Muir 1991).

Ground water:

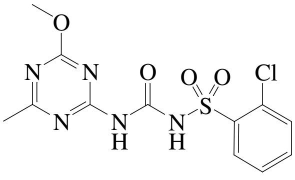
Sediment: aerobic half-life of 10–75 d for 0.1–5.4 μg/mL to biodegrade in activated sludge (Schwartz 1967; quoted, Muir 1991).

Soil: $t_{1/2}$ = 65 and 30 d soil at 15 and 29°C, respectively (Hartley & Kidd 1987; Herbicide Handbook 1989; quoted, Montgomery 1993; Tomlin 1994);

selected field $t_{1/2}$ = 30 d (Wauchope et al. 1992; Hornsby et al. 1996).

Biota:

17.1.1.18 Chlorsulfuron



Common Name: Chlorsulfuron
Synonym: DPX 4189, Finesse, Glean, Telar
Chemical Name: 2-chloro-*N*-(((4-methoxy-6-methyl-1,3,5-triazin-2-yl)amino)-carbonyl)-benzenesulfonamide; 1-(*o*-chlorophenyl)-3-(4-methoxy-6-methyl-*s*-triazin-2-yl)urea
Uses: herbicide to control broadleaf weeds and some grass weeds.
CAS Registry No: 64902-72-3
Molecular Formula: $C_{12}H_{12}ClN_5O_4S$
Molecular Weight: 357.773
Melting Point (°C):
176 (Lide 2003)
Boiling Point (°C):
192 (dec., Herbicide Handbook 1989; Montgomery 1993)
Density (g/cm³ at 20°C):
Molar Volume (cm³/mol):
Dissociation Constant pK_a:
3.6 (Herbicide Handbook 1989; Worthing & Hance 1991; Montgomery 1993; Tomlin 1994)
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
Entropy of Fusion, ΔS_{fus} (J/mol K):
Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F: 0.0330 (mp at 176°C)

Water Solubility (g/m³ or mg/L at 25°C or as indicated):
300 (at pH 5, Hartley & Kidd 1987; Worthing & Hance 1991; Tomlin 1994; Milne 1995)
27900 (at pH 7, Hartley & Kidd 1987; Worthing & Hance 1991; Tomlin 1994; Milne 1995)
28000 (at pH 7 with ionic strength 0.05, Herbicide Handbook 1989)
7000 (20–25°C, at pH 7, selected, Wauchope et al. 1992; quoted, Majewski & Capel 1995)
7000 (20–25°C, at pH 7, selected, Hornsby et al. 1996)
60, 7000 (at pH 5, pH 7, Montgomery 1993)
32000 (selected, Armbrust 2000)

Vapor Pressure (Pa at 25°C or as indicated):
6.10×10^{-4} (Hartley & Kidd 1987)
6.13×10^{-4} (Herbicide Handbook 1989)
3.00×10^{-9} (Worthing & Hance 1991; Tomlin 1994)
1.98×10^{-2} (20–25°C, Wauchope et al. 1992)
3.11×10^{-9} (Montgomery 1993)
6.13×10^{-4} (20–25°C, selected, Hornsby et al. 1996)

Henry's Law Constant (Pa·m³/mol at 25°C or as indicated):
3.60×10^{-11} (calculated-P/C, Montgomery 1993)
1.98×10^{-5} (20–25°C, calculated-P/C as per Wauchope et al. 1992, Majewski & Capel 1995)
6.79×10^{-6} (selected, Armbrust 2000)

Octanol/Water Partition Coefficient, log K_{OW}:
–0.84, 0.17, 1.09 (pH 8.4, pH 7.1, pH 4.5, UV, Ribo 1988)
–0.88, 1.05 (pH 8.4, pH 4.5, HPLC, Ribo 1988)
–1.34, 0.74 (pH 7, pH 4.5, Hay 1990)

2.20 (Grayson & Kleier 1990)
–1.0 (Montgomery 1993)
–0.88, 1.05, –1.34, 0.74, 2.20 (reported values, Sangster 1993)
–1.00 (at pH 7, Tomlin 1994)
0.74, –1.34 (lit. values, Hansch et al. 1995)
2.14 (LOGPSTAR or CLOGP data, Sabljic et al. 1995)

Bioconcentration Factor, log BCF:
0.622 (calculated-S as per Kenaga 1980, this work)

Sorption Partition Coefficient, log K_{OC}:
1.02 (Flanagan silt loam, Montgomery 1993)
1.60 (Tomlin 1994)
2.19 (calculated-MCI $^1\chi$, Sabljic et al. 1995)
1.60 (at pH 7, selected, Hornsby et al. 1996)
1.56 (selected, Armbrust 2000)

Environmental Fate Rate Constants, k, or Half-Lives, $t_{½}$:

Volatilization:

Photolysis: assuming first-order kinetics, calculated $t_{½}$ ~ 186 h for 33 µg/mL to degrade in distilled water, $t_{½}$ = 31 h for creek water, $t_{½}$ = 136 h for silica gel and $t_{½}$ = 115 h for montmorillonit under sunlight (Herrmann et al. 1985; quoted, Cessna & Muir 1991);

under indoor conditions $t_{½}$ = 92 h in methanol, $t_{½}$ = 78 h in distilled water but $t_{½}$ = 18 h in natural creek water (Herrmann et al. 1985);

reported $t_{½}$ = 18 h in distilled water at > 290 nm (Montgomery 1993)

aqueous photolysis rate constant, k = 5.0 × 10^{-4} h^{-1} (Armbrust 2000).

Oxidation:

Hydrolysis: $t_{½}$ = 4–8 wk at 20°C and pH 5.7–7.0 (Hartley & Kidd 1987; Worthing & Hance 1991; Montgomery 1993; Tomlin 1994);

stable aqueous hydrolysis rates at pH 7, 9; measured hydroxy radical rate constant for chlorsulfuron 6.9 × 10^{12} M^{-1}/h (Armbrust 2000).

Biodegradation: aerobic rate constant, k = 1.44 × 10^{-3} h^{-1} (Armbrust 2000).

Biotransformation:

Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants:

Half-Lives in the Environment:

Soil: hydrolysis rates will be increased by warm soil temperatures at low pH and in the presence of moisture with an average $t_{½}$ = 4–6 wk under growing conditions (Hartley & Kidd 1987; Herbicide Handbook 1989)

$t_{½}$ = 4–6 wk for degradation in soil via hydrolysis followed by microbial degradation (Hartley & Kidd 1987; quoted, Montgomery 1993; Tomlin 1994);

degradation rate constants: k = 0.033 d^{-1} at depth 0–20 cm with $t_{½}$ = 21 d, k = 0.0315 d^{-1} at depth 20–40 cm with $t_{½}$ = 22 d and for depth 40–60 cm with $t_{½}$ > 150 d (Soakwaters soil, Walker et al. 1989);

degradation k = 0.0116 d^{-1} at depth 0–20 cm with $t_{½}$ = 60 d, k = 0.0120 d^{-1} at depth 20–40 cm with $t_{½}$ = 58 d, and k = 0.0076 d^{-1} at depth 40–60 cm with $t_{½}$ = 91 d (Wharf ground soil, Walker et al. 1989);

degradation k = 0.0126 d^{-1} at depth 0–20 cm with $t_{½}$ = 55 d, k = 0.0073 d^{-1} at depth 20–40 cm with $t_{½}$ = 95 d, and k = 0.0056 d^{-1} at depth 40–60 cm with $t_{½}$ = 124 d (Cottage Field soil, Walker et al. 1989);

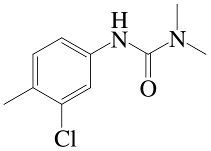
degradation k = 0.0147 d^{-1} at depth 0–20 cm with $t_{½}$ = 47 d, 0.0116 d^{-1} at depth 20–40 cm with $t_{½}$ = 60 d, and k = 0.0047 d^{-1} at depth 40–60 cm with $t_{½}$ = 147 d (Hunts Mill soil, Walker et al. 1989);

degradation 0.0094 d^{-1} (depth 0–20 cm with $t_{½}$ = 74 d), 0.0096 d^{-1} (depth 20–40 cm with $t_{½}$ = 72 d) and 0.0082 d^{-1} (depth 40–60 cm with $t_{½}$ = 85 d) (Bottom Barn soil, Walker et al. 1989);

degradation k = 0.0141 d^{-1} at depth 0–20 cm with $t_{½}$ = 49 d, k = 0.0126 d^{-1} at depth 20–40 cm with $t_{½}$ = 55 d, and k = 0.0089 d^{-1} at depth 40–60 cm with $t_{½}$ = 78 d (Long Ashton soil, Walker et al. 1989);

degradation k = 0.0144 d^{-1} at depth 0–20 cm with $t_{½}$ = 48 d, k = 0.0126 d^{-1} at depth 20–40 cm with $t_{½}$ = 55 d, and k = 0.0124 d^{-1} at depth 40–60 cm with $t_{½}$ = 56 d (Norfolk Agricultural Station soil, Walker et al. 1989) degradation k = 0.0248 d^{-1} at depth 0–20 cm with $t_{1/2}$ = 28 d, k = 0.0289 d^{-1} at depth 20–40 cm with $t_{1/2}$ = 24 d, and k = 0.0347 d^{-1} at depth 40–60 cm with $t_{1/2}$ = 20 d (Norfolk Agricultural Station soil, Walker et al. 1989); selected field $t_{1/2}$ = 40 d (Hornsby et al. 1996).

17.1.1.19 Chlorotoluron



Common Name: Chlorotoluron
Synonym: C 2242, Clortokem, Deltarol, Dicuran, Highuron, Higaluron, Tolurex
Chemical Name: 3-(3-chloro-*p*-tolyl)-1,1-dimethylurea; *N′*-(3-chloro-4-methylphenyl)-N,N-dimethylurea
Uses: herbicide to control pre- and post-emergent annual grasses and broadleaf weeds in winter cereals, particularly wheat and barley.
CAS Registry No: 15545-48-9
Molecular Formula: $C_{10}H_{13}ClN_2O$
Molecular Weight: 212.675
Melting Point (°C):
147 (Lide 2003)
Boiling Point (°C):
Density (g/cm^3 at 20°C):
1.40 (Tomlin 1994)
Molar Volume (cm^3/mol):
192 (modified Le Bas method at normal boiling point, Spurlock & Biggar 1994)
Dissociation Constant pK_a:
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
Entropy of Fusion, ΔS_{fus} (J/mol K):
Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F: 0.0635 (mp at 147°C)

Water Solubility (g/m^3 or mg/L at 25°C or as indicated):
10.0 (20°C, Spencer 1973)
70.0 (Martin & Worthing 1977)
10.0 (20°C, Khan 1980)
70.0 (20°C, Ashton & Crafts 1981)
56.4, 80.6, 99.1 (4, 25, 40°C, shake flask-liquid scintillation spectrometer LSS, Madhun et al. 1986)
70.0 (20°C, Hartley & Kidd 1987; Worthing & Walker 1991)
90.0 (Spurlock 1992; Spurlock & Biggar 1994)
10660 (calculated, Patil 1994)
74.0 (Tomlin 1994)
49.3 (predicted-AQUAFAC, Lee et al. 1996)

Vapor Pressure (Pa at 25°C or as indicated):
4.8×10^{-6} (20°C, Khan 1980)
1.7×10^{-5} (20°C, Ashton & Crafts 1981)
1.7×10^{-5} (20°C, Hartley & Kidd 1987)
1.7×10^{-5} (Tomlin 1994; selected, Halfon et al. 1996)

Henry's Law Constant (Pa·m^3/mol at 25°C or as indicated):
5.17×10^{-5} (20°C, calculated-P/C, this work)

Octanol/Water Partition Coefficient, log K_{OW}:
2.41 (shake flask-UV, Briggs 1981)
2.54 (Dao et al. 1983; Spurlock 1992; Spurlock & Biggar 1994)
2.33, 2.34, 2.32 (4, 25, 40°C, shake flask-liquid scintillation spectrometer LSS, Madhun et al. 1986)
2.41 (shake flask, Mitsutake et al. 1986)
2.0 (shake flask, pH 7, Baker et al. 1992)

2.241 (calculated, Evelyne et al. 1992)
2.41 (recommended, Sangster 1993)
2.25 (RP-HPLC-RT correlation, Sicbaldi & Finizio 1993)
0.26 (calculated, Patil 1994)
2.50 (Tomlin 1994)
2.41 (recommended, Hansch et al. 1995)
2.38, 2.44 (shake flask-UV, calculated-RP-HPLC-k′ correlation, Liu & Qian 1995)
2.25, 2.49, 2.42 (RP-HPLC-RT correlation, ClOGP, calculated-S, Finizio et al. 1997)
2.0 (RP-HPLC-RT correlation using short ODP column, Donovan & Pescatore 2002)

Bioconcentration Factor, log BCF:
1.75 (calculated-S, Kenaga 1980)
2.09, 2.16 (cuticle/water 24 h: tomato, pepper, Chaumat et al. 1991)
2.01, 2.15 (cuticle/water 24 h: box tree, pear, Chaumat et al. 1991)
1.30 (cuticle/water 24 h: vanilla, Chaumat et al. 1991)
2.09, 2.16 (cuticle/water: tomato, pepper, Evelyne et al. 1992)

Sorption Partition Coefficient, log K_{OC}:
2.62 (soil, calculated-S, Kenaga 1980)
1.78 (reported as log K_{OM}, Briggs 1981)
2.75, 2.62 (4°C, 25°C, Semiahmoo soil, in μmol/kg OC, batch equilibrium-sorption isotherm-liquid scintillation spectrometer LSS, Madhun et al. 1986)
2.57, 2.43 (4°C, 25°C, Adkins soil, in μmol/kg OC, batch equilibrium method-LSS, Madhun et al. 1986)
2.48, 2.18; 2.54, 2.50 (estimated-K_{OW}; solubility, Madhun et al. 1986)
2.81, 2.58 (exptl., calculated-K_{OW}, Liu & Qian 1995)
2.02 (soil, calculated-MCI $^1\chi$, Sabljic et al. 1995)
2.02; 2.05, 2.15 (soil, quoted obs.; estimated-class-specific model, estimated-general model using molecular descriptors, Gramatica et al. 2000)
2.00, 2.00 (soils: organic carbon OC $\geq$ 0.1%, OC $\geq$ 0.5%, average, Delle Site 2001)
2.14, 2.36 (Kishon river sediments, sorption isotherm, Chefetz et al. 2004)

Environmental Fate Rate Constants, k, or Half-Lives, $t_{1/2}$:
Volatilization:
Photolysis:
Oxidation:
Hydrolysis: calculated $t_{1/2}$ > 200 d at pH 5, 7, 9 and 30°C (Tomlin 1994).
Biodegradation: Biological degradation rate followed a first order kinetics with $t_{1/2}$ = 21.6 d by raw water microflora from River Nile, $t_{1/2}$ = 13,8 d by raw water microflora + sewage (El-Dib & Abou-Waly 1998)
Biotransformation: 4% of the selected 90 strains of micromycetes mostly isolated from soil-soil fungi, depleted 50% of chlorotoluron (100 mg/L) in 5-d experiment. (Vroumsia et al. 1996)
Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants:

Half-Lives in the Environment:
Air:
Surface water: Biological degradation $t_{1/2}$ = 21.6 d by raw water microflora from River Nile, $t_{1/2}$ = 13,8 d by raw water microflora + sewage (El-Dib & Abou-Waly 1998)
Ground water:
Sediment:
Soil: $t_{1/2}$ = 4 wk in the moist silty loam at (25 ± 1)°C (Smith & Briggs 1978);
$t_{1/2}$ ~ 200–4000 d in loamy sand and peat for 25–35°C as follows (Madhum & Freed 1987):
$t_{1/2}$ = 4340, 904, and 381 d at 25, 30, and 35°C, respectively, at herbicide concn at 5 μg/kg, while $t_{1/2}$ = 1335, 524, and 266 d at 25, 30, and 35°C, respectively, at herbicide concn at 100 μg/kg in an Adkins loamy sand; however, the half-lives in peat. $t_{1/2}$ = 2306, 1245, and 618 d at 25, 30, and 35°C, respectively, at herbicide concn at 5 μg/kg while $t_{1/2}$ = 1949, 1024, and 582 d at 25, 30, and 35°C, respectively, at herbicide concn at 100 μg/kg in a Semiahoo mucky peat (Madhun & Freed 1987)

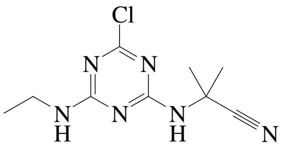
degradation by microorganism in biometer systems, $t_{½}$ = 93 d in silty sand standard metabolism experiments, $t_{½}$ = 140 d corrected standard conditions, $t_{½}$ = 110 d in simulated outdoor conditions; $t_{½}$ = 40 d in silty loam standard conditions, $t_{½}$ = 60 d corrected standard conditions, $t_{½}$ = 31 d in simulated outdoor conditions; at constant soil moisture and 20°C. Degradation by microorganism in small lysimeter systems: $t_{½}$ = 52 d outdoor fallow, $t_{½}$ = 14 d outdoor barley in silty sand, and $t_{½}$ = 49 d outdoor fallow, $t_{½}$ = 38 d outdoor barley in silty loam (Rüdel et al. 1993)

$t_{½}$ = 30–40 d in soil (Tomlin 1994);

$t_{½}$ = 135 d (selected, Halfon et al. 1996).

Biota:

17.1.1.20 Cyanazine



Common Name: Cyanazine
Synonym: Bladex, 90DF, DW 3418, Fortrok, Fortrol, Payze, SD 15418, WL 19805
Chemical Name: 2-(4-chloro-6-ethylamino-1,3,5-triazin-2-ylamino)-2-methyl-propionitrile
Uses: herbicide to control annual grasses and broadleaf weeds in cereals, cotton, maize, onions, peanuts, peas, potatoes, soybeans, sugar cane, and wheat fallow.
CAS Registry No: 21725-46-2
Molecular Formula: $C_9H_{13}ClN_6$
Molecular Weight: 240.692
Melting Point (°C):
168 (Lide 2003)
Boiling Point (°C):
Density (g/cm^3 at 20°C):
Molar Volume (cm^3/mol):
Dissociation Constant:
1.00 (pK_a, Weber et al. 1980; Willis & McDowell 1982)
12.9 (pK_b, Wauchope et al. 1992; Hornsby et al. 1996)
0.63, 1.1 (pK_a, Montgomery 1993)
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
Entropy of Fusion, ΔS_{fus} (J/mol K):
Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F: 0.0395 (mp at 168°C)

Water Solubility (g/m^3 or mg/L at 25°C or as indicated):
171 (Melnikov 1971; Wauchope 1978; Weber et al. 1980; Ashton & Crafts 1981)
171 (Martin & Worthing 1977; Herbicide Handbook 1978; Worthing & Walker 1987, Worthing & Hance 1991; Majewski & Capel 1995)
150 (selected, Schnoor & McAvoy 1981; Schnoor 1992)
171 (Hartley & Kidd 1987; Montgomery 1993; Tomlin 1994)
160 (23°C, Herbicide Handbook 1989)
171 (Budavari 1989; Milne 1995)
170 (20–25°C, selected, Wauchope et al. 1992; Hornsby et al. 1996)
6046 (calculated, Patil 1994)
45 (calculated-group contribution fragmentation method, Kühne et al. 1995)

Vapor Pressure (Pa at 25°C or as indicated. Additional data at other temperatures designated * are compiled at the end of this section):
2.13×10^{-7} (20°C, Ashton & Crafts 1973; 1981; Spencer 1982; Herbicide Handbook 1989)
2.67×10^{-7} (20–25°C, Weber et al. 1980)
5.33×10^{-7} (selected, Schnoor & McAvoy 1981; Schnoor 1992)
1.00×10^{-5} (20°C, extrapolated from gas saturation measurement, Grayson & Fosbracey 1982)
$\ln (P/Pa) = 25.7 - 10913/(T/K)$, temp range 65.7–92°C, (Antoine eq., gas saturation, Grayson & Fosbracey 1982)
2.00×10^{-7} (20°C, Hartley & Kidd 1987; Worthing & Hance 1991; Tomlin 1994; Majewski & Capel 1995)
5.21×10^{-6} (Worthing & Walker 1987)
1.33×10^{-6} (30°C, Herbicide Handbook 1989)
2.13×10^{-7} (20°C, Budavari 1989)
2.13×10^{-7} (20–25°C, selected, Wauchope et al. 1992; Hornsby et al. 1996)
2.13×10^{-7} (20°C, Montgomery 1993)

Henry's Law Constant (Pa·m^3/mol at 25°C or as indicated):

2816	(20–25°C, calculated-P/C, Montgomery 1993)
2.87×10^{-7}	(calculated-P/C as per Worthing & Walker 1987, Majewski & Capel 1995)
3.00×10^{-7}	(calculated-P/C, this work)

Octanol/Water Partition Coefficient, log K_{OW}:

2.18	(Kenaga & Goring 1980)
2.24	(shake flask-GC, Brown & Flagg 1981)
1.80, 1.66	(RP-HPLC-RT correlation, calculated, Finizio et al. 1991)
2.22	(selected, Magee 1991)
1.80, 2.24	(Montgomery 1993)
2.22	(recommended, Sangster 1993)
0.79	(calculated, Patil 1994)
2.10	(Tomlin 1994)
2.22	(recommended, Hansch et al. 1995)
2.04	(shake flask-UV, Liu & Qian 1995)
1.64, 1.29, 3.02	(RP-HPLC-RT correlation, CLOGP, calculated-S, Finizio et al. 1997)
1.70	(RP-HPLC-RT correlation using short ODP column, Donovan & Pescatore 2002)

Bioconcentration Factor, log BCF:

1.53	(calculated-S, Kenaga 1980)
1.00	(calculated-K_{OC}, Kenaga 1980)
1.48	(selected, Schnoor & McAvoy 1981; Schnoor 1992)

Sorption Partition Coefficient, log K_{OC}:

2.30	(Kenaga 1980; Kenaga & Goring 1980; Karickhoff 1981; Sabljic 1987; Bahnick & Doucette 1988)
2.41	(soil, calculated-S as per Kenaga & Goring 1980, Kenaga 1980)
2.26	(Georgia's Hickory Hill pond sediment, Brown & Flagg 1981)
2.71, 1.75, 1.85	(estimated-S, calculated-S and mp, calculated-K_{OW}, Karickhoff 1981)
0.48–1.48	(selected, sediment/water, Schnoor & McAvoy 1981; Schnoor 1992)
2.57, 2.26	(soil, quoted, Madhun et al. 1986)
2.36, 2.09; 2.33, 1.75	(estimated-reported K_{OW}s; estimated-reported solubilities, Madhun et al. 1986)
2.23	(soil, screening model calculations, Jury et al. 1987b)
2.35	(calculated-MCI χ, Bahnick & Doucette 1988)
2.30, 2.16	(reported, estimated as log K_{OM}, Magee 1991)
2.23, 2.26, 2.30	(soil, quoted values, Bottoni & Funari 1992)
2.28	(soil, 20–25°C, selected, Wauchope et al. 1992; quoted, Richards & Baker 1993; Hornsby et al. 1996)
1.58–2.63	(Montgomery 1993)
2.54	(selected, Lohninger 1994)
2.05, 2.11	(exptl., calculated-K_{OW}, Liu & Qian 1995)
2.28	(soil, calculated-MCI $^1\chi$, Sabljic et al. 1995)
2.28; 2.33, 2.25	(soil, quoted obs.; estimated-class-specific model, estimated-general model using molecular descriptors, Gramatica et al. 2000)
2.14, 2.19	(soils: organic carbon OC ≥ 0.1%, OC ≥ 0.5%, pH 5.6–8.0, average, Delle Site 2001)

Environmental Fate Rate Constants, k, or Half-Lives, $t_{½}$:

Volatilization:

Photolysis:

Oxidation:

Hydrolysis: alkaline chemical hydrolysis $t_{½} > 365$ d (Schnoor & McAvoy 1981; quoted, Schnoor 1992).

Biodegradation: aerobic $t_{½} = 14$ d for 0.06 μg/mL to degrade in pond water and $t_{½} > 28$ d in pond sediment both at 10–20°C (Roberts 1974; quoted, Muir 1991).

Biotransformation:

Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants:

Half-Lives in the Environment:

Air:

Surface water: aerobic $t_{½}$ = 14 d for 0.06 μg/mL to degrade in pond water at 10–20°C (Roberts 1974; quoted, Muir 1991).

Ground water: reported half-lives or persistence, $t_{½}$ = 10–29, 14 and 108 d (Bottoni & Funari 1992)

Sediment: aerobic $t_{½}$ > 28 d for 0.06 μg/mL to slowly degrade in pond sediment at 10–20°C (Roberts 1974; quoted, Muir 1991).

Soil: $t_{½}$ ~ 2 wk in soil (Beynon et al. 1972; quoted, Tomlin 1994);
persistence of 12 months in soil (Wauchope 1978);
$t_{½}$ = 13.5 d from screening model calculations (Jury et al. 1987b);
$t_{½}$ = 12–15 d in sandy loam soils and $t_{½}$ = 20–25 d in silt and clay loam soils (Herbicide Handbook 1989; quoted, Montgomery 1993);
disappearance $t_{½}$ = 181 d from the upper 15 cm on a clay loam Ontario soil in 1987 and $t_{½}$ = 90 d in 1988 with $t_{½}$(calc) = 27 and 12 d, respectively (Frank et al. 1991);
reported $t_{½}$ = 10–29 d, 13 d and 108 d (Bottoni & Funari 1992);
selected field $t_{½}$ = 14 d (Wauchope et al. 1992; quoted, Richards & Baker 1993; Hornsby et al. 1996)
soil $t_{½}$ = 19 d (Pait et al. 1992).

Biota: biochemical $t_{½}$ = 13.5 d from screening model calculations (Jury et al. 1987b).

TABLE 17.1.1.20.1
Reported vapor pressures of cyanazine at various temperatures

Grayson & Fosbracey 1982	
gas saturation-GC	
t/°C	**P/Pa**
65.7	0.0016
70.0	0.0025
77.5	0.0040
85.8	0.0101
87.8	0.0096
92.0	0.0181
20	$1. \times 10^{-5}$
$\ln P = A - B/(T/K)$	
	P/Pa
A	25.7
B	10913

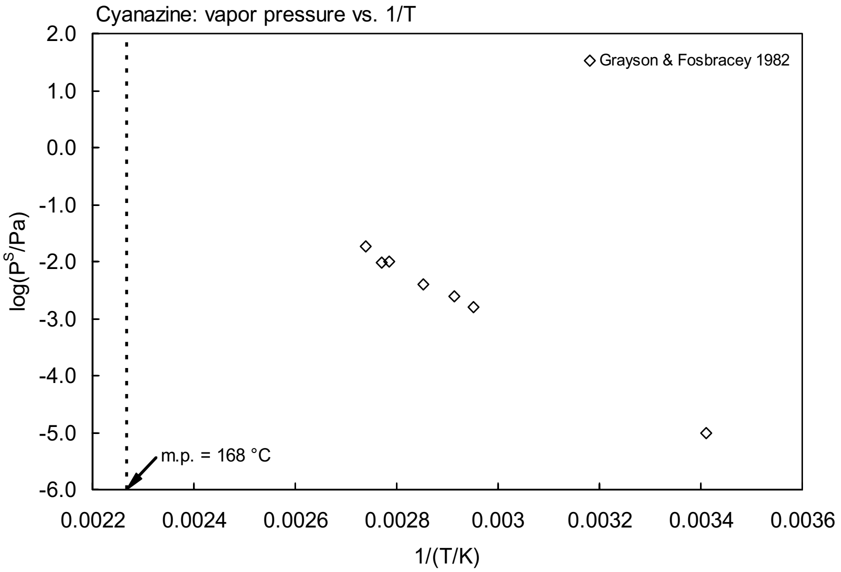
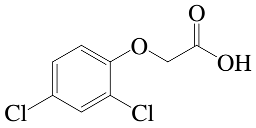


FIGURE 17.1.1.20.1 Logarithm of vapor pressure versus reciprocal temperature for cyanazine.

17.1.1.21 2,4-D

(See also Chapter 13, Carboxylic Acids)



Common Name: 2,4-D
Synonym: 2,4-Dichlorophenoxyacetic acid
Chemical Name: 2,4-dichlorophenoxyacetic acid
Uses: post-emergence control of annual and perennial broadleaf weeds in cereals, maize, sorgum, grassland, established turf, grass seed crops, orchards, cranberries, asparagus, sugar cane, rice, forestry, and on noncropland, etc.
CAS Registry No: 94-75-7
Molecular Formula: $C_8H_6Cl_2O_3$, $Cl_2C_6H_3OCH_2COOH$
Molecular Weight: 221.038
Melting Point (°C):
140.5 (Hartley & Kidd 1987; Howard 1991; Tomlin 1994; Lide 2003)
Boiling Point (°C):
160 (at 0.4 mmHg, Dean 1985)
215 (Neely & Blau 1985)
Density (g/cm^3 at 25°C):
1.565 (30°C, Neely & Blau 1985; Tomlin 1994)
1.416 (Montgomery 1993)
Molar Volume (cm^3/mol):
209.8 (calculated-Le Bas method at normal boiling point)
Dissociation Constant, pK_a:
2.73 (potentiometric method, Nelson & Faust 1969)
2.87 (spectrophotometric method, Cessna & Grover 1978)
2.80 (Reinert & Rogers 1984; selected, Wauchope et al. 1992)
2.64 (Dean 1985; Haag & Yao 1992; Lee et al. 1993)
2.61–3.31 (Howard 1991)
2.97 (Sangster 1993)
3.10 (Kollig 1993)
2.64–3.31 (Montgomery 1993)
Enthalpy of Vaporization, ΔH_V (kJ/mol):
93.89 (Rordorf 1989)
Enthalpy of Fusion ΔH_{fus} (kJ/mol):
38.074 (DSC method, Plato & Glasgow 1969)
39.6 (Rordorf 1989)
Entropy of Fusion, ΔS_{fus} (J/mol K):
Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F: 0.0736 (mp at 140.5°C)

Water Solubility (g/m^3 or mg/L at 25°C or as indicated):
890 (Hodgman 1952; Hamaker 1975; Verschueren 1983; Montgomery 1993)
522 (shake flask-UV, Leopold et al. 1960)
725 (Bailey & White et al. 1965)
725, 400, 900, 550 (Gunther et al. 1968)
900 (Herbicide Handbook 1974; Wauchope 1978; Kenaga 1980a,b; Kenaga & Goring 1980)
600 (20°C, Khan 1980)
620–900 (Weber et al. 1980)
470 (20–25°C, pH 5.6, Geyer et al. 1981)
633, 812 (15, 25°C, shake flask method, average values of 5 laboratories, OECD 1981)
620 (20°C, Hartley & Kidd 1983, 1987)

620 (Worthing & Walker 1983)
609 (Gerstl & Helling 1987)
400 (20°C, selected, Suntio et al. 1988)
703 (Gustafson 1989)
682 (Yalkowsky et al. 1987)
540–890 (Nyholm et al. 1992)
900, 600, 890, 703, 1072 (Wauchope et al. 1992)
890 (20–25°C, selected, Wauchope et al. 1992)
311 (pH 1, Tomlin 1994)

Vapor Pressure (Pa at 25°C or as indicated and reported temperature dependence equations):
8.0×10^{-5} (Hamaker 1975)
0.180–1.69 (transpiration method, Spencer 1976)
53.0 (160°C, Hartley & Kidd 1983, 1987)
8.0×10^{-5} (recommended, Neely & Blau 1985; Lyman 1985)
1.0 (20°C, selected, Suntio et al. 1988)
6.0×10^{-6} (selected, Nash 1989)
4.10×10^{-5}, 2.0×10^{-3}, 0.058, 1.10, 13.0 (25, 50, 70, 100, 125°C, gas saturation-GC, Rordorf 1989)
$\log (P_S/Pa) = 17.56 - 6544.1/(T/K)$; measured range 70.2–135°C (solid, gas saturation-GC, Rordorf 1989)
$\log (P_L/Pa) = 13.558 - 4904.6/(T/K)$; measured range 140–196°C (liquid, gas saturation-GC, Rordorf 1989)
0.20, 0.0032 (quoted, estimated from Henry's law constant, Howard 1991)
5.6×10^{-5} (selected, Mackay & Stiver 1991)
1.40, 3.2×10^{-3} (quoted, estimated from HLC, Howard 1991)
1.33×10^{-5}, 8.0×10^{-5}, 1.07×10^{-3}; 1.07×10^{-3} (20–25°C, quoted lit; selected, Wauchope et al. 1992)
0.627 (Montgomery 1993)
0.011 (Tomlin 1994)

Henry's Law Constant (Pa·m^3/mol at 25°C or as indicated):
1.36×10^{-5} (calculated-P/C, Jury et al. 1983)
1.39×10^{-5} (calculated-P/C, Jury et al. 1987a, Jury & Ghodrati 1989)
0.55 (20°C, calculated-P/C, Suntio et al. 1988)
0.0015 (calculated, Nash 1989)
1.03×10^{-3} (calculated-bond contribution, Howard 1991)
6.80, 0.853 (pH 1, pH 7 at 20°C, wetted wall column-GC, Rice et al. 1997b)
1.82×10^{-7} (quoted lit., Armbrust 2000)

Octanol/Water Partition Coefficient, log K_{OW}:
2.81 (shake flask-UV, Fujita et al. 1964)
2.59 (electrometric titration, Freese et al. 1979)
1.57 (Kenaga & Goring 1980; Kenaga 1980b)
2.74 (selected, Dao et al. 1983)
2.81 (20°C, Verschueren 1983)
1.57, 4.88 (shake flask-OECD 1981 Guidelines, Geyer et al. 1984)
2.65 (shake flask, log P Database, Hansch & Leo 1987)
2.50 (OECD 1981 method, Kerler & Schönherr 1988)
2.649 (liquid/liquid-countercurrent-chromatography, Ilchmann et al. 1993)
2.81 (recommended, Sangster 1993)
1.44–4.18 (quoted lit. range, Montgomery 1993)
2.58–2.83 (pH 1, Tomlin 1994)
2.81 (selected, Hansch et al. 1995)
0.59 (RP-HPLC-RT correlation, CLOGP, Calculated-S, Finizio et al. 1997)

Octanol/Air Partition Coefficient, log K_{OA}:

Bioconcentration Factor, log BCF:

1.11, –0.097 (calculated-S, K_{OW}, Kenaga 1980a)
–2.46, 1.30 (beef fat, fish, Kenaga 1980b)
0.778, 1.94 (alga *Chlorella*: exptl. 24 h exposure, calculated-S, Geyer et al. 1981)
0.778 (algae, Freitag et al. 1982)
< 1.00 (golden orfe, Freitag et al. 1982)
1.23 (activated sludge, Freitag et al. 1982)
0.0 (fish, microcosm conditions, Garten & Trabalka 1983;)
0.778, 1.23 (algae, calculated-K_{OW}, Geyer et al. 1984)
1.23 (algae, Geyer et al. 1984)
1.11 (calculated, Isensee 1991)
–5.00 (bluegill sunfish and channel catfish, Howard 1991)
–2.70 (frog tadpoles, Howard 1991)
–3.0, –2.52 (pH 7.8, seaweeds, Howard 1991)
0.778, 0.85 (quoted: alga, fish, Howard 1991)
0.0, 0.505 (catfish *Ictalurus melas*, water flea *Daphnia magna*, wet wt basis, Wang et al. 1996)

Sorption Partition Coefficient, log K_{OC}:

1.51 (Hamaker 1975)
1.30, 2.0 (quoted, calculated, Kenaga 1980a)
1.30, 2.11 (quoted, Kenaga & Goring 1980)
1.30 (quoted, Kenaga 1980b)
1.76 (quoted, average value of 3 soils, McCall et al. 1980)
2.25, 2.04, 2.35 (soil I-very strongly acid sandy soil pH 4.5–5.5, soil II-moderately or slightly acid loamy soil pH 5.6–6.5, soil III-slightly alkaline loamy soil pH 7.1–8.0, OECD 1981)
1.29 (soil, Neely & Blau 1985)
1.30 (soil, screening model calculations, Jury et al. 1987a,b; Jury & Ghodrati 1989)
1.61 (soil, quoted, Sabljic 1987)
1.75, 2.00 (quoted, calculated-MCI χ, Gerstl & Helling 1987)
2.59 (HPLC-k′ correlation, cyanopropyl column, mobile phase buffered to pH 3, Hodson & Williams 1988)
1.00, 1.23, 2.29 (sediment, Alfisol soil, Podzol soil, von Oepen et al. 1991)
1.30–1.78, 1.30–2.0, 1.72 (soil, quoted lit. values, Bottoni & Funari 1992)
1.30, 1.78, 1.51, 1.26, 1.72, 1.75, 1.76 (soil, quoted values, Wauchope et al. 1992)
1.30 (soil, selected, Wauchope et al. 1992)
0.68 (calculated-K_{OW}, Kollig 1993)
1.68–2.73 (Montgomery 1993)
1.66 (calculated-QSAR MCI ${}^1\chi$, Sabljic et al. 1995)
2.09, 1.04, 1.40, 0.778 (first generation Eurosoils ES-1, ES-2, ES-3, ES-4, shake flask/batch equilibrium-HPLC/UV, Gawlik et al. 1998, 1999)
1.65, 1.36, 1.37, 0.899 (second generation Eurosoils ES-1, ES-2, ES-3, ES-4, shake flask/batch equilibrium-HPLC/UV, Gawlik et al. 1999)
1.652 (second generation Eurosoil ES-1, HPLC-k′ correlation, Gawlik et al. 2000)
1.68 (soil, quoted, Armbrust 2000)
1.79, 1.77 (soils: organic carbon OC $\geq$ 0.1%, OC $\geq$ 0.5%, pH 2.8–8.0, average, Delle Site 2001)
2.16, 2.13 (soils: organic carbon OC $\geq$ 0.1%, OC $\geq$ 0.5%, pH 2.8–5.0, average, Delle Site 2001)
1.68, 1.68 (soils: organic carbon OC $\geq$ 0.1%, OC $\geq$ 0.5%, pH > 5.0, average, Delle Site 2001)

Environmental Fate Rate Constants, k, or Half-Lives, $t_{1/2}$:

Volatilization: volatilization from water is negligible, calculated volatilization $t_{1/2}$ = 660 d (from 1 cm) and $t_{1/2}$ = 7.1 yr (from 10 cm) from soil (Howard 1991).

Photolysis: aqueous photolysis $t_{1/2}$ = 2–4 d when irradiated at 356 nm, $t_{1/2}$ = 50 min in water when irradiated at 254 nm and $t_{1/2}$ = 29–43 d when exposed to September sunlight (Howard 1991);
aqueous photolysis rate constant, k = 2.2×10^{-3} h^{-1} (Armbrust 2000).
Oxidation:
photooxidation $t_{1/2}$ = 1.8–18 h, based on estimated rate constant for the vapor-phase reaction with hydroxyl radical in air (Howard et al. 1991)
k(aq.) = (1.0–2.3) M^{-1} s^{-1} for direct reaction with ozone in water at pH 1.5–2.9 and 21 ± 1°C, with $t_{1/2}$ = 3.9 h at pH 7 (Yao & Haag 1991).
k(calc) = 5.0×10^9 M^{-1} s^{-1} (Haag & Yao 1992)
k_{OH}(aq.) = 1.6×10^9 M^{-1} s^{-1} for reaction with hydroxyl radical in irradiated field water both in the laboratory and sunlit rice paddies (Mabury & Crosby 1996; quoted, Armbrust 2000);
k_{OH}(aq.) = 8.4×10^{12} M^{-1} h^{-1} at pH 5, 7, 9; measured hydroxyl radical rate constant for 2,4-D, (Armbrust 2000)
Hydrolysis: no hydrolyzable groups and rate constant at neutral pH is zero (Kollig et al. 1987; selected, Howard et al. 1991); generally resistant to hydrolysis, may become important at pH > 8 (Howard 1991).
Biodegradation:
k = 0.7–14.0 d^{-1} and $t_{1/2}$ = 10 to > 50 d in clear to murky river water with lag time ranges from 6–12 d (Nesbitt & Watson 1980a);
$t_{1/2}$ = 4 d in river with nutrient and suspended sediments and $t_{1/2}$ = 10 d with a lag time of 5 d for filtered river water (Nesbitt & Watson 1980b);
degradation kinetics not first-order, time for 50% decomposition in six soils: Commerce 5 d, Catlin 1.5 d, Keith 3.9 d, Cecil 3.0 d, Walla-Walla 2.5 d and Fargo 8.5 d, with an average time of 4 d (McCall et al. 1981)
aerobic degradation k = 0.3×10^{-3} h^{-1} with $t_{1/2}$ = 97.0 d for control system, k = 9.5×10^{-3} h^{-1} with $t_{1/2}$ = 3.1 d for metabolism, k = 16.2×10^{-3} h^{-1} with $t_{1/2}$ = 1.8 d for co-metabolism; anaerobic degradation k = 0.24×10^{-3} h^{-1} with $t_{1/2}$ = 120 d for control system, k = 0.21×10^{-3} h^{-1} with $t_{1/2}$ = 135 d for metabolism, k = 0.42×10^{-3} h^{-1} with $t_{1/2}$ = 69 d for co-metabolism, by a mixture of microorganisms from activated sludge, soil and sediment in cyclone fermentors (Liu et al. 1981)
k = (3.6–28.8) × 10^{-6} mL $cell^{-1}$ d^{-1} in natural water (Paris et al. 1981; quoted, Klečka 1985)
k < 0.14–0.07 d^{-1} in river water at 25°C (Nesbitt & Watson 1980; quoted, Klečka 1985)
k = (0.058 ± 0.006) d^{-1} in lake water at 29°C (Subba-Rao et al. 1982; quoted, Klečka 1985)
k = 0.08–0.46 d^{-1} in soil at 25°C (McCall et al. 1981; quoted, Klečka 1985);
$t_{1/2}$ (aq. aerobic) = 240–1200 h, based on unacclimated aerobic river die-away test data (Nesbitt & Watson 1980; selected, Howard et al. 1991);
$t_{1/2}$ (anaerobic) = 672–4320 h, based on unacclimated aqueous screening test data (Liu et al. 1981; selected, Howard et al. 1991);
k = 0.035 d^{-1} in die-away test, k = 0.029 d^{-1} in CO_2 evolution test, in soil and k = 6.9×10^{-1} mL (g bacteria)$^{-1}$ d^{-1} by activated sludge cultures (Scow 1982);
$t_{1/2}$ = 18 to over 50 d in clear river water, and $t_{1/2}$ = 10 to 25 d in muddy river water with lag times of 6 to 12 d; degradation with a mixture of microorganisms from activated sludge, soil, and sediments lead to half-lives of 1.8–3.1 d under aerobic conditions and 69–135 d under anaerobic conditions (Howard 1991)
k(aerobic) = 5.25×10^{-3} h^{-1} (Armbrust 2000).
Biotransformation:
Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants:
k_1 = 0.0092 h^{-1}; k_2 = 0.0092 h^{-1} (catfish *Ictalurus melas*, Wang et al. 1996)
k_1 = 0.8560 h^{-1}; k_2 = 0.2690 h^{-1} (Water flea *Daphnia magna*, Wang et al. 1996)

Half-Lives in the Environment:
Air: $t_{1/2}$ = 1.8–18 h, based on estimated rate constant for the reaction with OH radical (Howard et al. 1991);
photooxidation $t_{1/2}$ = 23.9 h for reactions with OH radical in air (Howard 1991).
Surface water: $t_{1/2}$ = 48–96 h, based on reported photolysis half-lives for aqueous solution irradiated at UV wavelength of 356 nm (Baur & Bovey 1974; selected, Howard et al. 1991);
degradation $t_{1/2}$ = 14 d in sensitized, filtered and sterilized river water, based on sunlight photolysis test of 1 μg mL^{-1} in distilled water (Zepp et al. 1975; quoted, Cessna & Muir 1991);
$t_{1/2}$ = 1.8 and 3.1 d for cometabolism and metabolism, respectively, easily degraded under aerobic conditions; $t_{1/2}$ = 69 and 135 d under anaerobic conditions (Liu et al. 1981;)

typical biodegradation $t_{1/2}$ = 10 to < 50 d with longer expected in oligotrophic waters, photolysis $t_{1/2}$ = 29–43 d for water solutions irradiated at sunlight (Howard 1991);
degraded relatively slowly when incubated in natural waters or in soil/sediment suspensions, with $t_{1/2}$ ~ 6 to 170 d (Muir 1991);
rate constant k(exptl) = (1.0–2.3) M^{-1} s^{-1} for direct reaction with ozone in water at pH 1.5–2.9 and 21°C, with $t_{1/2}$ = 3.9 h at pH 7 (Yao & Haag 1991);
rate constant k(calc) = 5×10^9 M^{-1} s^{-1} for the reaction with hydroxyl radical in aqueous solution (Haag & Yao 1992);
$t_{1/2}$ = 2–4 d when irradiated at λ = 356 nm in aqueous solution (Montgomery 1993).

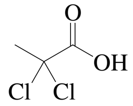
Ground water: $t_{1/2}$ = 480–4320 h, based on estimated unacclimated aqueous aerobic and anaerobic biodegradation half-lives (Howard et al. 1991)
reported $t_{1/2}$ = 4, 15, 1–35, 7–21 d (Bottoni & Funari 1992)

Sediment: $t_{1/2}$ < 1 d for degradation in sediments and lake muds (Howard 1991);
degraded relatively slowly when incubated in natural waters or in soil/sediment suspensions, with $t_{1/2}$ = 6 to 170 d (Muir 1991).

Soil: degradation $t_{1/2}$ = 5.0 and 4.0 d in Quachita Highlands' forest and grassland soil respectively, $t_{1/2}$ = 4 d in Gross Timbers Forest soil, average $t_{1/2}$ = 4 d in 3 soils (shake flask, Altom & Stritzke 1973);
field $t_{1/2}$ = 5.2 d in Arid range (Lane et al. 1977; quoted, Nash 1983);
field $t_{1/2}$ = 19 d in Dykland soil (Stewart & Gaul 1977; quoted, Nash 1983);
lab. $t_{1/2}$ = 5.5 d in Naff soil (Wilson & Cheng 1978; quoted, Nash 1983);
microagroecosystem $t_{1/2}$ = 11 d for granular application to bluegrass turf (Nash & Beall 1980)
non-persistent in soil with $t_{1/2}$ < 20 d (Willis & McDowell 1982);
microagroecosystem $t_{1/2}$ = 3 d in moist fallow soil (Nash 1983);
$t_{1/2}$ = 15 d in soil (Jury et al. 1983, 1987a,b; Jury & Ghodrati 1989);
persistence of one month in soil (Jury et al. 1987);
$t_{1/2}$ = 240–1200 h, based on estimated unacclimated aqueous aerobic biodegradation half-life (Howard et al. 1991);
biodegradation $t_{1/2}$ < 1 d to several weeks, $t_{1/2}$ = 3.9 and 11.5 d in 2 moist soils and $t_{1/2}$ = 9.4 to 254 d in the same soils under dry conditions (Howard 1991);
degraded relatively slowly when incubated in natural waters or in soil/sediment suspensions, with $t_{1/2}$ = 6 to 170 d (Muir 1991);
reported $t_{1/2}$ = 4,15, 1–35 and 7–21 d (Bottoni & Funari 1992);
field $t_{1/2}$ = 2–16 d, with a selected value of 10 d (Wauchope et al. 1992);
soil $t_{1/2}$ = 18 d (Pait et al. 1992);
rate constants for Amsterdam silt loam at soil depth 0–30 cm: k = 0.0053 d^{-1} at 10°C, k = 0.0046 d^{-1} at 17°C and k = 0.0127 d^{-1} at 24°C with corresponding first-order $t_{1/2}$ = 7, 7, and 2 d; at soil depth 30–60 cm: k = 0.00012 d^{-1} at 10°C, k = 0.0044 d^{-1} at 17°C and k = 0.0077 d^{-1} at 24°C with corresponding first-order $t_{1/2}$ = 273, 8, and 4 d; and at soil depth 60–120 cm: k = 0.00005 d^{-1} at 10°C, k = 0.0013 d^{-1} at 17°C and k = 0.0022 d^{-1} at 24°C with corresponding first-order $t_{1/2}$ = 593, 25, and 12 d (Veeh et al. 1996).

Biota: depuration $t_{1/2}$ = 13.8 h in daphnids, $t_{1/2}$ = 1.32 d in catfish (Ellgehausen et al. 1980).

17.1.1.22 Dalapon



Common Name: Dalapon
Synonym: Alatex, Basinex P, Crisapon, D-Granulat, Dawpon-Rae, Ded-Weed, Dowpon, DPA, Gramevin, Kenapon, Liropon, Proprop, Radapon
Chemical Name: 2,2-dichloropropanoic acid; 2,2-dichloropropionic acid; α-dichloropropanoic acid; α,α-dichloropropionic acid
Uses: selective systemic herbicide to control perennial and annual grasses on noncropland, fruits, vegetables, and some aquatic weeds.
CAS Registry No: 75-99-0
Molecular Formula: $C_3H_4Cl_2O_2$
Molecular Weight: 1432.969
Melting Point (°C): liquid
Boiling Point (°C):
185–190 (Herbicide Handbook 1989; Worthing & Hance 1991; Tomlin 1994)
98–99 (sodium salt at 20 mmHg, Budavari 1989)
Density (g/cm^3 at 20°C):
1.389 (Nelson & Faust 1969; quoted, Kenaga 1974; Montgomery 1993)
1.389 (22.8°C, Herbicide Handbook 1989)
1.4014 (Budavari 1989; Milne 1995)
Molar Volume (cm^3/mol):
Dissociation Constant pK_a:
1.84 (potentiometric titration, Nelson & Faust 1969; Freed 1976; Hornsby et al. 1996)
1.74 (Kenaga 1974; quoted, Howard 1991)
1.74–1.84 (Worthing & Hance 1991; Tomlin 1994)
2.06 (Yao & Haag 1991; Haag & Yao 1992)
1.84 (free acid, Montgomery 1993)
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
Entropy of Fusion, ΔS_{fus} (J/mol K):
Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F: 1.0

Water Solubility (g/m^3 or mg/L at 25°C or as indicated):
900000 (Woodford & Evans 1963; Bailey & White 1965)
> 800000 (Kenaga 1974)
502000 (Martin & Worthing 1977)
450000 (Weber et al. 1980; Budavari 1989)
501200 (Garten & Trabalka 1983)
431850 (selected, Gerstl & Helling 1987)
900000 (sodium salt, Worthing & Walker 1987, Worthing & Hance 1991)
500000 (Reinert 1989)
450000–900000 (Montgomery 1993)
900000 (20–25°C, selected, Hornsby et al. 1996)

Vapor Pressure (Pa at 25°C or as indicated):
16.0 (calculated from high temp., Foy 1976)
1.0×10^{-5} (Worthing & Hance 1991; Tomlin 1994)
0.0 (20–25°C, selected, Hornsby et al. 1996)

Henry's Law Constant ($Pa \cdot m^3/mol$ at 25°C):
6.50×10^{-3} (Hine & Mookerjee 1975)
0.608 (calculated, Montgomery 1993)

4.56×10^{-3} (calculated-P/C as per Howard 1991, Majewski & Capel 1995)

Octanol/Water Partition Coefficient, log K_{OW}:

0.76	(Kenaga 1974)
0.78	(Kenaga 1980)
1.34	(selected, Dao et al. 1983)
–2.76	(selected, Gerstl & Helling 1987)
1.48	(Reinert 1989)
0.78	(selected, Hansch et al. 1995)
1.47	(LOGSTAR or CLOGP data, Sabljic et al. 1995)

Octanol/Air Partition Coefficient, log K_{OA}:

Bioconcentration Factor, log BCF:

0.477	(dalapon sodium salt in fish, Kenaga 1974)
–0.444	(calculated-S, Kenaga 1980; quoted, Isensee 1991)
0.301	(estimated-K_{OW}, Lyman et al. 1982; quoted, Howard 1991)

Sorption Partition Coefficient, log K_{OC}:

0.477	(soil, calculated-S as per Kenaga & Goring 1980, Kenaga 1980)
0.97	(calculated-MCI χ, Gerstl & Helling 1987)
2.13	(Reinert 1989)
0.48, 2.13	(soil, quoted values, Bottoni & Funari 1992)
0.27–2.18	(calculated, Montgomery 1993)
0.40	(soil, calculated-MCI $^1\chi$, Sabljic et al. 1995)
0.0	(soil, 20–25°C, selected, Hornsby et al. 1996)

Environmental Fate Rate Constants, k, or Half-Lives, $t_{½}$:

Volatilization:

Photolysis:

Oxidation:

photooxidation $t_{½}$ = 289–2893 h in air, based on an estimated rate constant for the vapor-phase reaction with hydroxyl radical in air (Atkinson 1987; quoted, Howard et al. 1991);

k(aq.) = 4.6×10^8 M^{-1} s^{-1} for the reaction (photo-Fenton with reference to acetophenone) with hydroxyl radical in aqueous solutions at pH 3.4 and at 24 ± 1°C (Buxton et al. 1988; quoted, Faust & Hoigné 1990; Haag & Yao 1992)

k(aq.) $\leq$ 0.005 M^{-1} s^{-1} for direct reaction with ozone in water at pH 6.4 and 22°C, with a half-life of > 2 yr at pH 7 (Yao & Haag 1991).

k(aq.) = $(7.3 \pm 0.3) \times 10^7$ M^{-1} s^{-1} for the reaction (photo-Fenton with reference to acetophenone) with hydroxyl radical in aqueous solutions at pH 3.4 and at 24 ± 1°C (Haag & Yao 1992).

Hydrolysis:

Biodegradation: aqueous aerobic $t_{½}$ = 336–1440 h, based on unacclimated aerobic soil grab sample data (Corbin & Upchurch 1967; Kaufman & Doyle 1977; quoted, Howard et al. 1991);

rate constant k = 0.047 d^{-1} by soil incubation die-away studies (Rao & Davidson 1980; quoted, Scow 1982);

aqueous anaerobic $t_{½}$ = 1344–5760 h, based on estimated aqueous aerobic biodegradation half-life (Howard et al. 1991).

Biotransformation:

Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants:

Half-Lives in the Environment:

Air: $t_{½}$ = 289–2893 h, based on an estimated rate constant for the vapor-phase reaction with hydroxyl radical in air (Atkinson 1987; quoted, Howard et al. 1991).

Surface water: $t_{½}$ = 336–1440 h, based on estimated aqueous aerobic biodegradation half-life (Howard et al. 1991);

measured rate constant k ≤ 0.0005 M^{-1} s^{-1} for direct reaction with ozone in water at pH 6.4 and 22°C, with a $t_{1/2}$ ≥ 2 yr at pH 7 (Yao & Haag 1991).

Groundwater: $t_{1/2}$ = 672–2880 h, based on estimated aqueous aerobic biodegradation half-life (Howard et al. 1991).

reported $t_{1/2}$ = 30 d (Bottoni & Funari 1992)

Sediment:

Soil: $t_{1/2}$ = 7–8 d in soil (Kaufman 1966; quoted, Kaufman 1976);

persistence across 43 soils from < 2 wk to > 8 wk (Day et al. 1963; quoted, Kaufman 1976);

$t_{1/2}$ = 336–1440 h, based on unacclimated aerobic soil grab sample data (Corbin & Upchurch 1967; Kaufman & Doyle 1977; quoted, Howard et al. 1991);

estimated persistence of 8 months (Kearney et al. 1969; quoted, Jury et al. 1987);

persistence of 8 wk in soil (Edwards 1973; quoted, Morrill et al. 1982);

persistence of about 2 wk in growing season in most agricultural soils (Herbicide Handbook 1974; quoted, Kaufman 1976);

estimated first-order $t_{1/2}$ = 15 d from biodegradation rate constant k = 0.047 d^{-1} by soil incubation die-away studies (Rao & Davidson 1980; quoted, Scow 1982);

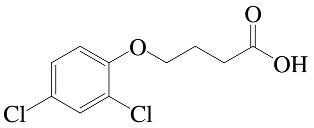
non-persistent in soil with $t_{1/2}$ < 20 d (Willis & McDowell 1982);

reported half-life or persistence, 30 d (Verschuren 1983; Bottoni & Funari 1992);

field $t_{1/2}$ = 30 d at 20–25°C (selected, Hornsby et al. 1996).

Biota:

17.1.1.23 2,4-DB



Common Name: 2,4-DB
Synonym: Butoxon, Butyrac, Butyrac 118, Embutox, Legumex D
Chemical Name: 4-(2,4-dichlorophenoxy)butanoic acid; 4-(2,4-dichlorophenoxy)butyric acid
Uses: herbicide for post-emergence control of many annual and perennial broadleaf weeds in lucerne, clovers, undersown cereals, grassland, forage legumes, soybeans, and groundnuts.
CAS Registry No: 94-82-6
Molecular Formula: $C_{10}H_{10}Cl_2O_3$
Molecular Weight: 249.090
Melting Point (°C):
  118 (Lide 2003)
Boiling Point (°C):
Density (g/cm^3 at 20°C):
Molar Volume (cm^3/mol):
  254.2 (calculate-Le Bas method at normal boiling point)
Dissociation Constant pK_a:
  5.95 (Bailey & White 1965; Que Hee et al. 1981)
  4.80 (Worthing & Walker 1987; Hornsby et al. 1996)
Enthalpy of Vaporization, ΔH_V (kJ/mol):
  91.29 (Rordorf 1989)
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
  33.6 (Rordorf 1989)
Entropy of Fusion, ΔS_{fus} (J/mol K):
Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F: 0.122 (mp at 118°C)

Water Solubility (g/m^3 or mg/L at 25°C or as indicated):
  82.3 (Bailey & White 1965)
  53 (rm. temp., Melnikov 1971)
  46 (Martin & Worthing 1977; Worthing & Walker 1987, Worthing & Hance 1991)
  46 (Weber et al. 1980)
  46 (Hartley & Kidd 1987; Budavari 1989;, Milne 1995)
  46 (20–25°C, selected, Hornsby et al. 1996)

Vapor Pressure (Pa at 25°C or as indicated and reported temperature dependence equations):
  negligible (Hartley & Kidd 1987)
  1.0×10^{-5}, 5.90×10^{-4}, 0.019, 0.38, 5.20 (25, 50, 70, 100, 125°C, gas saturation-GC, Rordorf 1989)
  $\log (P_S/Pa) = 17.692 - 6760.5/(T/K)$; measured range 80–120°C (solid, gas saturation-GC, Rordorf 1989)
  $\log (P_L/Pa) = 12.682 - 4768.7/(T/K)$; measured range 125–196°C (liquid, gas saturation-GC, Rordorf 1989)

Henry's Law Constant (Pa·m^3/mol):

Octanol/Water Partition Coefficient, log K_{OW}:
  3.53 (shake flask-HPLC/UV, Jafvert et al. 1990)
  3.53 (selected, Hansch et al. 1995)

Octanol/Air Partition Coefficient, log K_{OA}:

Bioconcentration Factor, log BCF:
  1.85 (calculated-S, Kenaga 1980)
  2.21 (calculated-log K_{OW} as per Mackay 1982, this work)

Sorption Partition Coefficient, log K_{OC}:

2.72	(soil, calculated-S, Kenaga 1980)
1.3	(organic carbon, Wauchope et al. 1991)
2.64	(20–25°C, estimated, Hornsby et al. 1996)

Environmental Fate Rate Constants, k, or Half-Lives, $t_{½}$:

Volatilization:

Photolysis:

Oxidation: photooxidation $t_{½}$ = 6–60 h in air, based on an estimated rate constant for the vapor-phase reaction with hydroxyl radicals in air (Atkinson 1987; quoted, Howard et al. 1991).

Hydrolysis: stable in distilled water for 40 d (Chau & Thomson 1978; quoted, Howard et al. 1991).

Biodegradation: aqueous aerobic $t_{½}$ = 24–168 h, based on unacclimated soil grab sample data (Smith 1978; quoted, Howard et al. 1991); aqueous anaerobic $t_{½}$ = 96–672 h, based on estimated unacclimated aqueous aerobic biodegradation half-life (Howard et al. 1991).

Biotransformation:

Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants:

Half-Lives in the Environment:

Air: $t_{½}$ = 6–60 h, based on an estimated rate constant for the vapor-phase reaction with hydroxyl radicals in air (Atkinson 1987; Howard et al. 1991).

Surface water: $t_{½}$ = 24–168 h, based on estimated unacclimated aqueous aerobic biodegradation half-life (Howard et al. 1991).

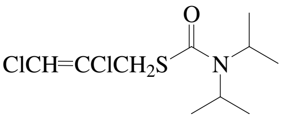
Groundwater: $t_{½}$ = 48–336 h, based on estimated unacclimated aqueous aerobic biodegradation half-life (Howard et al. 1991)
reported $t_{½}$ < 7 d (Bottoni & Funari 1992)

Sediment:

Soil: $t_{½}$ = 24–168 h, based on unacclimated soil grab sample data (Smith 1978; quoted, Howard et al. 1991)
selected $t_{½}$ = 10 d (Wauchope et al. 1991; quoted, Dowd et al. 1993);
$t_{½}$ < 7 d (Worthing & Hance 1991; Bottoni & Funari 1992);
field $t_{½}$ = 5 d (20–25°C, selected, Hornsby et al. 1996).

Biota:

17.1.1.24 Diallate



Common Name: Diallate
Synonym: Avadex, CP 15336, DATC, Pyradex
Chemical Name: *S*-(2,3-dichloroallyl)diisopropyl(thiocarbamate); *S*-(2,3-dichloro-2-propenyl)bis(1-methylethyl)-carbamothioate
Uses: pre-emergent and selective herbicide to control wild oats and blackgrass in barley, corn, flax, lentils, peas, potatoes, soybeans, and sugar beets.
CAS Registry No: 2303-16-4
Molecular Formula: $C_{10}H_{17}Cl_2NOS$
Molecular Weight: 270.219
Melting Point (°C):
  25–30 (Herbicide Handbook 1989; Montgomery 1993)
Boiling Point (°C):
  97 (at 0.15 mmHg, Herbicide Handbook 1989)
  108 (at 0.25 mmHg, Herbicide Handbook 1989; Montgomery 1993)
  150 (at 9 mmHg, Howard 1991; Milne 1995; Montgomery 1993)
Density (g/cm^3 at 20°C):
  1.188 (25°C, Hartley & Kidd 1987; Montgomery 1993)
Molar Volume (cm^3/mol):
  305.1 (calculated-Le Bas method at normal boiling point)
Dissociation Constant pK$_a$:
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
Entropy of Fusion, ΔS_{fus} (J/mol K):
Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F:

Water Solubility (g/m^3 or mg/L at 25°C or as indicated):
  40.0 (Günther et al. 1968)
  14.0 (Ashton & Crafts 1973, 1981)
  40.0 (rm. temp., Spencer 1973; Khan 1980)
  40.0 (Martin & Worthing 1977; Hartley & Kidd 1987; Montgomery 1993; Milne 1995)
  14.0 (Herbicide Handbook 1978; Herbicide Handbook 1989; Montgomery 1993)
  68.8 (22°C, shake flask-GC, Bowman & Sans 1979, 1983a,b)
  40.5 (20–25°C, shake flask-GC, Kanazawa 1981)
  52.5 (Garten & Trabalka 1983)
  14.0 (20–25°C, selected, Augustijn-Beckers et al. 1994; Hornsby et al. 1996)

Vapor Pressure (Pa at 25°C or as indicated):
  0.020 (Ashton & Crafts 1973; Herbicide Handbook 1989)
  0.0117 (20°C, Hartley & Graham-Bryce 1980)
  0.0337 (20°C, GC-RT correlation, Kim 1985)
  0.020 (Hartley & Kidd 1987)
  0.013 (20°C, selected, Suntio et al. 1988)
  0.020 (20°C, Montgomery 1993)
  0.020 (20–25°C, selected, Augustijn-Beckers et al. 1994; Hornsby et al. 1996)

Henry's Law Constant (Pa·m^3/mol at 25°C or as indicated):
  0.250 (20°C, calculated-P/C, Suntio et al. 1988)
  0.385 (calculated-P/C, Howard 1991)
  0.253 (20–25°C, calculated-P/C, Montgomery 1993)

0.108 (calculated-P/C, this work)

Octanol/Water Partition Coefficient, log K_{OW}:
5.23 (estimated, USEPA 1988; quoted, Howard 1991)
3.29 (calculated, Montgomery 1993)
3.67 (LOGPSTAR or CLOGP data, Sabljic et al. 1995)

Octanol/Air Partition Coefficient, log K_{OA}:

Bioconcentration Factor, log BCF:
2.15 (calculated-S, Kenaga 1980; quoted, Howard 1991; Isensee 1991)
2.08 (calculated-K_{OC}, Kenaga 1980)

Sorption Partition Coefficient, log K_{OC}:
3.28 (soil, Grover 1974)
2.96. 2.46, 2.59, 2.49, 2.65 (Melfort loam, Weyburn sandy loam, Regina clay, Indian Head sandy loam, Asquith loamy sand, Grover et al. 1979)
3.28 (soil, measured value, Kenaga 1980; Kenaga & Goring 1980)
3.00 (soil, calculated-S as per Kenaga & Goring 1980, Kenaga 1980)
2.77 (calculated-MCI χ, Bahnick & Doucette 1988)
2.28 (Montgomery 1993)
3.52 (selected, Lohninger 1994)
2.70 (20–25°C, selected, Augustijn-Beckers et al. 1994; Hornsby et al. 1996)
3.28 (soil, calculated-MCI $^1\chi$, Sabljic et al. 1995)
3.28; 3.21, 2.66 (soil, *cis*-isomer, quoted exptl.; estimated-class-specific model, estimated-general model using molecular descriptors, Gramatica et al. 2000)
3.28; 3.21, 2.65 (soil, *trans*-isomer, quoted exptl.; estimated-class-specific model, estimated-general model using molecular descriptors, Gramatica et al. 2000)

Environmental Fate Rate Constants, k, or Half-Lives, $t_{1/2}$:
Volatilization:
Photolysis: $t_{1/2}$ = 4 h, < 1% of 135 μg/mL to degrade in distilled water under > 300 nm light (Ruzo & Casida 1985; quoted, Cessna & Muir 1991).
Oxidation: photooxidation $t_{1/2}$ = 0.58–5.8 h, based on an estimated rate constant for the vapor-phase reaction with hydroxyl radicals in air (Atkinson 1987; quoted, Howard et al. 1991).
Hydrolysis: neutral hydrolysis rate constant $k = (1.2 \pm 0.7) \times 10^{-5}\ h^{-1}$ with a calculated first-order $t_{1/2}$ = 6.6 yr at pH 7 (Ellington et al. 1987, 1988);
first-order $t_{1/2}$ = 6.6 yr, based on measured first-order base catalyzed hydrolysis rate constant at pH 7 (Ellington et al. 1987; quoted, Howard et al. 1991)
$t_{1/2}$ = 2400 d at pH 2, $t_{1/2}$ = 2500 d at pH 7 and $t_{1/2}$ = 32 d at pH 12 in natural waters (Capel & Larson 1995).
Biodegradation: aqueous aerobic $t_{1/2}$ = 252–2160 h, based on aerobic soil die-away test data (Anderson & Domsch 1976; Smith 1970; quoted, Howard et al. 1991); aqueous anaerobic $t_{1/2}$ = 1008–8640 h, based on aerobic soil die-away test data (Anderson & Domsch 1976; Smith 1970; quoted, Howard et al. 1991)
$t_{1/2}$(aerobic) = 11 d, $t_{1/2}$(anaerobic) = 42 d in natural waters (Capel & Larson 1995)
Biotransformation:
Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants:

Half-Lives in the Environment:
Air: $t_{1/2}$ = 0.58–5.8 h, based on an estimated rate constant for the vapor-phase reaction with hydroxyl radicals in air (Atkinson 1987; quoted, Howard et al. 1991).
Surface water: $t_{1/2}$ = 252–2160 h, based on aerobic soil die-away test data (Anderson & Domsch 1976; Smith 1970; quoted, Howard et al. 1991)
Biodegradation $t_{1/2}$(aerobic) = 11 d, $t_{1/2}$(anaerobic) = 42 d, hydrolysis $t_{1/2}$ = 2400 d at pH 2, $t_{1/2}$ = 2500 d at pH 7 and $t_{1/2}$ = 32 d at pH 12 in natural waters (Capel & Larson 1995)

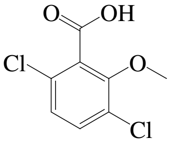
Ground water: $t_{1/2}$ = 504–4320 h, based on aerobic soil die-away test data (Anderson & Domsch 1976; Smith 1970; quoted, Howard et al. 1991).

Sediment:

Soil: $t_{1/2}$ = 252–2160 h, based on aerobic soil die-away test data (Anderson & Domsch 1976; Smith 1970; quoted, Howard et al. 1991; Montgomery 1993);
$t_{1/2}$ = 30 d (Hartley & Kidd 1987; quoted, Montgomery 1993);
selected field $t_{1/2}$ = 30 d (Augustijn-Beckers et al. 1994; Hornsby et al. 1996).

Biota:

17.1.1.25 Dicamba



Common Name: Dicamba
Synonym: Banex, Banvel, Banvel D, Brush buster, Dianat, MDBA, Mediben
Chemical Name: 3,6-dichloro-2-methoxybenzoic acid; 3,6-dichloro-*o*-anisic acid
Uses: systemic pre-emergent and post-emergent herbicide to control both annual and perennial broadleaf weeds.
CAS Registry No: 1918-00-9
Molecular Formula: $C_8H_6Cl_2O_3$
Molecular Weight: 221.038
Melting Point (°C):

115	(Lide 2003)

Boiling Point (°C):
Density (g/cm^3 at 20°C):

1.570	(25°C, Hartley & Kid 1987; Worthing & Hance 1991; Montgomery 1993; Tomlin 1994; Milne 1995)

Molar Volume (cm^3/mol):

207.9	(calculated-Le Bas method at normal boiling point)

Dissociation Constant pK_a:

1.94	(Kearney & Kaufman 1975; Spencer 1982; Lee et al. 1993)
1.90	(Cessna & Grover 1978; Weber et al. 1980; Willis & McDowell 1982; Howard 1991; Montgomery 1993; Armbrust 2000)
1.95	(Worthing & Hance 1991; Montgomery 1993; Caux et al. 1993)
1.87	(Tomlin 1994)
1.91	(Hornsby et al. 1996)

Enthalpy of Vaporization, ΔH_V (kJ/mol):

77.85	(Rordorf 1989)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

22.59	(DSC method, Plato & Glasgow 1969)
19.1	(Rordorf 1989)

Entropy of Fusion, ΔS_{fus} (J/mol K):
Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F: 0.131 (mp at 115°C)

Water Solubility (g/m^3 or mg/L at 25°C or as indicated):

7900	(Freed 1966; Verschueren 1983)
4500	(Martin & Worthing 1977; quoted, Kenaga 1980; Kenaga & Goring 1980; Khan 1980; Ashton & Crafts 1981; Weber et al. 1980; Hartley & Graham-Bryce 1980)
6500	(Hartley & Kidd 1987; Herbicide Handbook 1989; Caux et al. 1993)
6500	(Worthing & Walker 1987, Worthing & Hance 1991; Montgomery 1993; Tomlin 1994; Milne 1995)
5600	(20°C, selected, Suntio et al. 1988)
4410, 221	(quoted, calculated-group contribution fragmentation method, Kühne et al. 1995)
8310	(selected., Armbrust 2000)

Vapor Pressure (Pa at 25°C or as indicated and reported temperature dependence equations):

0.00454	(Ashton & Crafts 1973; 1981)
0.00267	(Baur & Bovey 1974; Spencer 1976)
0.49	(20°C, Hartley & Graham-Bryce 1980; Khan 1980)
< 0.00013	(20–25°C, Weber et al. 1980; Willis & McDowell 1982)
0.00453	(Herbicide Handbook 1983, 1989; Worthing & Hance 1991)
0.0045	(Hartley & Kidd 1987; Tomlin 1994)
0.50	(100°C, Budavari 1989)

2.90×10^{-3}, 6.40×10^{-2}, 0.88, 8.60, 63.0 (25, 50, 70, 100, 125°C, gas saturation-GC, Rordorf 1989)

log (P_S/Pa) = 14.706 – 5139.1/(T/K); measured range 60.1–110°C (solid, gas saturation-GC, Rordorf 1989)
log (P_L/Pa) = 11.911 – 4067.0/(T/K); measured range 115–176°C (liquid, gas saturation-GC, Rordorf 1989)

0.50	(20°C, selected, Taylor & Spencer 1990)
0.0045	(20°C, Montgomery 1993)

Henry's Law Constant (Pa·m³/mol at 25°C or as indicated):

0.00012	(20°C, calculated-P/C, Suntio et al. 1988)
0.0248	(calculated-P/C, Taylor & Glotfelty 1988)
0.0918	(Suntio et al. 1988; quoted, Howard 1991; Majewski & Capel 1995)
2.2×10^{-5}	(calculated-P/C, Nash 1989)
1.22×10^{-4}	(20–25°C, calculated-P/C, Montgomery 1993)
0.00012, 0.000154	(20, 25°C, quoted, Caux et al. 1993)
4.46×10^{-5}	(quoted lit., Armbrust 2000)

Octanol/Water Partition Coefficient, log K_{OW}:

0.477	(Rao & Davidson 1980)
2.41	(selected, Dao et al. 1983)
2.21	(shake flask, Log P Database, Hansch & Leo 1985, 1987)
–1.69	(selected, Gerstl & Helling 1987)
3.01	(selected, Travis & Arms 1988)
2.46	(Reinert 1989)
2.49	(shake flask-HPLC/UV, Jafvert et al. 1990)
2.46	(EPA Environmental Fate one-liner database Version 3.04, Lee et al. 1993)
2.21	(recommended, Sangster 1993)
0.48	(Montgomery 1993)
–0.80	(pH 7, Tomlin 1994)
2.21	(recommended, Hansch et al. 1995)

Bioconcentration Factor, log BCF:

0.699	(calculated-S, Kenaga 1980)
–2.00	(calculated-K_{OC}, Kenaga 1980)
–4.58	(beef biotransfer factor logB_b, correlated-K_{OW}, Oehler & Ivie 1980)
–4.60	(milk biotransfer factor logB_m, correlated-K_{OW}, Oehler & Ivie 1980)
1.450	(estimated-K_{OW} per Hansch & Leo 1985, Lyman et al. 1982)
0.903	(estimated-S per Suntio et al. 1988, Lyman et al. 1982)

Sorption Partition Coefficient, log K_{OC}:

–0.398	(soil, quoted exptl., Kenaga 1980)
1.63	(soil, calculated-S as per Kenaga & Goring 1980, Kenaga 1980)
0.342	(av. soils/sediments, Rao & Davidson 1980)
–0.40, 2.08	(quoted, calculated-MCI χ, Gerstl & Helling 1987)
0.34	(soil, screening model calculations, Jury et al. 1987b)
2.67	(K_{OC} = 470 reported, Reinert 1989)
0.643	(soil, estimated, Shirmohammadi et al. 1989)
–1.00	(selected, USDA 1989; quoted, Neary et al. 1993)
0.30	(organic carbon, Wauchope et al. 1991)
–0.40, 1.62, 0.18, 0.34	(soil, quoted values, Bottoni & Funari 1992)
1.50; 1.46	(soil, quoted exptl.; calculated-MCI χ and fragment contribution Meylan et al. 1992)
–0.40, 0.34	(Montgomery 1993)
0.30	(Tomlin 1994)
1.50	(quoted or calculated-QSAR MCI $^1\chi$, Sabljic et al. 1995)
1.114	(quoted lit., Armbrust 2000)

Sorption Partition Coefficient, log K_{OM}:

2.74	(organo-clay DODMA140-SAz, sorption isotherm, Zhao et al. 1996)

2.57	(organo-clay DODMA-SAz, sorption isotherm-HPLC/UV, Zhao et al. 1996)
2.48	(organo-clay HDTMA-SAz, sorption isotherm-HPLC/UV, Zhao et al. 1996)
2.59	(organo-clay HDTMA-SWy, sorption isotherm-HPLC/UV, Zhao et al. 1996)

Environmental Fate Rate Constants, k, or Half-Lives, $t_{½}$:

Volatilization:

Photolysis: aqueous photolysis rate constant $k = 7.5 \times 10^{-4}\ h^{-1}$ (Armbrust 2000).

Oxidation: photooxidation $t_{½}$ = 2.4–6.0 d, based on estimated rate constant for the vapor-phase reaction with hydroxyl radicals in the atmosphere (Atkinson 1985; quoted, Howard 1991);
measured hydroxy radical reaction rate constant for dicamba $4.8 \times 10^{12}\ M^{-1}$ /h (Armbrust 2000).

Hydrolysis: $t_{½}$ > 133 d for 2 μg mL^{-1} to hydrolyze in dark sterile pond water at 37–39°C (Scifres et al. 1973; quoted, Muir 1991);
stable aqueous hydrolysis rates at pH 5, 7, 9 (Armbrust 2000).

Biodegradation: $t_{½}$ = 60 d to > 160 d for 100 μg mL^{-1} to degrade in pond sediment/water under lighted conditions at 20–30°C (Scifres et al. 1973; quoted, Muir 1991); under lab. conditions using nonsterile sandy loam, silty clay, or heavy clay soil, 50% of applied dicamba degraded within 2 weeks; however in sterilized (via heating) soil, over 90% of applied dicamba was recovered after 4 weeks, suggesting that microbes were responsible for the decomposition (Smith 1973; quoted, Howard 1991);
$t_{½}$ > 25 d for 5.85 mg of labeled dicamba to plants to degrade following washoff from plants and sands in model ecosystem (derived from data of Yu et al. 1975; Muir 1991);
$k = 0.022\ d^{-1}$ by soil incubation die-away studies (Rao & Davidson 1980; quoted, Scow 1982);
rate of biodegradation in soil generally increases with temperature and soil moisture (up to 50%) and tends to be faster when the soil is slightly acidic (Herbicide Handbook 1983; quoted, Howard 1991);
aerobic rate constant $k = 1.60 \times 10^{-3}\ h^{-1}$ (Armbrust 2000).

Biotransformation:

Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants:

Half-Lives in the Environment:

Air: $t_{½}$ ~ 2.42 d for reaction with hydroxyl radicals (estimated, Eisenreich et al. 1981; quoted, Caux et al. 1993
$t_{½}$ = 2.42–6.0 d, based on estimated rate constant for the vapor-phase reaction with hydroxyl radicals in the atmosphere (Atkinson 1985; quoted, Howard 1991).

Surface water:

Ground water: $t_{½}$ = 23.5 d determined under batch conditions at 28°C, $t_{½}$ = 38 d at 20°C, and $t_{½}$ = 151 d at 12°C and were all higher than $t_{½}$ ~ 13.5 d from the decrease in column effluent concentrations over time (Comfort et al. 1992);
reported $t_{½}$ = 14–433, 201 and 25 d (Bottoni & Funari 1992)
$t_{½}$ < 7 d in surface water (Caux et al. 1993).

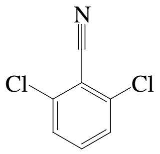
Sediment:

Soil: estimated persistence of 2 months (Kearney et al. 1969; quoted, Jury et al. 1987a);
$t_{½}$ = 59, 19, and 17 d with disappearance rates: k = 0.0117, 0.036 and 0.041 d^{-1} at pH 4.3, 5.3 and 6.5 (Hamaker 1972; quoted, Nash 1988);
persistence of 2 months in soil (Edwards 1973; quoted, Morrill et al. 1982);
degradation $t_{½}$ = 32 d and 17 d in Quachita Highlands = forest and grassland soil respectively, $t_{½}$ = 26 d in Gross Timbers Forest soil, average $t_{½}$ = 25 d in 3 soils (Altom & Stritzke 1973);
first-order $t_{½}$ ~ 31.5 d in soil from biodegradation rate constant $k = 0.022\ d^{-1}$ by soil incubation die-away studies (Rao & Davidson 1980; quoted, Scow 1982);
nonpersistent in soils with $t_{½}$ < 20 d (Willis & McDowell 1982);
mean $t_{½}$ = 14 d under lab. conditions from review of persistence literature, while the mean $t_{½}$ = 8 d under field conditions (Rao & Davidson 1982; quoted, Howard 1991);
non-persistent with $t_{½}$ < 20 d in soil (Willis & McDowell 1982);
$t_{½}$ = 14 d from screening model calculations (Jury et al. 1987b);
$t_{½}$ < 14 d under conditions amenable to rapid metabolism (Herbicide Handbook 1989);
selected $t_{½}$ = 14 d (Wauchope et al. 1991; quoted, Dowd et al. 1993);
$t_{½}$ < 14–25 d (Worthing & Hance 1991; quoted, Montgomery 1993);

reported $t_{½}$ = 20 d, 25 d and 14–433 d (Bottoni & Funari 1992);
$t_{½}$ = 4–555 d with a mean $t_{½}$ = 24 d (Caux et al. 1993);
$t_{½}$ < 14 d (Tomlin 1994).

Biota: biochemical $t_{½}$ = 14 d from screening model calculations (Jury et al. 1987b);
average $t_{½}$ = 25 d in the forest (USDA 1989; quoted, Neary et al. 1993);
biological $t_{½}$ = 0.64 h (Caux et al. 1993).

17.1.1.26 Dichlobenil



Common Name: Dichlobenil
Synonym: Barrier 2G, Barrier 50W, Casoron, DBN, DCB, Decabane, Du-Sprex, Dyclomec, NIA 5996, Niagara 5006, Niagara 5996, Norosac
Chemical Name: 2,6-dichlorobenzonitrile
Uses: soil applied herbicide to control many annual and perennial broadleaf weeds.
CAS Registry No: 1194-65-6
Molecular Formula: $C_7H_3Cl_2N$
Molecular Weight: 172.012
Melting Point (°C):
144.5 (Lide 2003)
Boiling Point (°C):
270 (Verloop 1972; Khan 1980; Worthing & Hance 1991; Tomlin 1994; Milne 1995)
Density (g/cm^3 at 20°C):
> 1.0 (Milne 1995)
Molar Volume (cm^3/mol):
148.9 (calculated-Le Bas method at normal boiling point)
Dissociation Constant pK_a:
Enthalpy of Vaporization, ΔH_V (kJ/mol):
65.74 (Rordorf 1989)
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
25.94 (DSC method, Plato & Glasgow 1969)
34.33 (Verloop 1972)
24.2 (Rordorf 1989)
Entropy of Fusion, ΔS_{fus} (J/mol K):
Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F: 0.0672 (mp at 144.5°C)

Water Solubility (g/m^3 or mg/L at 25°C or as indicated):
18 (20°C, Günther et al. 1968; Weber 1972; Verloop 1972; Spencer 1982; Verschueren 1983)
25 (Günther et al. 1968; Montgomery 1993)
18 (Martin & Worthing 1977; Herbicide Handbook 1978)
18 (Wauchope 1978; Khan 1980; Burkhard & Guth 1981)
18 (20°C, Ashton & Crafts 1981; Hartley & Kidd 1987; Herbicide Handbook 1989)
18 (20°C, Worthing & Walker 1987, Worthing & Hance 1991; Tomlin 1994)
21.2 (20–25°C, selected, Wauchope et al. 1992; Lohninger 1994; Hornsby et al. 1996)
18, 25 (20°C, 25°C, Milne 1995)

Vapor Pressure (Pa at 25°C or as indicated and reported temperature dependence equations):
0.072 (20°C, effusion manometer technique, Barnsley & Rosher 1961)
0.0733 (20°C, Verloop 1972; Khan 1980; Ashton & Crafts 1981; Herbicide Handbook 1989)
0.0667 (20°C, Weber 1972; Worthing & Walker 1987)
0.0004 (20°C, Spencer 1976)
0.0666 (20°C, effusion method, Spencer 1976)
0.0733 (20–25°C, Weber et al. 1980)
0.073 (20°C, Hartley & Kidd 1987)
0.070 (20°C, selected, Suntio et al. 1988)
0.110, 1.80, 20.0, 160, 970 (25, 50, 70, 100, 125°C, gas saturation-GC, Rordorf 1989)
$\log (P_S/Pa) = 14.787 - 4698.2/(T/K)$; measured range 32.4–125°C (solid, gas saturation-GC, Rordorf 1989)

log (P_L/Pa) = 11.754 – 3434.1/(T/K); measured range 32.4–125°C (liquid, gas saturation-GC, Rordorf 1989)

0.133	(20–25°C, selected, Wauchope et al. 1992; Hornsby et al. 1996)
0.0733	(Montgomery 1993)
0.088	(20°C, gas saturation, Tomlin 1994)

Henry's Law Constant (Pa·m^3/mol at 25°C or as indicated):

0.700	(20°C, volatilization rate, Burkhard & Guth 1981)
0.669	(20°C, calculated-P/C, Suntio et al. 1988)
0.637	(20°C, calculated-P/C, Muir 1991)
0.669	(20–25°C, calculated-P/C, Montgomery 1993)

Octanol/Water Partition Coefficient, log K_{OW}:

2.90	(Rao & Davidson 1980; selected, Suntio et al. 1988, Magee 1991)
2.57; 2.65	(RP-HPLC-RT correlation; shake flask, Eadsforth & Moser 1983)
3.06	(shake flask, Geyer et al. 1984)
2.94	(Hansch & Leo 1985)
1.63	(Reinert 1989)
2.98	(selected, Dao et al. 1983, Gerstl & Helling 1987)
2.90	(shake flask, Log P Database, Hansch & Leo 1987)
2.90	(recommended, Sangster 1993)
2.70	(Tomlin 1994)
2.74	(recommended, Hansch et al. 1995)
2.95	(RP-HPLC-RT correlation, Nakamura et al. 2001)
2.98	(RP-HPLC-RT correlation using short ODP column, Donovan & Pescatore 2002)

Bioconcentration Factor, log BCF:

1.74	(fish in static water, Kenaga 1975; Kenaga & Goring 1980)
2.08	(calculated-S, Kenaga 1980; quoted, Isensee 1991)
1.08	(calculated-K_{OC}, Kenaga 1980)
1.18–1.60	(fish, Freitag et al. 1982)
1.30	(algae, Freitag et al. 1982)
1.72	(estimated-S, Lyman et al. 1982; quoted, Howard 1991)
2.03–2.32	(Montgomery 1993)

Sorption Partition Coefficient, log K_{OC} at 25°C or as indicated:

2.91	(potting soil with 22% organic content, Massini 1961)
2.08	(sandy loam with 5% organic content, Massini 1961)
2.37	(soil, Hamaker & Thompson 1972–1987)
2.95	(soil, calculated-S as per Kenaga & Goring 1980, Kenaga 1980)
2.35	(Rao & Davidson 1980)
2.94	(soil, estimated-S, Lyman et al. 1982; quoted, Howard 1991)
2.37, 1.45	(quoted, calculated-MCI χ, Gerstl & Helling 1987)
2.96	(Reinert 1989)
2.37; 2.31	(reported as log K_{OM}; estimated as log K_{OM}, Magee 1991)
2.21, 2.57–2.96	(soil, quoted values, Bottoni & Funari 1992)
2.60	(soil, 20–25°C, estimated, Wauchope et al. 1992; Hornsby et al. 1996)
2.60	(estimated-chemical structure, Lohninger 1994)
2.31	(soil, calculated-MCI $^1\chi$, Sabljic et al. 1995)

Environmental Fate Rate Constants, k, or Half-Lives, $t_{½}$:

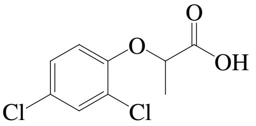
Volatilization: $t_{½}$ ~ 7.4 d, based on Henry's law constant for a model river 1-m deep with a wind velocity of 3 m/s and flowing at 1 m/s (estimated, Lyman et al. 1982; quoted, Howard 1991);
$t_{½}$ ~ 11 d from 1 m depth of water at 20°C (estimated, Muir 1991).

Photolysis: photolytic $t_{½}$ = 15 d in water (Tomlin 1994).

Oxidation: photooxidation $t_{1/2}$ = 92 d in air, based on estimation for the vapor-phase reaction with hydroxyl radicals in atmosphere (Atkinson 1987; quoted, Howard 1991).
Hydrolysis:
Biodegradation: $t_{1/2}$ ~ 7 d for 5 μg/mL to biodegrade in sediment suspension at 30°C (Miyazaki et al. 1975; quoted, Muir 1991).
Biotransformation:
Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants:

Half-Lives in the Environment:
Air: $t_{1/2}$ = 92 d, based on estimation for the vapor-phase reaction with hydroxyl radicals in atmosphere (Atkinson 1987; quoted, Howard 1991).
Surface water:
Ground water: reported $t_{1/2}$ = 44–360 d (Bottoni & Funari 1992)
Sediment: $t_{1/2}$ ~ 7 d for 5 μg/mL to biodegrade in sediment suspension at 30°C (Miyazaki et al. 1975; quoted, Muir 1991).
Soil: estimated persistence of 4 months (Kearney et al. 1969; quoted, Jury et al. 1987);
$t_{1/2}$ = 1–6 months in soil depending on soil type (Beynon & Wright 1972; Verloop 1972; quoted, Tomlin 1994);
persistence of 4 months in soil (Edwards 1973; quoted, Morrill et al. 1982);
persistence of 4 months (Wauchope 1978);
$t_{1/2}$ = 1.5 to 12 months depending upon soil type (Herbicide Handbook 1989);
selected $t_{1/2}$ = 60 d (Wauchope et al. 1992; Hornsby et al. 1996);
reported $t_{1/2}$ = 45–360 d (Bottoni & Funari 1992).
Biota:

17.1.1.27 Dichlorprop



Common Name: Dichlorprop
Synonym: Cornox RK, dichloroprop, Dikofag DP, 2,4-DP, Hedonal DP, Polymone
Chemical Name: (±)-2-(2,4-dichlorophenoxy) propanoic acid; (±)-2-(2,4-dichlorophenoxy) propionic acid
Uses: herbicide and growth regulator to control annual broadleaf and grass weeds; also to control aquatic weeds and chemical maintenance of embankments and roadside verges.
CAS Registry No: 120-36-5
Molecular Formula: $C_9H_8Cl_2O_3$
Molecular Weight: 235.064
Melting Point (°C):

117.5	(Lide 2003)

Boiling Point (°C):
Density (g/cm^3 at 20°C):

1.64	(25°C, Bailey & White 1965)
1.42	(Herbicide Handbook 1989; Tomlin 1994)

Molar Volume (cm^3/mol):

232.0	(calculated-Le Bas method at normal boiling point)
165.6	(calculated-density)

Dissociation Constant pK_a:

2.855	(Cessna & Grover 1978)
2.86	(Wauchope et al. 1992; Hornsby et al. 1996)
3.00	(Tomlin 1994)

Enthalpy of Vaporization, ΔH_V (kJ/mol):

127.9	(Rordorf 1989)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

34.31	(DSC method, Plato 1972)
30.9	(Rordorf 1989)

Entropy of Fusion, ΔS_{fus} (J/mol K):

Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F: 0.124 (mp at 117.5°C)

Water Solubility (g/m^3 or mg/L at 25°C or as indicated):

350	(20°C, Woodford & Evans 1963; Spencer 1973)
350	(Martin & Worthing 1977)
350	(20°C, Hartley & Kidd 1987; Worthing & Walker 1987, 1991)
710	(28°C, Herbicide Handbook 1989)
50	(ester, 20–25°C, estimated, Wauchope et al. 1992; Lohninger 1994; Hornsby et al. 1996)

Vapor Pressure (Pa at 25°C or as indicated and reported temperature dependence equations):

4.50×10^{-4} (20°C, Hartley & Kidd 1987)
2.90×10^{-7}, 4.10×10^{-5}, 2.8×10^{-3}, 0.11, 2.80 (25, 50, 70, 100, 125°C, gas saturation-GC, Rordorf 1989)
$\log (P_S/Pa) = 21.26 - 8289.2/(T/K)$; measured range 95.7–118°C (solid, gas saturation-GC, Rordorf 1989)
$\log (P_L/Pa) = 17.174 - 6682.8/(T/K)$; measured range 120–150°C (liquid, gas saturation-GC, Rordorf 1989)
4.00×10^{-4} (20–25°C, estimated, Wauchope et al. 1992; Hornsby et al. 1996)
$< 1.0 \times 10^{-5}$ (20°C, Tomlin 1994)

Henry's Law Constant (Pa·m^3/mol at 25°C):

2.69×10^{-4} (calculated-P/C, this work)

Octanol/Water Partition Coefficient, log K_{OW}:

2.75 (RP-HPLC-k′ correlation, Braumann et al. 1983)
3.43 (shake flask-GC, Ilchmann et al. 1993)
2.06 to –0.22 (pH 4–7, shake flask-LSC, Riise & Salbu 1992)
1.77 (Tomlin 1994)
3.43 (recommended, Sangster 1993; Hansch et al. 1995)

Bioconcentration Factor, log BCF:

1.36 (calculated-S, Kenaga 1980)

Sorption Partition Coefficient, log K_{OC}:

2.23 (soil, calculated-S, Kenaga 1980)
3.00 (soil, 20–25°C, estimated, Wauchope et al. 1992; Lohninger 1994; Hornsby et al. 1996)
2.05, 2.07, 1.70, 1.79, 1.73 (5 soils: soil A 30.4% OC and pH 4.4, soil B14.6% OC pH 4.1, soil C/loam 3.3% OC pH 5.0, soil D/silty clay 1.3% OC pH 5.1, soil E/sand 1.4% OC pH 5.3, batch equilibrium-sorption isotherms, Riise Salbu 1992)
1.08–1.60 (Tomlin 1994)

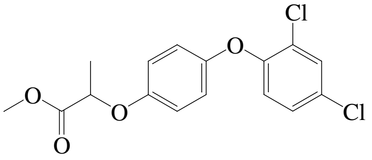
Environmental Fate Rate Constants, k, or Half-Lives, $t_{½}$:

Photolysis: photodegradation $t_{½}$ = 10 to 19 d on 3 Spanish natural dry soils; $t_{½}$ = 22 to 59 d on 10% peat-amened dry soils; degradation $t_{½}$ ~ 2–6 d on moist soils at field capacity and saturation soils for degradation at 0,1 and 2 exposures days; and $t_{½}$ = 16–37 d on moist soils at field capacity and saturated soils for degradation at 2,4 and 10 exposure days (Romero et al. 1998)

Half-Lives in the Environment:

Soil: $t_{½}$ = 12 d and 8 d in Quachita Highlands = forest and grassland soil, respectively, $t_{½}$ = 10 d in gross timbers forest soil, average $t_{½}$ = 10 d in 3 soils (Altom & Stritzke 1973);
selected field $t_{½}$ = 10 d (Wauchope et al. 1992; Hornsby et al. 1996);
$t_{½}$ ~ 8 d in soil (Tomlin 1994)
photodegradation $t_{½}$ = 10–19 d in 3 Spanish natural dry soils, $t_{½}$ = 22–59 d in the 10% peat-amended dry soils; degradation $t_{½}$ ~ 2–6 d on moist soils at field capacity and saturation soils for degradation at 0,1 and 2 exposures days; and $t_{½}$ = 16–37 d on moist soils at field capacity and saturated soils for degradation at 2,4 and 10 exposure days (Romero et al. 1998)

17.1.1.28 Diclofop-methyl



Common Name: Diclofop-methyl
Synonym: Hoelon, dichlordiphenoprop, Hoegrass, Illoxan
Chemical Name: methyl 2-[4-(2′,4′-dichlorophenoxy)-phenoxy]propanoate
Uses: herbicide to control post-emergent wild oats, wild millets, and other annual grass weeds in wheat, barley, rye, red fescue, and broadleaf weeds in crops such as soybeans, sugar cane, fodder beet, flax, legumes, oilseed rape, sunflowers, clover, lucerne, groundnuts, brassicas, carrots, celery, beet root, parsnips, lettuce, spinach, potatoes, tomatoes, fennel, alliums, herbs, etc.
CAS Registry No: 51338-27-3
Molecular Formula: $C_{16}H_{14}Cl_2O_4$
Molecular Weight: 341.186
Melting Point (°C):
 40 (Lide 2003)
Boiling Point (°C):
 175–176 (at 0.1 mmHg, Hartley & Kidd 1987; Herbicide Handbook 1989)
Density (g/cm^3):
 1.30 (40°C, Hartley & Kidd 1987; Worthing & Walker 1987; Herbicide Handbook 1989)
 1.035 (Herbicide Handbook 1989)
Acid Dissociation Constants, pK_a:
 3.1 (Wauchope et al. 1992; Hornsby et al. 1996)
Molar Volume (cm^3/mol):
 349.6 (calculated-Le Bas method at normal boiling point)
 329.7 (calculated-density)
Dissociation Constant pK_a:
 3.1 (Wauchope et al. 1992; Hornsby et al. 1996)
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
Entropy of Fusion, ΔS_{fus} (J/mol K):
Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F: 0.713 (mp at 40°C)

Water Solubility (g/m^3 or mg/L at 25°C or as indicated):
 3.0 (22°C, Hartley & Kidd 1987; Worthing & Walker 1987; Worthing & Hance 1991)
 3.0 (22°C, Herbicide Handbook 1989)
 0.80 (20–25°C, selected, Wauchope et al. 1992; Hornsby et al. 1996)
 0.80 (20°C, pH 7, Tomlin 1994)
 4.23 (Majewski & Capel 1995)
 4.06 (calculated-group contribution method, Kühne et al. 1995)
 3.0 (Lohninger 1994; Milne 1995)
 0.8 (selected, Halfon et al. 1996)

Vapor Pressure (Pa at 25°C or as indicated):
 3.44×10^{-5} (20°C, Worthing 1983, 1987; Hartley & Kidd 1987)
 3.40×10^{-5} (20°C, Worthing & Walker 1987, Worthing & Hance 1991)
 3.47×10^{-5}, 1.6×10^{-4}, 3.87×10^{-3} (20°C, 30°C, 54.3°C, Herbicide Handbook 1989)
 5.91×10^{-5} (selected, Wauchope et al. 1992; Hornsby et al. 1996)
 2.5×10^{-4}, 7.7×10^{-3} (20°C, 50°C, Tomlin 1994)
 4.80×10^{-5} (quoted, Majewski & Capel 1987)
 4.7×10^{-4} (selected, Halfon et al. 1996)

Henry's Law Constant (Pa·m^3/mol at 25°C):

0.00387	(calculated-P/C, Majewski & Capel 1995)
0.199	(calculated-P/C, this work)

Octanol/Water Partition Coefficient, log K_{OW}:

4.80	(shake flask, Log P Database, Hansch & Leo 1987)
4.601	(Stevens et al. 1988)
4.58	(Worthing & Hance 1991)
4.60	(shake flask, pH 7, Baker et al. 1992)
4.80	(recommended, Sangster 1993)
4.5775	(Tomlin 1994)
4.80	(recommended, Hansch et al. 1995)
5.52	(Pomona-database, Müller & Kördel 1996)
4.87	(RP-HPLC-RT correlation using short ODP column, Donovan & Pescatore 2002)

Bioconcentration Factor, log BCF or log K_B:

2.74	(calculated-S as per Kenaga 1980, this work)

Sorption Partition Coefficient, log K_{OC}:

4.69, 4.20	(Wauchope et al. 1992)
4.15–4.39	(soil, quoted values, Bottoni & Funari 1992)
4.20	(20–25°C, soil, recommended, Wauchope et al. 1992; Hornsby et al. 1996)
4.25	(soil, HPLC-screening method, mean value of different stationary and mobile phases, Kördel et al. 1993, 1995b)
4.15–4.39	(soil, Tomlin 1994)
4.20	(estimated-chemical structure, Lohninger 1994)
4.25; 3.61	(HPLC-screening method; calculated-PCKOC fragment method, Müller & Kördel 1996)

5.505, 5.334, 4.122, 4.737, 4.182 (first generation Eurosoils ES-1, ES-2, ES-3, ES-4, ES-5, shake flask/batch equilibrium-HPLC/UV, Gawlik et al. 1998)

4.002, 3.731, 3.453, 3.257, 3.715 (second generation Eurosoils ES-1, ES-2, ES-3, ES-4, ES-5, shake flask-batch equilibrium-HPLC/UV and HPLC-k′ correlation, Gawlik et al. 2000)

Environmental Fate Rate Constants, k, or Half-Lives, $t_{½}$:

Volatilization:

Photolysis:

Oxidation:

Hydrolysis:

Biodegradation: first-order rate constants k = –0.0883, –0.225, –0.266 h^{-1} in nonsterile sediment and k = –0.0158, –0.0139, –0.0134 h^{-1} in sterile sediment by shake-tests at Davis Bayou, k = –0.0457, –0.103, –0.120 h^{-1} in nonsterile water and k = –0.00233, –0.00722, –0.00785 h^{-1} in sterile water by shake-tests at Davis Bayou (Walker et al. 1988)

$t_{½}$ = 10 d in sandy soils and $t_{½}$ ~ 30 d in sandy clay soils under aerobic conditions (Herbicide Handbook 1989)

Biotransformation:

Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants:

Half-Lives in the Environment:

Air:

Surface water: $t_{½}$ = 363 d at 25°C and pH 5, $t_{½}$ = 31.7 d at pH 7 and $t_{½}$ = 0.52 d at pH 9 (Tomlin 1994).

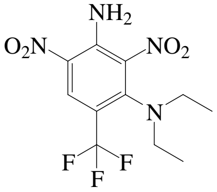
Ground water: reported $t_{½}$ = 6–9, 23–38 and 150 d (Bottoni & Funari 1992)

Sediment:

Soil: $t_{½}$ = 10 d in sandy soils and $t_{½}$ ~ 30 d in sandy clay soils while under anaerobic conditions, results were similar except that the very rapid cleavage of the ester bond by hydrolysis within one hour to propionic acid derivatives was experienced and within 2 d, up to 86% of the parent compound was metabolized into various free acid metabolites and up to 3.7% of phenol metabolites (Herbicide Handbook 1989);

$t_{½}$ = 6–9 d, 23–38 d and 150 d (Bottoni & Funari 1992);
selected field $t_{½}$ = 30 d at pH 7.0 (Wauchope et al. 1992; Hornsby et al. 1996)
V = 1–57 d and $t_{½}$ = 30–281 d for various soils in field trials (Tomlin 1994).
$t_{½}$ = 30 d (selected, Halfon et al. 1996).
Biota: $t_{½}$ = 3–7 d for wheat (Herbicide Handbook 1989)
$t_{½}$ = 3 d in sugar beet (Tomlin 1994).

17.1.1.29 Dinitramine



Common Name: Dinitramine
Synonym: Cobex, Cobexo
Chemical Name: *N,N*-diethyl-2,6-dinitro-4-trifluoromethyl-*m*-phenylenediamine
Uses: herbicide for selective pre-plant soil incorporating control of many annual grass and broadleaf weeds in cotton, soybeans, peas, groundnuts, beans, sunflowers, safflowers, carrots, turnips, fennel, chicory, etc. and in transplanted tomatoes, capsicums, aubergines, and brassicas.
CAS Registry No: 29091-05-2
Molecular Formula: $C_{11}H_{13}N_4O_4F_3$
Molecular Weight: 322.241
Melting Point (°C):
98 (Lide 2003)
Boiling Point (°C):
Density (g/cm^3 at 20°C):
1.50 (25°C, Ashton & Crafts 1981; Hartley & Kidd 1987)
Molar Volume (cm^3/mol):
265.7 (calculated-Le Bas method at normal boiling point)
Dissociation Constant pK_a:
4.5 (Haag & Yao 1992)
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
Entropy of Fusion, ΔS_{fus} (J/mol K):
Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F: 0.192 (mp at 98°C)

Water Solubility (g/m^3 or mg/L at 25°C or as indicated):
1.1 (Martin & Worthing 1977; Kenaga 1980; Kenaga & Goring 1980; Khan 1980; Isensee 1991)
1.0 (Wauchope 1978; Verschueren 1983)
1.0 (20°C, Ashton & Crafts 1981; Hartley & Kidd 1987)
1.1 (Worthing & Walker 1987, 1991)
1.1 (20–25°C, selected, Augustijn-Beckers et al. 1994; Hornsby et al. 1996)
1.0 (20°C, Tomlin 1994; Milne 1995)

Vapor Pressure (Pa at 25°C or as indicated):
0.00048 (Khan 1980; Ashton & Crafts 1981)
0.00048 (Verschueren 1983)
0.000479 (Hartley & Kidd 1987; Worthing & Hance 1991; Tomlin 1994)
0.00040 (20°C, selected, Suntio et al. 1988)
0.00048 (20–25°C, selected, Augustijn-Beckers et al. 1994; Hornsby et al. 1996)

Henry's Law Constant (Pa·m^3/mol at 25°C or as indicated):
0.160 (20°C, calculated-P/C, Suntio et al. 1988)

Octanol/Water Partition Coefficient, log K_{OW}:
4.31 (selected, Dao et al. 1983)
4.30 (Worthing & Hance 1991; Tomlin 1994)
4.30 (Milne 1995)
4.30 (recommended, Hansch et al. 1995)
3.89 (LOGPSTAR or CLOGP data, Sabljic et al. 1995)

Bioconcentration Factor, log BCF:

2.77	(calculated-S, Kenaga 1980; quoted, Isensee 1991)
2.45	(calculated-K_{OC}, Kenaga 1980)

Sorption Partition Coefficient, log K_{OC}:

3.60	(soil, Harvey 1974)
3.61	(soil, calculated-S as per Kenaga & Goring 1980, Kenaga 1980)
3.60	(20–25°C, estimated, Augustijn-Beckers et al. 1994; Hornsby et al. 1996)
3.84	(estimated-chemical structure, Lohninger 1994)
3.63	(soil, calculated-MCI $^1\chi$, Sabljic et al. 1995)
3.63; 3.42	(soil, quoted exptl.; estimated-general model using molecular descriptors, Gramatica et al. 2000)

Environmental Fate Rate Constants, k, or Half-Lives, $t_{½}$:

Volatilization:

Photolysis: $t_{½} < 1$ h in distilled water, river water and ocean water under sunlight (Newsom & Woods 1973; quoted, Cessna & Muir 1991).

Oxidation:

Hydrolysis:

Biodegradation: $t_{½}$ = 22 d for 0.5 μg/mL to biodegrade in flooded soil with approximately 1 cm of water on top of the soil (Savage 1978; quoted, Muir 1991).

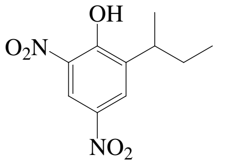
Biotransformation:

Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants:

Half-Lives in the Environment:

Soil: $t_{½}$ = 22 d for 0.5 μg/mL to biodegrade in flooded soil with approximately 1 cm of water on top of the soil (Savage 1978; quoted, Muir 1991);
persistence of 3 months in soil (Wauchope 1978);
selected field $t_{½}$ = 30 d (Augustijn-Beckers et al. 1994; Hornsby et al. 1996);
$t_{½}$ = 10–66 d (Tomlin 1994).

17.1.1.30 Dinoseb



Common Name: Dinoseb

Synonym: Anatox, Aretit, Basanite, Butaphene, Caldon, Chemox, Dibutox, Dinitrall, DNBP, DN-289, DNOSAP, DNOSBP, DNSBP, Dow General, Dyanap, Dytop

Chemical Name: 2-*sec*-butyl-4,6-dinitrophenol

Uses: herbicides/insecticides; pre- or post-emergence control of broadleaf weeds in cereals, maize, lucerne, clover, trefoil, grass leys, potatoes, peas, onions, garlics, peas, leeks, soya beans, orchards, groundnuts, strawberries, vineyards and other crops; for control of strawberry runners and raspberry suckers and overwintering forms of insect pests on fruit trees; also used as a desiccant for leguminous seed crops; destruction of potato haulms; as a pre-harvest hop defoliant, etc.

CAS Registry No: 88-85-7

Molecular Formula: $C_{10}H_{12}N_2O_5$

Molecular Weight: 240.212

Melting Point (°C):
40 (Lide 2003)

Boiling Point (°C):
362 (estimated, Grain 1982)

Density (g/cm^3 at 20°C):
1.265 (45°C, Hartley & Kidd 1987; Herbicide Handbook 1989; Milne 1995)

Molar Volume (cm^3/mol):
218.0 (calculated-Le Bas method at normal boiling point)

Dissociation Constant pK$_a$:
4.62 (radiometer/pH meter, Cessna & Grover 1978; Hornsby et al. 1996)
4.61 (radiometer/pH meter, Cessna & Grover 1978)
4.62 (Worthing & Walker 1987, 1991)
4.50 (Yao & Haag 1991)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

Entropy of Fusion, ΔS_{fus} (J/mol K):

Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F: 0.713 (mp at 40°C)

Water Solubility (g/m^3 or mg/L at 25°C or as indicated):
50 (Günther 1968; Spencer 1982; Thomas 1982)
52 (Kearney & Kaufman 1975; Khan 1980)
50 (Martin & Worthing 1977; Kenaga 1980)
52 (Ashton & Crafts 1981; Herbicide Handbook 1989)
100 (rm. temp., Worthing & Walker 1983, Worthing & Hance 1991)
52 (20°C, Hartley & Kidd 1987; Milne 1995)
52 (20–25°C, selected, Hornsby et al. 1996)

Vapor Pressure (Pa at 25°C or as indicated):
130 (151.5°C, Khan 1980)
133 (151.1°C, Ashton & Crafts 1981)
0.0008, 0.0067 (supercooled liquid, estimated, Grain 1982)
0.0067 (Thomas 1982)
0.0023 (30°C, Spencer 1982)
10 (20°C, selected, Suntio et al. 1988)
0.183 (60°C, Worthing & Hance 1991)
0.0067 (20–25°C, selected, Hornsby et al. 1996)

Henry's Law Constant ($\mathrm{Pa\cdot m^3/mol}$ at 25°C or as indicated):

51.1	(20°C, calculated-P/C, Suntio et al. 1988)

Octanol/Water Partition Coefficient, $\log K_{OW}$:

3.59	(Hansch & Leo 1979)
3.69	(calculated, Zitko et al. 1976)
3.69	(Hansch & Leo 1985)
4.10	(RP-PHLC-RT correlation, Klein et al. 1988)
3.14	(shake flask/slow stirring-GC, De Bruijn et al. 1989)
3.0, 3.57	(pH 7, pH 2, shake flask, Brooke et al. 1990)
3.69	(recommended, Sangster 1993)
3.56	(recommended, Hansch et al. 1995)

Bioconcentration Factor, log BCF:

1.83	(calculated-S, Kenaga 1980a; quoted, Howard 1991)
0.778	(calculated-K_{OC}, Kenaga 1980)
1.51	(measured, Kenaga 1980; quoted, Isensee 1991)

Sorption Partition Coefficient, $\log K_{OC}$:

2.85	(soil, Thomas 1982)
2.09	(soil, Kenaga 1980a; Kenaga & Goring 1980)
2.71	(soil, calculated-S as per Kenaga & Goring 1980, Kenaga 1980a)
3.82	(HPLC-k′ correlation, cyanopropyl column, mobile phase buffered to pH 3, Hodson & Williams 1988)
2.68	(estimated as $\log K_{OM}$, Magee 1991)
1.80, 2.04, 2.08	(soil, literature values, Bottoni & Funari 1992)
2.70	(selected, Lohninger 1994)
2.09	(soil, calculated-MCI $^1\chi$, Sabljic et al. 1995)
1.48	(soil, 20–25°C, estimated, Hornsby et al. 1996)

Adsorption coefficient, K_d ($\mathrm{L\cdot kg^{-1}}$):

6.4, 64	(homoionic K^+-kaolinite, K^+-montmorillonite clay minerals, Haderlein et al. 1996)

Environmental Fate Rate Constants, k, or Half-Lives, $t_{1/2}$:

Volatilization: initial rate constant $k = 1.1 \times 10^{-3}\ h^{-1}$ and predicted rate constant $k = 2.6 \times 10^{-3}\ h^{-1}$ from soil with $t_{1/2}$ = 266.5 h (Thomas 1982).

Photolysis:

Oxidation:

photooxidation $t_{1/2}$ = 12.2–122 h in air, based on estimated rate constant for the reaction with hydroxyl radical in air (Atkinson 1987; quoted, Howard et al. 1991)

k(aq.) = $(0.003\text{–}2) \times 10^5\ M^{-1}\ s^{-1}$ for direct reaction with ozone in water at pH 1.9–5.0 and 24 ± 1°C, with $t_{1/2}$ = 0.16 s at pH 7 (Yao & Haag 1991).

k(calc) = $4 \times 10^9\ M^{-1}\ s^{-1}$ for the reaction with hydroxyl radical in aqueous solutions at 24 ± 1°C (Haag & Yao 1992).

Hydrolysis:

Biodegradation: aqueous aerobic $t_{1/2}$ = 1032–2952 h, based on aerobic soil mineralization data for one soil (Doyle et al. 1978; quoted, Howard et al. 1991) and aqueous anaerobic $t_{1/2}$ = 96–360 h, based on anaerobic soil die-away test data for isopropalin (Gingerich & Zimdahl 1976; quoted, Howard et al. 1991).

Biotransformation:

Bioconcentration, Uptake (k_1) and Elimination Constants (k_2):

Half-Lives in the Environment:

Air: $t_{1/2}$ = 12.2–122 h, based on estimated rate constant for the reaction with hydroxyl radical in air (Atkinson 1987; quoted, Howard et al. 1991).

Surface water: $t_{1/2}$ = 1032–2952 h, based on aerobic soil mineralization data for one soil (Doyle et al. 1978; quoted, Howard et al. 1991);

measured rate constant k = (0.003–2) × 10^5 M^{-1} s^{-1} for direct reaction with ozone in water at pH 1.9 -5.0 and 24 ± 1°C, with $t_{½}$ = 0.16 s at pH 7 (Yao & Haag 1991).

Ground water: $t_{½}$ = 96–5904 h, based on estimated unacclimated aqueous aerobic and anaerobic biodegradation half-lives (Howard et al. 1991)

reported $t_{½}$ = 30 d (Bottoni & Funari 1992)

Sediment:

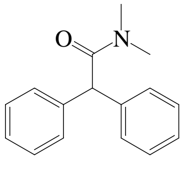
Soil: $t_{½}$ = 1032–2952 h, based on aerobic soil mineralization data for one soil (Doyle et al. 1978; quoted, Howard et al. 1991);

reported $t_{½}$ = 30 d (Bottoni & Funari 1992);

field $t_{½}$ = 30 d at 20–25°C (estimated, Hornsby et al. 1996).

Biota:

17.1.1.31 Diphenamid



Common Name: Diphenamid
Synonym: Difenamide, Dimid, Dymid, Enide, Fenam, Rideon
Chemical Name: *N,N*-dimethyldiphenylacetamide; *N,N*-dimethyl-α-phenyl-benzeneacetamide
Uses: herbicide for pre-emergence control of annual grasses and some broadleaf weeds in cotton, sweet potatoes, tomatoes, vegetables, capsicums, okra, soybeans, groundnuts, tobacco, pome fruit, stone fruit, citrus fruit, bush fruit, strawberries, forestry nurseries, and ornamental plants, shrubs, and trees.
CAS Registry No: 957-51-7
Molecular Formula: $C_{16}H_{17}NO$
Molecular Weight: 239.312
Melting Point (°C):
135 (Lide 2003)
Boiling Point (°C):
Density (g/cm^3 at 20°C):
1.17 (23.3°C, Hartley & Kidd 1987; Tomlin 1994; Milne 1995)
Molar Volume (cm^3/mol):
284.2 (calculated-Le Bas method at normal boiling point)
Dissociation Constant pK$_a$:
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
27.405 (DSC method, Plato & Glasgow 1969)
Entropy of Fusion, ΔS_{fus} (J/mol K):
Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F: 0.0833 (mp at 135°C)

Water Solubility (g/m^3 or mg/L at 25°C or as indicated):
240 (Melnikov 1971)
260 (27°C Spencer 1973, 1982; Khan 1980; Worthing & Walker 1987)
260 (Martin & Worthing 1977; Weber et al. 1980; Kenaga 1980)
260 (27°C, Hartley & Kidd 1987; Herbicide Handbook 1989; Tomlin 1994)
280 (20–25°C, selected, Hornsby et al. 1996)

Vapor Pressure (Pa at 25°C or as indicated):
$< 1.33 \times 10^{-4}$ (Weber et al. 1980)
negligible (20°C, Hartley & Kidd 1987; Tomlin 1994)
4.0×10^{-6} (20–25°C, selected, Hornsby et al. 1996)

Henry's Law Constant (Pa·m^3/mol at 25°C or as indicated):

Octanol/Water Partition Coefficient, log K_{OW}:

Bioconcentration Factor, log BCF:
1.43 (calculated-S, Kenaga 1980)

Sorption Partition Coefficient, log K_{OC}:
2.32 (soil, calculated-S, Kenaga 1980)
2.32 (selected, Lohninger 1994)
2.32 (soil, 20–25°C, selected, Hornsby et al. 1996)

Environmental Fate Rate Constants, k, or Half-Lives, $t_{½}$:

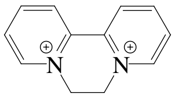
Photolysis: $t_{½}$ = 2.25 h in distilled water (Tanaka et al. 1981; quoted, Cessna & Muir 1991);

Half-Lives in the Environment:

Soil: estimated persistence of 8 months (Kearney et al. 1969; Edwards 1973; quoted, Morrill et al. 1982; Jury et al. 1987);
persistence under warm damp conditions is ca. 3–6 months (Herbicide Handbook 1989; Tomlin 1994)
field $t_{½}$ = 30 d at 20–25°C (selected, Hornsby et al. 1996).

Biota:

17.1.1.32 Diquat



Common Name: Diquat
Synonym: Aquacide, Deiquat, Dextrone, Ortho, Pathclear, Preeglone, Reglone, Weedol, Weedtrine-D
Chemical Name: 1,1′-ethylene-2,2′-dipyridine
Uses: nonselective contact herbicide to control broadleaf weeds in fruit and vegetable crops.
CAS Registry No: 2764-72-9
Molecular Formula: $C_{12}H_{14}N_2$
Molecular Weight: 186.236
Melting Point (°C): 335–340 (Spencer 1982)
Boiling Point (°C):
Density (g/cm^3 at 20°C):

1.22–1.27	(Ashton & Crafts 1981; Herbicide Handbook 1989; Montgomery 1993; Tomlin 1994)

Molar Volume (cm^3/mol):

230.6	(calculated-Le Bas method at normal boiling point)
149.6	(calculated-density)

Dissociation Constant pK_a:
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
Entropy of Fusion, ΔS_{fus} (J/mol K):
Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F:

Water Solubility (g/m^3 or mg/L at 25°C):

700000	(Khan 1980; Spencer 1982)
670000	(Weber et al. 1980)
700000	(Verschueren 1983)
700000	(Worthing & Hance 1991; Tomlin 1994)
700000	(Montgomery 1993)

Vapor Pressure (Pa at 25°C or as indicated):

< 0.00533	(Agrochemicals Handbook 1983)
$< 1.3 \times 10^{-5}$	(Worthing & Hance 1991; Tomlin 1994)
$< 1.3 \times 10^{-5}$	(20°C, Montgomery 1993)

Henry's Law Constant (Pa·m^3/mol at 25°C or as indicated):

$< 6.38 \times 10^{-9}$	(20–25°C, calculated-P/C, Montgomery 1993)
$< 3.42 \times 10^{-9}$	(calculated-P/C, this work)

Octanol/Water Partition Coefficient, log K_{OW}:

–3.05	(Garten & Trabalka 1983)
2.78	(Reinert 1989)
–4.60	(20°C, Worthing & Hance 1991; Tomlin 1994)
–4.60	(Montgomery 1993)

Bioconcentration Factor, log BCF:

–2.84	(calculated-S as per Kenaga 1980, this work)
–5.92	(calculated-log K_{OW} as per Mackay 1982, this work)

Sorption Partition Coefficient, log K_{OC}:

2.84	(Reinert 1989)
0.420	(calculated, Montgomery 1993)
0.425	(calculated-S as per Kenaga 1980, this work)

Environmental Fate Rate Constants, k, or Half-Lives, $t_{½}$:

Volatilization:

Photolysis: $t_{½}$ = 192 h for 10 µg/mL to degrade in distilled water under 240–260 nm light (Funderburk et al. 1960; quoted, Cessna & Muir 1991);

$t_{½}$ < 5 wk for 4 µg/mL to degrade in distilled water under sunlight (Slade & Smith 1967; quoted, Cessna & Muir 1991);

dry diquat photodecomposed by UV light with $t_{½}$ = 48 h (Funderburk & Bozarth 1967; quoted, Montgomery 1993);

$t_{½}$ ~ 48 h when associated with aerosols (Howard 1991);

$t_{½}$ = 3 wk for 3% of 5 µg/mL to degrade in distilled water under sunlight (Smith & Grove 1969; quoted, Cessna & Muir 1991).

Oxidation:

k(aq.) = $5.9 \times 10^9\ M^{-1}\ s^{-1}$ for the reaction (Fenton with reference to acetophenone) with hydroxyl radical in aqueous solutions at pH 3.1 and at 24 ± 1°C (Buxton et al. 1988; quoted, Faust & Hoigné 1990; Haag & Yao 1992)

k(aq.) = $(0.6 \pm 0.2)\ M^{-1}\ s^{-1}$ for direct reaction with ozone in water at pH 3.1 and 22°C, with a half-life of 15 h at pH 7 (Yao & Haag 1991).

k(aq.) = $(8.0 \pm 1.8) \times 10^8\ M^{-1}\ s^{-1}$ for the reaction (Fenton with reference to acetophenone) with hydroxyl radical in aqueous solutions at pH 3.1 and at 24 ± 1°C (Haag & Yao 1992).

Hydrolysis: $t_{½}$ = 74 d under simulated sunlight at pH 7 (Montgomery 1993; Tomlin 1994).

Biodegradation: $t_{½}$ ~ 50 d to biodegrade in lake water (Hiltibran 1972; quoted, Muir 1991);

$t_{½}$ > 158 d for 1.5 µg/mL of infested sediment-water microcosm to biodegrade in sediment and $t_{½}$ ~ 2 d in water both at 25°C (derived from Simsiman & Chesters 1976; Muir 1991).

Biotransformation:

Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants:

Half-Lives in the Environment:

Air:

Surface water: $t_{½}$ ~ 50 d to biodegrade in lake water (Hiltibran 1972; quoted, Muir 1991);

$t_{½}$ ~ 2 d of ^{14}C-diquat in water of a weed-infested simulated lake impoundment containing Lake Mendota sediment, the rapid disappearance is attributed to adsorption by sediments, suspended particulate matter and aquatic plants (shake flask-scintillation spectrometry, Simsiman & Chesters 1976)

measured rate constant k = $(0.6 \pm 0.2)\ M^{-1}\ s^{-1}$ for direct reaction with ozone in water at pH 3.1 and 22°C, with $t_{½}$ = 15 h at pH 7 (Yao & Haag 1991).

Ground water:

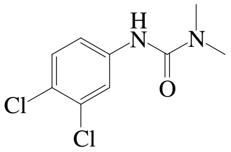
Sediment: Slow microbial degradation due to tight bonding of adsorbed Diquat to the clay minerals on the sediment (shake flask-liquid scintillation spectrometry, Simsiman & Chesters 1976)

$t_{½}$ > 158 d for 1.5 µg/mL of infested sediment-water microcosm to biodegrade (derived from results of Simsiman & Chesters 1976; Muir 1991).

Soil:

Biota:

17.1.1.33 Diuron



Common Name: Diuron
Synonym: AF 101, Cekiuron, Crisuron, Dailon, DCMU, Diater, dichlorofonidim, Di-on, Direx, DMU, Drexel, Duran, Dynex, Herbatox, Karmex, Marmer, NA 2767, Telvar, Unidron, Urox D, Vonduron
Chemical Name: 3-(3,4-dichlorophenyl)-1,1-dimethylurea; *N'*-(3,4-dichlorophenyl)-*N,N*-dimethylurea
Uses: pre-emergence herbicide in soils to control germinating broadleaf grasses and weeds in crops such as apples, cotton, grapes, pears, pineapple, and alfalfa; also used as sugar cane flowering depressant.
CAS Registry No: 330-54-1
Molecular Formula: $C_9H_{10}Cl_2N_2O$
Molecular Weight: 233.093
Melting Point (°C):
158 (Lide 2003)
Boiling Point (°C):
180 (decomposes, Montgomery 1993)
Density (g/cm^3 at 20°C):
Molar Volume (cm^3/mol):
223.8 (calculated-Le Bas method at normal boiling point)
188.0 (modified Le Bas method at normal boiling point, Spurlock & Biggar 1994a)
Dissociation Constant pK$_a$:
–1 to –2 (Montgomery 1993)
Enthalpy of Vaporization, ΔH_V (kJ/mol):
66.0 (Rordorf 1989)
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
33.89 (DSC method, Plato & Glasgow 1969)
27.3 (Rordorf 1989)
Entropy of Fusion, ΔS_{fus} (J/mol K):
Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F: 0.0496 (mp at 158°C)

Water Solubility (g/m^3 or mg/L at 25°C or as indicated):
42.0 (Günther et al. 1968; Melnikov 1971; Spencer 1973. 1982; Khan 1980; Ashton & Crafts 1981)
42.0 (20°C, Weber 1972; Weber et al. 1980)
37.3 (shake flask-UV, Freed et al. 1976; Freed 1976)
42.0 (Martin & Worthing 1977; Hartley & Kidd 1987; Worthing & Walker 1987, Worthing & Hance 1991; Herbicide Handbook 1989; Tomlin 1994; Milne 1995)
42.4 (shake flask, Briggs 1981)
22.0 (shake flask-HPLC, Ellgehausen et al. 1981)
38.7 (generator column-HPLC/RI, Swann et al. 1983)
120 (RP-HPLC-RT correlation, Swann et al. 1983)
19.6, 40.1, 53.4 (4, 25, 40°C, shake flask-liquid scintillation spectrometer LSS, Madhun et al. 1986)
42.0 (20–25°C, selected, Wauchope et al. 1992; Hornsby et al. 1996)
40.0 (20°C, Montgomery 1993)

Vapor Pressure (Pa at 25°C or as indicated and reported temperature dependence equations):
1.6×10^{-5} (estimated, Nex & Swezey 1954)
3.8×10^{-6} (20°C, Johnson & Julin 1974)
4.1×10^{-4} (50°C, Khan 1980; Ashton & Crafts 1981)
$< 1.3 \times 10^{-4}$ (20–25°C, Weber et al. 1980)
2.5×10^{-4} (Thomas 1982)

2.1×10^{-5} (Jury et al. 1983; quoted, Taylor & Glotfelty 1988; Taylor & Spencer 1990)
3.6×10^{-4} (Jury et al. 1983; quoted, Howard 1991)
2.7×10^{-4} (selected, Nkedi-Kizza et al. 1985)
4.1×10^{-4} (50°C, Hartley & Kidd 1987; Worthing & Hance 1991; Herbicide Handbook 1989)
2.0×10^{-4} (20°C, selected, Suntio et al. 1988)
5.30×10^{-4}, 1.0×10^{-2}, 0.130, 1.20, 79 (25, 50, 70, 100, 125°C, gas saturation-GC, Rordorf 1989)
$\log (P_S/Pa) = 13.339 - 4953.8/(T/K)$; measured range 36.2–90.2°C (solid, gas saturation-GC, Rordorf 1989)
$\log (P_L/Pa) = 9.800335 - 3445.24/(T/K)$; measured range not specified (liquid, gas saturation-GC, Rordorf 1989)
9.2×10^{-6} (20–25°C, selected, Wauchope et al. 1992; Hornsby et al. 1996)
1.1×10^{-6} (Tomlin 1994)

Henry's Law Constant (Pa·m^3/mol at 25°C or as indicated):
1.4×10^{-4} (calculated-P/C, Jury et al. 1984, 1987a,b; Jury & Ghodrati 1989)
1.2×10^{-4} (20°C, calculated-P/C, Suntio et al. 1988)
1.3×10^{-4} (calculated-P/C, Taylor & Glotfelty 1988)
0.274 (calculated-P/C, Howard 1991)
2.1×10^{-5} (20°C, calculated-P/C, Muir 1991)
1.5×10^{-4} (20–25°C, calculated-P/C, Montgomery 1993)

Octanol/Water Partition Coefficient, log K_{OW}:
2.60 (calculated-f const., Rekker 1977)
2.81 (Rao & Davidson 1980)
2.68 (shake flask-UV, Briggs 1981)
2.89 (shake flask-HPLC, Ellgehausen et al. 1981)
2.60 (Elgar 1983)
2.77 (Hansch & Leo 1985)
2.69, 2.65, 2.63 (4, 25, 40°C, shake flask-liquid scintillation spectrometer LSS, Madhun et al. 1986)
2.86 (shake flask, Mitsutake et al. 1986)
1.97–2.81 (Montgomery 1993)
2.78 (recommended, Sangster 1993)
2.45 (RP-HPLC-RT correlation, Sicbaldi & Finizio 1993)
2.80 (Aquasol Database 1994; quoted, Pinsuwan et al. 1995)
2.81 (shake flask, Spurlock & Biggar 1994a)
2.85 ± 1.70 (Tomlin 1994)
2.58, 2.73 (shake flask-UV, RP-HPLC-k′ correlation, Liu & Qian 1995)
2.68 (recommended, Hansch et al. 1995)
2.45 (RP-HPLC-RT correlation, Finizio et al. 1997)

Bioconcentration Factor, log BCF:
1.40 (measured, Isensee 1976)
1.88 (calculated-S, Kenaga 1980)
1.34 (calculated-K_{OC}, Kenaga 1980)
2.16 (*Pimephales promelas*, Call et al. 1987)
2.41, 2.48 (cuticle/water: tomato, pepper, Chaumat et al. 1991)
2.41, 2.51 (cuticle/water: box tree, laurel, Chaumat et al. 1991)
2.55, 2.28 (cuticle/water: pear, ivy, Chaumat et al. 1991)
1.18, 1.64 (cuticle/water: cleavers, vanilla, Chaumat et al. 1991)
2.45, 2.48 (cuticle/water: tomato, pepper, Evelyne et al. 1992)

Bioaccumulation Factor, log BF:
–1.70 (adipose tissue in both male & female Albino rats, Hodge et al. 1967)

Sorption Partition Coefficient, log K_{OC}:
2.60 (soil, Hamaker & Thompson 1972; Farmer 1976; Hance 1976)

2.75 (soil, calculated-S as per Kenaga & Goring 1977, Kenaga 1980)
2.59 (average of 3 soils, HPLC-RT correlation, McCall et al. 1980)
2.15–2.52 (Peck et al. 1980)
2.21 (soil, converted from reported K_{OM} multiplied 1.724, Briggs 1981)
3.06, 2.41 (estimated-S, solubility and mp, Karickhoff 1981)
1.58, 2.42 (estimated-K_{OW}, Karickhoff 1981)
2.58 (average of 84 soils, Rao & Davidson 1982)
2.18 (soil, Thomas 1982)
2.83 (Webster soil, Nkedi-Kizza 1983)
2.49 (soil slurry method, Swann et al. 1983)
2.48 (RP-HPLC-RT correlation, Swann et al. 1983)
3.03, 2.94 (4°C, 25°C, Semiahmoo soil, batch equilibrium method-LSS, Madhun et al. 1986)
2.82, 2.68 (4°C, 25°C, Adkins soil, batch equilibrium method-LSS, Madhun et al. 1986)
2.86, 2.44, 2.48; 2.81, 2.74, 2.44 (estimated-K_{OW}; solubility, Madhun et al. 1986)
2.50 (calculated-MCI χ, Gerstl & Helling 1987)
2.58 (soil, screening model calculations, Jury et al. 1987a,b; Jury & Ghodrati 1989)
2.35, 2.57 (2 subsurface soils from Oklahoma, Bouchard & Wood 1988)
2.94, 2.68 (mucky peat soil, loam sand soil, quoted, Howard 1991)
2.18, 2.48–2.49, 2.59, 2.66 (soil, quoted values, Bottoni & funari 1992)
2.68 (soil, 20–25°C, selected, Wauchope et al. 1992; Hornsby et al. 1996)
2.21–2.87 (Montgomery 1993)
2.68 (selected, Lohninger 1994)
2.60 (Tomlin 1994)
2.70 (calculated-K_{OW}, Liu & Qian 1995)
2.40 (soil, calculated-MCI $^1\chi$, Sabljic et al. 1995)
3.07, 2.37, 2.82, 2.51, 2.96 (calculated-K_{OW}; HPLC-screening method with different LC-columns, Szabo et al. 1999)
2.48, 2.42 (soil, estimated-class-specific model, estimated-general model using molecular descriptors, Gramatica et al. 2000)
2.44, 2.43, 2.57 (soils: organic carbon OC ≥ 0.1%, OC ≥ 0.5%, 0.1 ≤ OC < 0.5%, average, Delle Site 2001)
2.78‘ (sediment: organic carbon OC ≥ 0.5%, average, Delle Site 2001)

Environmental Fate Rate Constants, k, or Half-Lives, $t_{1/2}$:

Volatilization: 2.5×10^{-3} h^{-1} (initial) and 5.3×10^{-4} h^{-1} (predicted) from soil with $t_{1/2}$ = 1307 h (Thomas 1982); the calculated $t_{1/2}$ = 1918 d due to volatilization from soil when incorporated into 1 cm of soil (Jury et al. 1983; quoted, Howard 1991).

Photolysis: $t_{1/2}$ = 2.25 h for 80–84% of 40 μg/mL to degrade in distilled water under 300 nm light (Tanaka et al. 1981; quoted, Cessna & Muir 1991); in surface waters should be photolyzed within a few days (Howard 1991).

Oxidation: photooxidation $t_{1/2}$ = 0.12 d in air, based on estimation for the vapor-phase reaction with hydroxyl radical in the atmosphere (Atkinson 1987; quoted, Howard 1991).

Hydrolysis: $t_{1/2}$ > 4 months for 4660 μg/mL to hydrolyze in phosphate buffer at pH 5–9 and 20°C (El-Dib & Aly 1976; quoted, Muir 1991).

Biodegradation: $t_{1/2}$ = 328 d for a 100 d leaching and screening test in 0–10 cm depth of soil (Rao & Davidson 1980; quoted, Jury et al. 1983, 1984, 1987a);

$t_{1/2}$ = 3–10 d for 40 μg/mL to biodegrade in pond sediment of anaerobic media at 30°C (Attaway et al. 1982a quoted, Muir 1991);

$t_{1/2}$ < 17 d for 40 μg/mL to biodegrade in pond sediment at 30°C (Attaway et al. 1982b; quoted, Muir 1991);

67–99% will be degraded in 10 wk under aerobic conditions by mixed cultures isolated from pond water and sediments forming 6–7 products (Ellis & Camper 1982; quoted, Howard 1991; Muir 1991);

$t_{1/2}$ < 70 d at 30°C (Ellis & Camper 1982; quoted, Muir 1991; Montgomery 1993);

$t_{1/2}$ ~ 5 d for 0.22 μg/mL to biodegrade in pond sediment of anaerobic media (Stepp et al. 1985; quoted, Muir 1991);

$t_{1/2}$(aerobic) ~ 20 d for 0.0005–10 μg/mL to biodegrade in filtered sewage water at 20°C (Wang et al. 1985; quoted, Muir 1991).

Biotransformation: ~ 7% of a selection of 90 strains of micromycetes mostly isolated from soil-soil fungi, depleted over 50% of diuron (20 mg/L) in 5-d experiment (Vroumsia et al. 1996)

Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants:

Half-Lives in the Environment:

Air: $t_{1/2}$ = 0.12 d, based on estimation for the vapor-phase reaction with hydroxyl radical in the atmosphere (Atkinson 1987; quoted, Howard 1991).

Surface water: should be photolyzed within a few days (Howard 1991).

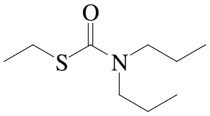
Ground water: reported half-lives or persistence, $t_{1/2}$ = 20–70, 90–180, 200, and 328 d (Bottoni & Funari 1992)

Sediment: $t_{1/2}$ = 3–10 d for 40 μg/mL to biodegrade in pond sediment of anaerobic media at 30°C (Attaway et al. 1982a; quoted, Muir 1991);
$t_{1/2}$ < 17 d for 40 μg/mL to biodegrade in pond sediment at 30°C (Attaway et al. 1982b);
$t_{1/2}$ ~ 5 d for 0.22 μg/mL to biodegrade in pond sediment of anaerobic media (Stepp et al. 1985)

Soil: estimated persistence of 10 months in soil (Kearney et al. 1969; quoted, Jury et al. 1987);
persistence of 8 months in soil (Edwards 1973; quoted, Morrill et al. 1982);
$t_{1/2}$ = 7.0 months at 15°C and $t_{1/2}$ = 5.5 months at 30°C in soils (Freed & Haque 1973);
persistence of 10 months (Wauchope 1978);
rate constant k = 0.0031 d^{-1} with $t_{1/2}$ = 328 d under field conditions (Rao & Davidson 1980);
calculated $t_{1/2}$ = 1918 d due to volatilization from soil when incorporated into 1 cm of soil (Jury et al. 1983; quoted, Howard 1991);
$t_{1/2}$ ~ 200–4000 d in loamy sand and peat at 25–35°C as follows (Madhum & Freed 1987):
$t_{1/2}$ = 705, 414, and 225 d at 25, 30, and 35°C, respectively, at herbicide concn at 5 μg/kg, while $t_{1/2}$ = 1392, 630, and 406 d at 25, 30, and 35°C, respectively, at herbicide concn at 100 μg/kg in an Adkins loamy sand; however, the half-lives were considerable higher in peat. $t_{1/2}$ = 3991, 2164, and 1165 d at 25, 30, and 35°C, respectively, at herbicide concn at 5 μg/kg while $t_{1/2}$ = 3416, 1832, and 896 d at 25, 30, and 35°C, respectively, at herbicide concn at 100 μg/kg in a Semiahoo mucky peat (Madhun & Freed 1987)
$t_{1/2}$ = 328 d from screening model calculations (Jury et al. 1987a,b; Jury & Ghodrati 1989);
reported $t_{1/2}$ = 20–70 d, 90–180 d, 200 d and 328 d (Bottoni & Funari 1992);
$t_{1/2}$ = 75–102 d in 0–40 cm soil cores taken, from cultivated field, $t_{1/2}$ = 55–65 d from meadow and $t_{1/2}$ = 29–35 d from gravel track (Hassink et al. 1994);
selected field $t_{1/2}$ = 90 d (Wauchope et al. 1992; Hornsby et al. 1996).

Biota: biochemical $t_{1/2}$ = 328 d from screening model calculations (Jury et al. 1987a,b; Jury & Ghodrati 1989).

17.1.1.34 EPTC



Common Name: EPTC
Synonym: Eptam, Eradicane, FDA 1541, R 1608, Torbin
Chemical Name: carbamic acid, dipropylthio-, *S*-ethyl ester; *S*-ethyldipropyl(thiocarbamate); *S*-ethyldipropylcarbamothioate
Uses: selective systemic herbicide for pre-emergence control of perennial and annual grasses, broadleaf weeds.
CAS Registry No: 759-94-4
Molecular Formula: $C_9H_{19}NOS$
Molecular Weight: 189.318
Melting Point (°C): liquid
Boiling Point (°C):

235.0	(Khan 1980; Herbicide Handbook 1989)
127.0	(at 20 mmHg, Hartley & Kidd 1987; Budavari 1989; Worthing & Hance 1991; Montgomery 1993; Tomlin 1994; Milne 1995)

Density (g/cm^3 at 20°C):

0.9546	(30°C, Spencer 1982; Hartley & Kidd 1987; Montgomery 1993; Tomlin 1994; Milne 1995)
0.960	(25°C, Herbicide Handbook 1989; Montgomery 1993)

Molar Volume (cm^3/mol):

236.5	(calculated-Le Bas method at normal boiling point)

Dissociation Constant pK_a:
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
Entropy of Fusion, ΔS_{fus} (J/mol K):
Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F: 1.0

Water Solubility (g/m^3 or mg/L at 25°C or as indicated):

375	(shake flask-GC, Freed et al. 1967)
365	(Martin & Worthing 1977)
370	(20°C, Khan 1980; Ashton & Crafts 1981; Herbicide Handbook 1989)
370–375	(Weber et al. 1980)
375	(20°C, Spencer 1982)
370	(Beste & Humburg 1983; Jury et al. 1983, 1984)
375	(Hartley & Kidd 1987; Montgomery 1993; Tomlin 1994)
375	(24°C, Worthing & Walker 1987, Worthing & Hance 1991)
365	(20°C, Budavari 1989; Milne 1995)
344	(20–25°C, selected, Wauchope et al. 1992; Hornsby et al. 1996; Lohninger 1994)

Vapor Pressure (Pa at 25°C or as indicated):

4.666	(extrapolated, Patchett et al. 1964)
20.66	(Bailey & White 1965)
1.84	(20°C, effusion method, Hamaker & Kerlinger 1971)
2.16, 2.63, 3.69, 8.266	(23, 24, 28, 40°C, Hamaker 1972)
4.532	(Khan 1980; Ashton & Crafts 1981; Herbicide Handbook 1989)
2.62	(20°C, volatilization rate, Burkhard & Guth 1981)
2.80	(Patchett et al. 1983)
0.612	(20°C, GC-RT correlation, Kim 1985)
4.70	(Hartley & Kidd 1987)
2.00	(20°C, selected, Suntio et al. 1988)
4.532	(35°C, Budavari 1989)
4.50	(Worthing & Hance 1991)

4.532 (20–25°C, selected, Wauchope et al. 1992; Hornsby et al. 1996)
4.532 (20°C, Montgomery 1993)
0.00001 (Tomlin 1994)

Henry's Law Constant (Pa·m^3/mol at 25°C or as indicated):

1.32 (20°C, volatilization rate, Burkhard & Guth 1981)
1.463 (calculated-P/C, Jury et al. 1983, 1984, 1987a,b; Jury & Ghodrati 1989)
1.02 (20°C, calculated-P/C, Suntio et al. 1988)
1.463 (calculated-P/C, Taylor & Glotfelty 1988)
1.013 (20–25°C, calculated-P/C, Montgomery 1993)
1.023 (calculated-P/C, this work)

Octanol/Water Partition Coefficient, log K_{OW}:

1.76 (selected, Dao et al. 1983)
3.21 (shake flask, Log P Database, Hansch & Leo 1987)
3.20 (Worthing & Hance 1991; Montgomery 1993; Tomlin 1994; Milne 1995)
3.21 (recommended, Sangster 1993)
3.21 (recommended, Hansch et al. 1995)
3.45 (RP-HPLC-RT correlation, Finizio et al. 1997)

Bioconcentration Factor, log BCF:

1.34 (calculated-S, Kenaga 1980; quoted, Isensee 1991)
1.08 (calculated-K_{OC}, Kenaga 1980)

Sorption Partition Coefficient, log K_{OC}:

2.38 (soil, Hamaker & Thompson 1972)
2.45 (soil, Hamaker & Thompson 1972)
2.23 (soil, calculated-S as per Kenaga & Goring 1980, Kenaga 1980)
2.58 (soil, screening model calculations, Jury et al. 1987a,b; Jury & Ghodrati 1989)
2.23–2.38, 2.45 (quoted values, Bottoni & Funari 1992)
2.30 (soil, 20–25°C, selected, Wauchope et al. 1992)
2.38 (Montgomery 1993)
2.30 (selected, Lohninger 1994)
2.45 (selected, Wienhold & Gish 1994)
2.38 (soil, calculated-MCI $^1\chi$, Sabljic et al. 1995)
2.23, 1.98 (soil, estimated-class specific model, estimated-general model using molecular descriptors, Gramatica et al. 2000)
2.03, 2.00 (soils: organic carbon OC ≥ 0.1%, OC ≥ 0.5%, average, Delle Site 2001)

Environmental Fate Rate Constants, k, or Half-Lives, $t_{½}$:

Volatilization: $t_{½}$ = 3.7 d (Jury et al. 1983).

Photolysis: rate constant $k = 5.2 \times 10^{-3}$ s^{-1} for a light intensity corresponding to a 12-h average NO_2 photolysis rate with a black lamp spectral distribution (Kwok et al. 1992);
photodegradation $t_{½}$ = 14.0 and 18.5 min in water solution under irradiation with UV light at 254 nm (Abu-Qare & Duncan 2002).

Oxidation: second order rate constants $k_{OH} = (3.10–3.40) \times 10^{-11}$ cm^3 molecule^{-1} s^{-1} for gas-phase reaction with OH radical, $k_{NO3} = 0.92 \times 10^{-14}$ cm^3 molecule^{-1} s^{-1} with NO_3 radical and $k_{O3} < 1.3 \times 10^{-19}$ cm^3 molecule^{-1} s^{-1} with O_3 at 298 K (Kwok et al. 1992);
calculated lifetime of 6 h for the vapor-phase reaction with OH radical in the troposphere (Atkinson et al. 1992; Kwok et al. 1992).

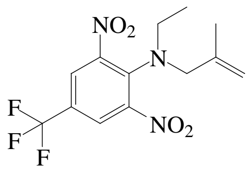
Hydrolysis:

Biodegradation: $t_{½}$ = 30 d for a 100 d leaching and screening test in 0–10 cm depth of soil (Nash 1980; quoted, Jury et al. 1983, 1984, 1987a; quoted, Grover 1991).

Biotransformation:
Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants:

Half-Lives in the Environment:
Air: calculated tropospheric lifetimes are: > 8 h due to photolysis, 5.8 d due to reaction with OH radical, 5.0 d with NO_3 radical and > 125 d with O_3 (Kwok et al. 1992);
calculated lifetime of 6 h for the vapor-phase reaction with OH radical in the troposphere (Atkinson et al. 1992; Kwok et al. 1992).
Surface water: $t_{½}$ = 14.0 and 18 min for elimination in water under irradiation with UV light at 254 nm (Abu-Qare & Duncan 2002).
Ground water: reported half-lives or persistence, $t_{½}$ = 7 and 30 d (Bottoni & Funari 1992)
Sediment:
Soil: estimated persistence of 4 months in soil (Kearney et al. 1969; quoted, Jury et al. 1987a);
$t_{½}$ = 30 d from screening model calculations (Jury et al. 1987a,b; Jury & Ghodrati 1989);
$t_{½}$ ~ 1 wk in moist loam soil at 21 to 27°C (Herbicide Handbook 1974, 1989);
reported $t_{½}$ = 7, 30 d (Bottoni & Funari 1992);
selected field $t_{½}$ = 6 d (Wauchope et al. 1992; quoted, Richards & Baker 1993; Hornsby et al. 1996).
Biota: biochemical $t_{½}$ = 30 d from screening model calculations (Jury et al. 1987a,b; Jury & Ghodrati 1989)

17.1.1.35 Ethalfluralin



Common Name: Ethalfluralin
Synonym: Benzenamine, Somilan, Sonalan, Sonalen
Chemical Name: *N*-ethyl-*N*-(2-methyl-2-propenyl)-2.6-dinitro-(trifluoromethyl)-benzenamine
CAS Registry No: 55283-68-6
Uses: herbicide
Molecular Formula: $C_{13}H_{14}F_3N_3O_4$
Molecular Weight: 333.263
Melting Point (°C):
57 (Lide 2003)
Boiling Point (°C):
256 (decomposes, Hartley & Kidd 1987; Tomlin 1994; Milne 1995)
Density (g/cm^3 at 20°C):
1.32 (Ashton & Crafts 1981; Herbicide Handbook 1989)
Molar Volume (cm^3/mol):
Dissociation Constant pK$_a$:
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
Entropy of Fusion, ΔS_{fus} (J/mol K):
Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F: 0.485 (mp at 57°C)

Water Solubility (g/m^3 or mg/L at 25°C):

0.21	(Ashton & Crafts 1981)
0.20	(pH 7, Spencer; Hartley & Kidd 1987; Worthing & Walker 1987)
0.30	(pH 7, Herbicide Handbook 1989)
0.30	(selected, Wauchope et al. 1992; Hornsby et al. 1996)
0.30	(pH 7, Tomlin 1994; Milne 1995)
0.40	(Majewski & Capel 1995)

Vapor Pressure (Pa at 25°C or as indicated):

1.10×10^{-4}	(Worthing & Walker 1983, 1987; Hartley & Kidd 1987)
0.0109	(Spencer 1982; Herbicide Handbook 1989)
0.0117	(selected, Wauchope et al. 1992; Hornsby et al. 1996)
0.0117	(Tomlin 1994)
2.22×10^{-4}	(20–25°C, Majewski & Capel 1995)

Henry's Law Constant (Pa·m^3/mol at 25°C):

0.183	(calculated-P/C, Majewski & Capel 1995)
13	(calculated-P/C, Wolt 1997)

Octanol/Water Partition Coefficient, log K_{OW}:

5.11	(pH 7, Tomlin 1994; Milne 1995)
4.92	(quoted values; selected, Wolt 1997)

Octanol/Air Partition Coefficient, log K_{OA}:

Bioconcentration Factor, log BCF or log K_B:

Sorption Partition Coefficient, log K_{OC}:

3.60	(selected, soil, Wauchope et al. 1992; Hornsby et al. 1996)
3.60–3.90	(soil, Tomlin 1994)
3.61–3.92	(soil, Wolt 1997)

Environmental Fate Rate Constants, k, or Half-Lives, $t_{½}$:

Volatilization:

Photolysis: $t_{½}$ = 6.3 h in aqueous phase and $t_{½}$ = 2 h in vapor phase (Tomlin 1994);

Aqueous photolysis $t_{½}$ = 6.3 h in pH 5 sterile buffer solution; soil photolysis $t_{½}$ = 14.2 d in air-dry sandy loam soil when exposed to a xenon light source; air photolysis $t_{½}$ = 2 h when exposed to a light source simulating summer sunlight at 34°C (Wolt 1997).

Oxidation:

Hydrolysis: no hydrolysis after 33 d at pH 3, 6 and 9 (51°C, Tomlin 1994); stable in sterile, buffered solutions across a range of pH (Wolt 1997).

Biodegradation:.

Biotransformation: $t_{½}$ = 45 d for aerobic metabolism in sandy loam soils and $t_{½}$ = 14 d for more rapid metabolism anaerobically in the same soil (quoted, Tomlin 1994; Wolt 1997).

Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants:

Half-Lives in the Environment:

Air: air photolysis $t_{½}$ = 2 h when exposed to a light source simulating summer sunlight at 34°C (Wolt 1997).

Surface water: water photolysis $t_{½}$ = 6.3 h in pH 5 sterile buffer solution; $t_{½}$ = 2 d for dissipation from the water column in a pond water-sediment system under outdoor conditions (Wolt 1997).

Ground water:

Sediment: $t_{½}$ = 38 h in anaerobic pond water sediment system (Wolt 1997).

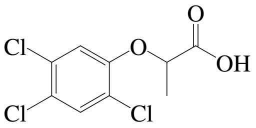
Soil: reported field $t_{½}$ = 30–60 d, 60 d, 25–46 d; recommended $t_{½}$ = 60 d (Wauchope et al. 1992; Hornsby et al. 1996);

$t_{½}$ = 45 d for aerobic metabolism in sandy loam soils and $t_{½}$ = 14 d for more rapid metabolism anaerobically in the same soil (Tomlin 1994);

terrestrial filed dissipation $t_{½}$ = 4–146 d, $t_{½}$ = 45 d in moist aerobic soil, $t_{½}$ = 14 d in anaerobic soil shifted to anaerobic conditions (Wolt 1997).

Biota:

17.1.1.36 Fenoprop



Common Name: Fenoprop
Synonym: Silvex, 2,4,5-TP, Kuron, Kurosal, Fruitone T
Chemical Name: 2-(2,4,5-trichlorophenoxy) propionic acid
CAS Registry No: 93-72-1
Uses: herbicide/growth regulator
Molecular Formula: $C_9H_7Cl_3O_3$
Molecular Weight: 269.509
Melting Point (°C):
181.6 (Lide 2003)
Boiling Point (°C):
Density (g/cm^3 at 20°C):
Molar Volume (cm^3/mol):
Dissociation Constant pK_a:
2.84 (Worthing 1983, 1987; Augustijn-Beckers et al. 1994)
Enthalpy of Vaporization, ΔH_V (kJ/mol):
75.75 (Rordorf 1989)
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
44.6 (Rordorf 1989)
Entropy of Fusion, ΔS_{fus} (J/mol K):
Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F: 0.0291 (mp at 181.6°C)

Water Solubility (g/m^3 or mg/L at 25°C):
140 (Kenaga & Goring 1980, Kenaga 1980a,b, Spencer 1982)
140 (Worthing & Walker 1983, 1987; Budavari 1989)
200 (Verschueren 1983)
176 (Hartley & Kidd 1987)
12.0 (calculated-MCI χ, Patil 1994)
140 (selected, Augustijn-Beckers et al. 1994; Hornsby et al. 1996)

Vapor Pressure (Pa at 25°C or as indicated and reported temperature dependence equations):
2.30×10^{-3}, 4.40×10^{-2}, 0.55, 4.90, 34.0 (25, 50, 70, 100, 125°C, gas saturation-GC, Rordorf 1989)
$\log (P_S/\text{Pa}) = 13.953 - 4948/(T/K)$; measured range 85.4–181°C (gas saturation-GC, Rordorf 1989)
$\log (P_L/\text{Pa}) = 11.727 - 3956.9/(T/K)$; measured range 181–211°C (gas saturation-GC, Rordorf 1989)
$< 1.33 \times 10^{-6}$ (estimated, Augustijn-Beckers et al. 1994; Hornsby et al. 1996)

Henry's Law Constant (Pa·m^3/mol):

Octanol/Water Partition Coefficient, log K_{OW}:
2.44 (Kenaga 1980a)
3.86 (estimated, Garten & Trabalka 1983)
3.13 (counter-current chromatography, Ilchmann et al. 1993)
2.75 (calculated-MCI χ, Patil 1994)
3.80 (selected, Hansch et al. 1995)

Octanol/Air Partition Coefficient, log K_{OA}:

Bioconcentration Factor, log BCF or log K_B:
1.76 (calculated, Kenaga 1980a)
1.58, 2.23 (calculated-solubility, K_{OW}, Kenaga 1980b)

1.76 (fish, flowing water, Garten & Grabalka 1983)
2.35 (Isensee 1991)

Sorption Partition Coefficient, log K_{OC}:

3.41 (soil, Kenaga & Goring 1980)
2.46 (calculated-K_{OW}, Kenaga 1980b)
1.91 (soil: calculated-MCI χ, Meylan et al. 1992)
2.48 (soil, selected, Augustijn-Beckers et al. 1994; Hornsby et al. 1996)
3.28 (soil, calculated-MCI χ, Sabljic et al. 1995)

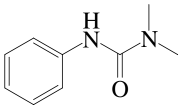
Environmental Fate Rate Constants, k, or Half-Lives, $t_{½}$:

Biodegradation: $t_{½} > 205$ d for ring cleavage in soil suspensions (Verschueren 1983)

Half-Lives in the Environment:

Soil: persistence 47–205 d in soil (Alexander et al. 1961)
degradation $t_{½} = 21$ d and 14 d in Quachita Highlands' forest and grassland soil respectively, $t_{½} = 15$ d in gross timbers forest soil, average $t_{½} = 17$ d in 3 soils (Altom & Stritzke 1973);
$t_{½} = 5$–11 d in a microagroecosystem study (Nash 1983);
$t_{½} > 205$ d for ring cleavage in soil suspensions (Verschueren 1983);
field $t_{½} = 21$ d (Augustijn-Beckers et al. 1994; Hornsby et al. 1996)

17.1.1.37 Fenuron



Common Name: Fenuron
Synonym: Dozer, Dybar, Falisilvan, Fenidim, Fenulon, Urab
Chemical Name: 1,1-dimethyl-3-phenylurea; *N,N*-dimethyl-*N′*-phenylurea
Uses: herbicide to control woody plants and deep-rooted perennial weeds, often used in combination with chlorpropham to extend its weed control spectrum and range of crops.
CAS Registry No: 101-42-8
Molecular Formula: $C_9H_{12}N_2O$
Molecular Weight: 164.203
Melting Point (°C):

132	(Lide 2003)

Boiling Point (°C):
Density (g/cm^3 at 20°C):

1.13	(25°C, Hartley & Kidd 1987)
1.08	(Worthing & Hance 1991; Tomlin 1994)

Molar Volume (cm^3/mol):

182.0	(calculated-Le Bas method at normal boiling point)
159.0	(modified Le Bas method, Spurlock & Biggar 1994a)

Dissociation Constant pK_a:
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

24.267	(DSC method, Plato & Glasgow 1969)

Entropy of Fusion, ΔS_{fus} (J/mol K):
Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F: 0.0892 (mp at 132°C)

Water Solubility (g/m^3 or mg/L at 25°C or as indicated):

2600	(Freed 1966)
2400	(Günther et al. 1968)
3850	(Martin & Worthing 1977; Kenaga 1980; Kenaga & Goring 1980; Verschueren 1983)
3850	(Khan 1980; Weber et al. 1980; Ashton & Crafts 1981; Willis & McDowell 1982)
3700	(shake flask-HPLC, Ellgehausen et al. 1981)
3850	(Hartley & Kidd 1987; Worthing & Walker 1987, Worthing & Hance 1991; Tomlin 1994)
3000	(20°C, selected, Suntio et al. 1988)
3900	(Spurlock 1992; Spurlock & Biggar 1994b)
3850	(20–25°C, selected, Augustijn-Beckers et al. 1994; Hornsby et al. 1996)

Vapor Pressure (Pa at 25°C or as indicated):

0.0213	(60°C, Khan 1980; Verschueren 1983)
0.0210	(60°C, Hartley & Kidd 1987)
0.0050	(20°C, selected, Suntio et al. 1988)
0.0210	(60°C, Worthing & Hance 1991; Tomlin 1994)
0.0267	(20–25°C, selected, Augustijn-Beckers et al. 1994; Hornsby et al. 1996)

Henry's Law Constant (Pa·m^3/mol at 25°C at 25°C or as indicated):

0.00027	(20°C, calculated-P/C, Suntio et al. 1988)

Octanol/Water Partition Coefficient, log K_{OW}:

0.98	(shake flask-UV, Hansch & Anderson 1967)
1.00	(Leo et al. 1971)
1.00	(shake flask-UV, Lord et al. 1980)

0.96 (shake flask-UV, Briggs 1981; Karickhoff 1981)
0.88 (shake flask-HPLC, Ellgehausen et al. 1981)
0.62 (HPLC-k′ correlation, McDuffie 1981)
0.70 (Elgar 1983)
1.18 (RP-HPLC-k′ correlation, Braumann et al. 1983)
1.00 (shake flask-HPLC, Spurlock & Biggar 1994a)
0.98 (recommended, Sangster 1993)
1.18 (RP-HPLC-RT correlation, Sicbaldi & Finizio 1993)
0.98 (recommended, Hansch et al. 1995)
1.18 (RP-HPLC-RT correlation, Finizio et al. 1997)

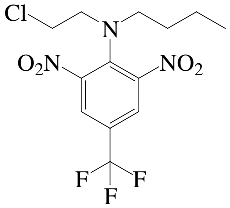
Bioconcentration Factor, log BCF:
0.778 (calculated-S, Kenaga 1980)
0.0 (calculated-K_{OC}, Kenaga 1980)
1.34 (earthworms, Lord et al. 1980)
0.699, 0.602 (cuticle/water: tomato, pepper, Evelyne et al. 1992)

Sorption Partition Coefficient, log K_{OC}:
1.43 (soil, Hamaker & Thompson 1972)
1.67 (soil, calculated-S as per Kenaga & Goring 1980, Kenaga 1980)
0.88 (reported as log K_{OM}, Briggs 1981)
0.61 (estimated-K_{OW}, Karickhoff 1981)
1.80, 1.86 (estimated-S, Karickhoff 1981)
0.72, 0.84 (estimated-S and mp, Karickhoff 1981)
1.74 (calculated-MCI χ, Gerstl & Helling 1987)
1.62 (20–25°C, selected, Augustijn-Beckers et al. 1994; Hornsby et al. 1996)
1.40 (soil, calculated-MCI $^1\chi$, Sabljic et al. 1995)
1.40; 1.40, 1.70 (soil, quoted obs.; estimated-class-specific model, estimated-general model using molecular descriptors, Gramatica et al. 2000)
1.42, 1.41 (soils: organic carbon OC ≥ 0.1%, OC ≥ 0.5%, average, Delle Site 2001)

Environmental Fate Rate Constants, k, or Half-Lives, $t_{1/2}$:
Biodegradation: aerobic $t_{1/2} \geq 10$ d for 0.01 μg/mL to biodegrade in river water (Eichelberger & Lichtenberg 1971; quoted, Muir 1991).

Half-Lives in the Environment:
Air:
Surface water: aerobic $t_{1/2} \geq 10$ d for 0.01 μg/mL to biodegrade in river water (Eichelberger & Lichtenberg 1971; quoted, Muir 1991);
persistence of up to 4 weeks in river water (Eichelberger & Lichtenberg 1971).
Ground water:
Sediment:
Soil: $t_{1/2}$ = 4.5 months at 15°C and 2.2 months at 30°C in soils (Freed & Haque 1973);
persistence of 8 months in soil (Edwards 1973; quoted, Morrill et al. 1982);
selected field $t_{1/2}$ = 60 d (Augustijn-Beckers et al. 1994; Hornsby et al. 1996).
Biota:

17.1.1.38 Fluchloralin



Common Name: Fluchloralin
Synonym: BAS-392H, Basalin
Chemical Name: *N*-(2-chloroethyl)-2,6-dinitro-*N*-propyl-4-(trifluoromethyl)benzenamine; N-(2-chloroethyl)α,α,α-trifluoro-2,6-dinitro-*N*-propyl-*p*-toluidine
Uses: herbicide for pre-plant or pre-emergence control of annual grass and broadleaf weeds in cotton, groundnuts, jute, potatoes, rice soybeans, and sunflowers, etc.
CAS Registry No: 33245-39-5
Molecular Formula: $C_{12}H_{13}ClF_3N_3O_4$
Molecular Weight: 355.697
Melting Point (°C):

42	(Lide 2003)

Boiling Point (°C):
Density (g/cm^3 at 20°C):
Molar Volume (cm^3/mol):

326.1	(calculated-Le Bas method at normal boiling point)

Dissociation Constant pK_a:
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
Entropy of Fusion, ΔS_{fus} (J/mol K):
Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F: 0.681 (mp at 42°C)

Water Solubility (g/m^3 or mg/L at 25°C or as indicated):

1.00	(20°C, Weber 1972; Ashton & Crafts 1981)
1.00	(Edwards 1977)
< 1.0	(Martin & Worthing 1977; Herbicide Handbook 1978, 1989)
0.70	(20°C, Spencer 1982)
< 1.0	(Worthing & Walker 1987, 1991; Tomlin 1994)
10	(Budavari 1989; Milne 1995)
0.90	(20–25°C, selected, Augustijn-Beckers et al. 1994; Hornsby et al. 1996)
0.50	(selected, Lohninger 1994)

Vapor Pressure (Pa at 25°C or as indicated):

0.0033 (20°C, Weber 1972; Worthing & Walker 1987)
0.373 (20°C, Ashton & Crafts 1981)
0.0008, 0.0033, 0.0133, 0.533 (20, 30, 40, 50°C, gas saturation, Spencer 1982)
0.0035 (Herbicide Handbook 1983; quoted, Nash 1988)
0.0037, 0.0033 (20°C, 30°C, Herbicide Handbook 1989)
0.004 (20°C, Worthing & Hance 1991; Tomlin 1994)
0.004 (20–25°C, selected, Augustijn-Beckers et al. 1994; Hornsby et al. 1996)

Henry's Law Constant (Pa·m^3/mol at 25°C or as indicated):

1.174	(20°C, calculated-P/C, Muir 1991)
1.343	calculated-P/C, this work)

Octanol/Water Partition Coefficient, log K_{OW}:

4.63	(selected, Magee 1991)

4.70 (CLOGPSTAR or CLOGP data, Sabljic et al. 1995)

Bioconcentration Factor, log BCF:

> 2.79, 2.40 (calculated-S, calculated-K_{OC}, Kenaga 1980)

Sorption Partition Coefficient, log K_{OC}:

3.56 (soil, Harvey 1974)
3.60 (soil, Kenaga 1980)
> 3.64 (soil, calculated-S as per Kenaga & Goring 1980, Kenaga 1980)
4.25 (calculated-MCI χ, Bahnick & Doucette 1988)
3.56; 3.58 (reported as log K_{OM}, estimated as log K_{OM}, Magee 1991)
3.48 (20–25°C, estimated, Augustijn-Beckers et al. 1994; Hornsby et al. 1996)
3.80 (estimated-chemical structure, Lohninger 1994)
3.55 (soil, calculated-MCI ${}^1\chi$, Sabljic et al. 1995)
3.55; 4.02 (soil, quoted obs.; estimated-general model using molecular descriptors, Gramatica et al. 2000)

Environmental Fate Rate Constants, k, or Half-Lives, $t_{½}$:

Volatilization: estimated $t_{½}$ ~ 1 d from 1 m depth of water (20°C, Muir 1991).

Photolysis: $t_{½}$ = 13 d for 84% of 5 μg/mL to degrade in distilled water under sunlight (Nilles & Zabik 1974; quoted, Cessna & Muir 1991);
$t_{½}$ = 8 h for 50% of 2000 μg/mL to degrade in methanol under sunlight (Plimmer & Klingebiel 1974; quoted, Cessna & Muir 1991).

Oxidation:

Hydrolysis:

Biodegradation: $t_{½}$ = 8 d for 0.5 μg/mL to biodegrade in soil at 20–42°C (Savage 1978; quoted, Muir 1991);
$t_{½}$ = 3.6 wk for 2.0 μg/mL to biodegrade in soil at 25°C (Brewer et al. 1982; quoted, Muir 1991).

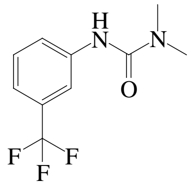
Biotransformation:

Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants:

Half-Lives in the Environment:

Soil: $t_{½}$ = 8 d for 0.5 μg/mL to biodegrade in soil at 20–42°C (Savage 1978; quoted, Muir 1991);
$t_{½}$ = 1.5 d on Bosket silt loam, $t_{½}$ = 4 d on Sharkey clay for the first 3 to 5 days when sprayed onto soil surface, rate of loss much slower for the remainder of the 7- or 12-d sampling period with $t_{½}$ = 13 d on Bosket silt loam, $t_{½}$ = 8 d on Sharkey clay (Savage & Jordon 1980)
measured dissipation rate k = 0.099–0.13 d^{-1} (derived from Savage & Jordan 1980, Nash 1988);
field studies, $t_{½}$ = 12.2 wk - 1978 first study; $t_{½}$ = 13.0 wk -1978 second study; $t_{½}$ = 17.6 wk -1979, in a Crowley silt loam at Stuttgart, Arkansas (Brewer et al. 1982)
Laboratory studies: $t_{½}$ = 28.7 wk at 4°C, 10.5 wk at 25°C for soils of field capacity moisture (27% w/w for Crowley silt loam) and $t_{½}$ = 20.8 wk at 4°C, $t_{½}$ = 8.4 wk at 25°C for flooded soil of Crowley silt loam; $t_{½}$ = 29.3 wk at 4°C, $t_{½}$ = 10.5 wk at 25°C for soil of field capacity moisture (34% w/w for Sharkey silty clay) and $t_{½}$ = 20.8 wk at 4°C and $t_{½}$ = 4.3 wk at 25°C for flooded soil, Sharkey silty clay (Brewer et al. 1982);
$t_{½}$ = 3.6 wk for 2.0 μg/mL to biodegrade in soil at 25°C (derived form Brewer et al. 1982, Muir 1991);
estimated dissipation rate k = 0.29, and 0.120 d^{-1} (Nash 1988);
estimated field $t_{½}$ ~ 60 d (Augustijn-Beckers et al. 1994; Hornsby et al. 1996).

17.1.1.39 Fluometuron



Common Name: Fluometuron
Synonym: CIBA 2059, Cotoran, Cottonex, Higalcoton, Lanex, Meturon, Pakhtaran
Chemical Name: 1,1-dimethyl-3-(α,α,α-trifluoro-*m*-tolyl)urea; N,N-dimethyl-N′-[3-(trifluoromethyl)phenyl]urea
Uses: herbicide to control many annual broadleaf weeds in sugar cane and cotton.
CAS Registry No: 2164-17-2
Molecular Formula: $C_{10}H_{11}F_3N_2O$
Molecular Weight: 232.201
Melting Point (°C):

163–164.5	(Hartley & Kidd 1987; Herbicide Handbook 1989; Worthing & Hance 1991; Montgomery 1993; Tomlin 1994; Milne 1995)
164	(Lide 2003)

Boiling Point (°C):
Density (g/cm^3 at 20°C):

1.390	(Hartley & Kidd 1987; Worthing & Hance 1991; Montgomery 1993; Tomlin 1994; Milne 1995)

Molar Volume (cm^3/mol):

229.7	(calculated-Le Bas method at normal boiling point)
167.1	(calculated-density)

Dissociation Constant pK_a:

–1.00	(Sangster 1993)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

29.706	(DSC method, Plato 1972)

Entropy of Fusion, ΔS_{fus} (J/mol K):

Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F: 0.0433 (mp at 164°C)

Water Solubility (g/m^3 or mg/L at 25°C or as indicated):

90	(Melnikov 1971; Spencer 1973, 1982; quoted, Wauchope 1978; Khan 1980; Weber et al. 1980)
90	(20°C, Martin & Worthing 1977; Herbicide Handbook 1978,89)
106	(shake flask-UV, Briggs 1981)
90	(Herbicide Handbook 1983)
105	(20°C, Hartley & Kidd 1987; Worthing & Walker 1987, 1991)
110	(20–25°C, selected, Wauchope et al. 1992; Hornsby et al. 1996)
80	(Montgomery 1993)
110	(Tomlin 1994)

Vapor Pressure (Pa at 25°C or as indicated):

6.70×10^{-5}	(20–25°C, Weber et al. 1980)
6.70×10^{-5}	(Herbicide Handbook 1983)
6.70×10^{-5}	(20°C, Hartley & Kidd 1987; Herbicide Handbook 1989; Montgomery 1993)
6.60×10^{-5}	(20°C, Worthing & Hance 1991)
1.25×10^{-4}	(20–25°C, selected, Wauchope et al. 1992; Hornsby et al. 1996)
1.25×10^{-4}	(Tomlin 1994)

Henry's Law Constant ($Pa \cdot m^3/mol$ at 25°C or as indicated):

< 0.283	(20–25°C, calculated-P/C, Montgomery 1993)
1.73×10^{-4}	(calculated-P/C, this work)

Octanol/Water Partition Coefficient, log K_{OW}:

1.34	(Briggs 1969)
2.42	(shake flask-UV, Briggs 1981)
1.88	(shake flask-UV, pH 5, Barak et al. 1983)
2.40	(selected, Gerstl & Helling 1987)
2.23	(Worthing & Hance 1991; Tomlin 1994; Milne 1995)
2.23, 2.38	(Montgomery 1993)
2.03	(RP-HPLC-RT correlation, Sicbaldi & Finizio 1993)
2.20	(recommended, Sangster 1993)
2.42	(recommended, Hansch et al. 1995)
2.03	(RP-HPLC-RT correlation, Finizio et al. 1997)

Bioconcentration Factor, log BCF:

1.67	(calculated-S, Kenaga 1980)
0.954	(calculated-K_{OC}, Kenaga 1980)

Sorption Partition Coefficient, log K_{OC}:

2.24	(soil, Abernethy & Davidson 1971; Davidson & McDougal 1973; Savage & Wauchope 1974; Carringer et al. 1975; Wood & Davidson 1975)
2.30	(soil, Kenaga 1980)
2.57	(soil, calculated-S as per Kenaga & Goring 1980, Kenaga 1980)
1.82	(soil, converted from reported K_{OM} multiplied by 1.724, Briggs 1981)
2.30	(calculated-MCI χ, Gerstl & Helling 1987)
2.00	(soil, 20–25°C, selected, Wauchope et al. 1992; Hornsby et al. 1996)
1.46–2.08	(Montgomery 1993)
2.00	(estimated-chemical structure, Lohninger 1994)
1.49–2.07	(Tomlin 1994)
2.00	(soil, calculated-MCI $^{1}\chi$, Sabljic et al. 1995)
2.33; 2.66., 2.03, 2.64, 2.36, 1.94	(quoted lit., calculated-K_{OW}; HPLC-screening method with different LC-columns, Szabo et al. 1999)
2.14, 2.51	(soil, estimated-class-specific model, estimated-general model using molecular descriptors, Gramatica et al. 2000)

Environmental Fate Rate Constants, k, or Half-Lives, $t_{1/2}$:

Volatilization:

Photolysis: $t_{1/2}$ = (11 ± 2 h) in 10 ppm aqueous solutions under summer sunlight of 9.1 h/d exposure and $t_{1/2}$ = (33 ± 16) h under spring sunlight of 3.7 h/d exposure (Burkhard et al. 1975).

Oxidation:

Hydrolysis: $t_{1/2}$ = 1.6 yr at 20°C and pH 1, $t_{1/2}$ = 2.4 yr at pH 5, and $t_{1/2}$ = 2.8 yr at pH 9 (Montgomery 1993).

Biodegradation:

Biotransformation:

Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants:

Half-Lives in the Environment:

Air:

Surface water: $t_{1/2}$ = 730–1010 d at pH 5–9 and 20°C in aqueous solutions (Herbicide Handbook 1989).

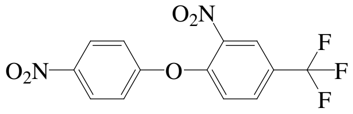
Ground water:

Sediment:

Soil: measured dissipation rate k = 0.023–0.043 d^{-1} (Horowitz & Herzlinger 1974: quoted, Nash 1988);
estimated dissipation rate k = 0.0012, and 0.011 d^{-1} (Nash 1988);
persistence of 4 months in soil (Wauchope 1978);
selected field $t_{1/2}$ = 85 d (Wauchope et al. 1992; Hornsby et al. 1996);
soil $t_{1/2}$ = 30 d (Pait et al. 1992);
median $t_{1/2}$ ~ 30 d in soil (Herbicide Handbook 1989; Tomlin 1994).

Biota:

17.1.1.40 Fluorodifen



Common Name: Fluorodifen
Synonym: Preforan, Soyex
Chemical Name: 4-nitrophenyl α,α,α-trifluoro-2-nitro-*p*-tolyl ether
Uses: herbicide.
CAS Registry No: 15457-05-3
Molecular Formula: $C_{13}H_7F_3N_2O_5$
Molecular Weight: 328.200
Melting Point (°C):
94 (Spencer 1982; Milne 1995; Lide 2003)
Boiling Point (°C):
Density (g/cm^3 at 20°C):
Molar Volume (cm^3/mol):
282.6 (calculated-Le Bas method at normal boiling point)
Dissociation Constant pK_a:
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
Entropy of Fusion, ΔS_{fus} (J/mol K):
Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F: 0.210 (mp at 94°C)

Water Solubility (g/m^3 or mg/L at 25°C or as indicated):

2.0	(20°C, Spencer 1973, 1982)
< 2.0	(Weber et al. 1980)
2.0	(shake flask-HPLC, Ellgehausen et al. 1981)
2.0	(20°C, Worthing & Walker 1987, Worthing & Hance 1991)

Vapor Pressure (Pa at 25°C or as indicated):

9.33×10^{-6}	(20°C, Spencer 1982)

Henry's Law Constant (Pa·m^3/mol):

Octanol/Water Partition Coefficient, log K_{OW}:

3.30	(shake flask-HPLC, Ellgehausen et al. 1980; Geyer et al. 1991)
4.40	(20 ± 2°C, shake flask-UV, Briggs 1981)
3.65	(shake flask-HPLC, Ellgehausen et al. 1981)
3.60	(HPLC-RT correlation, Nandihalli et al. 1993)
3.65	(recommended, Sangster 1993)
3.65	(recommended, Hansch et al. 1995)

Bioconcentration Factor, log BCF:

2.019	(algae, log BF-bioaccumulation factor, Ellgehausen et al. 1980)
2.386	(catfish, log BF-bioaccumulation factor, Ellgehausen et al. 1980)
1.178	(daphnids, log BF-bioaccumulation factor, Ellgehausen et al. 1980)

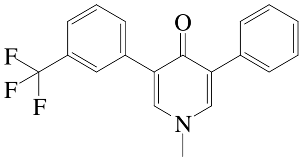
Sorption Partition Coefficient, log K_{OC}:

3.13	(calculated-MCI χ, Gerstl & Helling 1987)

Environmental Fate Rate Constants, k, or Half-Lives. $t_{½}$:

Half-Lives in the Environment:

17.1.1.41 Fluridone



Common Name: Fluridone
Synonym: Brake, EL-171, Fluridon, Pride, Sonar
Chemical Name: 1-methyl-3-phenyl-5-[3-(trifluoromethyl)phenyl] 4(1H)-pyridinone; 1-methyl-3-phenyl-5-(α,α,α-trifluoro-m-tolyl)-4-pyridone
Uses: herbicide to control annual grass and broadleaf weeds and certain perennial species in cotton; also used to control aquatic weeds and plants in lakes, ponds, ditches, etc.
CAS Registry No: 59756-60-4
Molecular Formula: $C_{19}H_{14}F_3NO$
Molecular Weight: 329.315
Melting Point (°C):
155 (Lide 2003)
Boiling Point (°C):
Density (g/cm^3 at 20°C):
Molar Volume (cm^3/mol):
333.5 (calculated-Le Bas method at normal boiling point)
Dissociation Constant:
12.3 (pK_b, Wauchope et al. 1992)
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
Entropy of Fusion, ΔS_{fus} (J/mol K):
Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F: 0.0530 (mp at 155°C)

Water Solubility (g/m^3 or mg/L at 25°C or as indicated):
12.0 (20°C, Weber 1972; Worthing & Walker 1987)
12.0 (Kenaga 1980)
12.0 (Herbicide Handbook 1983, 1989; Budavari 1989; Milne 1995)
12.0 (Hartley & Kidd 1987; Worthing & Walker 1987, Worthing & Hance 1991)
10.0 (20–25°C, selected, Wauchope et al. 1992; Hornsby et al. 1996)
10.0 (selected, Lohninger 1994)

Vapor Pressure (Pa at 25°C or as indicated):
1.31×10^{-5} (20°C, Weber 1972; Worthing & Walker 1987)
1.00×10^{-5} (Herbicide Handbook 1983)
0.013 (Hartley & Kidd 1987; Worthing & Hance 1991)
1.33×10^{-5} (Herbicide Handbook 1989)
1.33×10^{-5} (20–25°C, selected, Wauchope et al. 1992; Hornsby et al. 1996)
1.30×10^{-5} (Tomlin 1994)

Henry's Law Constant (Pa·m^3/mol at 25°C or as indicated):
3.59×10^{-4} (20°C, calculated-P/C, Muir 1991)

Octanol/Water Partition Coefficient, log K_{OW}:
1.87 (Reinert 1989)
1.87 (Worthing & Hance 1991; Tomlin 1994; Milne 1995)
2.98 (shake flask, Takahashi et al. 1993; quoted, Sangster 1993)
3.16 (LOGPSTAR or CLOGP data, Sabljic et al. 1995)

Bioconcentration Factor, log BCF:

2.18 (calculated-S, Kenaga 1980; quoted, Isensee 1991)
0.778 (measured, West et al. 1983; quoted, Isensee 1991)

Sorption Partition Coefficient, log K_{OC} at 25°C or as indicated:

1.60 (soil, Kenaga 1980)
2.97–3.39 (pond sediment, Muir et al. 1980)
3.36, 2.95 (lake and river sediment, Muir et al. 1980)
2.94 (Reinert 1989)
2.90, 3.81, 3.03 (Norfolk sand pH 6.0, Norfold with montmorillonite pH 5.9, Norfolk sand with added organic matter pH 5.3, Reinert 1989)
3.43, 2.57, 2.43 (California soil at pH 6, 7, 7.3, Reinert 1989)
3.00 (20–25°C, selected, Wauchope et al. 1992; Hornsby et al. 1996)
3.00 (selected, Lohninger 1994)
2.85 (soil, calculated-MCI $^1\chi$, Sabljic et al. 1995)

Environmental Fate Rate Constants, k, or Half-Lives, $t_{1/2}$:

Volatilization: estimated $t_{1/2}$ = 10,000 d from 1 m depth of water at 20°C (Muir 1991).

Photolysis: $t_{1/2}$ ~ 23 h to degrade in distilled water under > 290 nm light (West et al. 1979; quoted, Cessna & Muir 1991);

$t_{1/2}$ ~ 6 h for 5 μg/mL to degrade in nonsterile pond water under sunlight (Muir & Grift 1982; quoted, Cessna & Muir 1991);

$t_{1/2}$ = 27 d for 85% of 10 μg/mL to degrade in distilled water and for 85% of 10 μg/mL to degrade in lake water at pH 8.4 both under sunlight (Sanders & Mosier 1983; quoted, Cessna & Muir 1991; Howard et al. 1991)

resistance to decomposition by UV light with $t_{1/2}$ = 23 h in deionized water (Herbicide Handbook 1989).

Oxidation: photooxidation $t_{1/2}$ = 0.359–3.20 h, based on estimated rate constant for reaction with hydroxyl radicals (Atkinson 1987; quoted, Howard et al. 1991) and ozone (Atkinson & Carter 1984; quoted, Howard et al. 1991).

Hydrolysis: $t_{1/2}$ > 113 d for 1 μg/mL to hydrolyze in pond water at 4°C (Ghassemi et al. 1981; quoted, Muir 1991); $t_{1/2}$ = 23 h in water (Tomlin 1994).

Biodegradation: aqueous aerobic $t_{1/2}$ = 44–192 d, based on soil die-away test data and field study soil persistence (Banks et al. 1979; quoted, Howard et al. 1991);

$t_{1/2}$ = 12 months for 5 μg/mL to biodegrade in static sediment and water, and $t_{1/2}$ ~ 9 months in aerobic and anaerobic sediment and water all at 25°C (Muir & Grift 1982; quoted, Muir 1991);

aqueous anaerobic $t_{1/2}$ = 176 d to 2.1 yr, based on estimated unacclimated aqueous aerobic biodegradation half-life (Howard et al. 1991);

microbial degradation $t_{1/2}$ > 343 d at pH 7.3 with 2.6% organic matter in a silt loam soil (Tomlin 1994).

Biotransformation:

Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants:

k_1 = 0.9–1.3 h^{-1} (*Chironomus tentans* larvae in pond sediment-water system, 96-h exposure, calculated by using first-order kinetic and concn factors, Muir et al. 1983)

k_1 = 0.70–5.6 h^{-1} (*Chironomus tentans* larvae in river sediment-water system, 96-h exposure, calculated by using first-order kinetic and concn factors, Muir et al. 1983)

k_1 = 1.7–3.40 h^{-1} (*Chironomus tentans* larvae in sediment (sand)-water system, 96-h exposure, calculated by using first-order kinetic and concn factors, Muir et al. 1983)

k_1 = 1.7–2.1 h^{-1} (*Chironomus tentans* larvae in sediment (sand)-water system, 96-h exposure, calculated by using initial uptake data of 0–12 h, Muir et al. 1983)

k_2 = 0.052 h^{-1} (*Chironomus tentans* larvae in pond sediment-water system, calculated by concentration decay curve, Muir et al. 1983)

k_2 = 0.118 h^{-1} (*Chironomus tentans* larvae in river water system, calculated by concentration decay curve, Muir et al. 1983)

k_2 = 0.055 h^{-1} (*Chironomus tentans* larvae in river sediment-water system, calculated by concentration decay curve, Muir et al. 1983)

k_2 = 0.041 h^{-1} (*Chironomus tentans* larvae in sediment (sand)-water system, calculated by concentration decay curve, Muir et al. 1983)

Half-Lives in the Environment:

Air: $t_{1/2}$ = 0.359–3.20 h, based on estimated rate constant for reaction with hydroxyl radicals (Atkinson 1987; quoted, Howard et al. 1991) and ozone (Atkinson & Carter 1984; quoted, Howard et al. 1991).

Surface water: $t_{1/2}$ ~ 21 d in water (Hartley & Kidd 1987);
$t_{1/2}$ = 288–864 h, based on estimated photolysis half-life in water (Howard et al. 1991);
anaerobic $t_{1/2}$ = 9 months and aerobic $t_{1/2}$ ~ 20 d (Tomlin 1994).

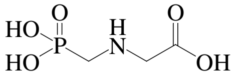
Ground water: $t_{1/2}$ = 2112–9216 h, based on estimated unacclimated aqueous aerobic biodegradation half-life (Howard et al. 1991).

Sediment: $t_{1/2}$ = 12 months for 5 μg/mL to biodegrade in static sediment and water, and $t_{1/2}$ ~ 9 months in aerobic and anaerobic sediment and water all at 25°C (Muir & Grift 1982; quoted, Muir 1991).

Soil: measured dissipation rate k = 0.0041 d^{-1} (Banks et al. 1979; quoted, Nash 1988) with estimated $t_{1/2}$ = 44–192 d (Banks et al. 1979; quoted, Howard et al. 1991);
estimated dissipation rate k = 0.0067 and 0.025 d^{-1} (Nash 1988);
selected field $t_{1/2}$ = 21 d (Wauchope et al. 1992; Hornsby et al. 1996);
$t_{1/2}$ ~ 90 d in the hydrosoil (Tomlin 1994).

Biota: elimination $t_{1/2}$ = 13.2 h in pond sediment-water, $t_{1/2}$ = 5.9 h in river water, $t_{1/2}$ = 12.5 h in river sediment-water, $t_{1/2}$ = 16.9 in sand-water systems (*Chironomus tentans* larvae, Muir et al. 1983)

17.1.1.42 Glyphosate



Common Name: Glyphosate
Synonym: Mon-0573, 0468, 2139; Polado, Roundup
Chemical Name: *N*-(phosphoromethyl)glycine
Uses: nonselective, post-emergent, broad spectrum herbicide to control annual and perennial grasses, sedges, broadleaf, and emerged aquatic weeds; also used to control insects on fruit trees.
CAS Registry No: 1071-83-6
Molecular Formula: $C_3H_8NO_5P$
Molecular Weight: 169.074
Melting Point (°C):

230	(dec., Montgomery 1993; Milne 1995; Lide 2003)

Boiling Point (°C):
Density (g/cm^3 at 20°C):

1.74	(Herbicide Handbook 1989; Montgomery 1993)

Molar Volume (cm^3/mol):
Dissociation Constant pK_a:

5.70	(Worthing & Hance 1991)
2.60, 5.90, 10.40	(pK_1, pK_2, pK_3, Yao & Haag 1991; Haag & Yao 1992)
2.32, 5.86, 10.86	(pK_1, pK_2, pK_3, Montgomery 1993; Hornsby et al. 1996)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
Entropy of Fusion, ΔS_{fus} (J/mol K):
Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F: 0.0097 (mp at 230°C)

Water Solubility (g/m^3 or mg/L at 25°C):

10000	(Spencer 1973, 1982; Herbicide Handbook 1978; Ashton & Crafts 1981)
12000	(Martin & Worthing 1977; Worthing & Walker 1987, Worthing & Hance 1991; Tomlin 1994)
15700	(Herbicide Handbook 1989)
12000	(Budavari 1989; Montgomery 1993; Milne 1995)

Vapor Pressure (Pa at 25°C or as indicated):

2.59×10^{-5}	(45°C, Herbicide Handbook 1989)
4.00×10^{-5}	(Worthing & Hance 1991)
0.001	(Montgomery 1993; quoted, Majewski & Capel 1995)
negligible	(Tomlin 1994)
0.0	(selected, Halfon et al. 1996)

Henry's Law Constant (Pa m^3/mol at 25°C):

1.41×10^{-5}	(calculated-P/C, Montgomery 1993)

Octanol/Water Partition Coefficient, log K_{OW}:

–1.70	(shake flask, pH 5.3, Martin & Edgington 1981)
–4.10	(shake flask, pH 2.5, Stevens et al. 1988)
–3.25	(Reinert 1989)
–4.59	(Worthing & Hance 1991)
–1.60	(Montgomery 1993)
–4.10, –1.70	(pH 2.5, pH 5.3, quoted, Sangster 1993)
–1.70	(pH 5.3, selected, Hansch et al. 1995)
0.94	(RP-HPLC-RT correlation, Finizio et al. 1997)

Bioconcentration Factor, log BCF:

0.477	(calculated-S, Kenaga 1980; quoted, Isensee 1991)
2.26	(calculated-K_{OC}, Kenaga 1980)

Sorption Partition Coefficient, log K_{OC}:

3.42	(soil, Sprankle et al. 1975; Hance 1976; Nomura & Hilton 1977)
1.40	(soil, calculated-S as per Kenaga & Goring 1980, Kenaga 1980)
1.22	(selected, USDA 1989; quoted, Neary et al. 1993)
–0.43	(Reinert 1989)

3.69, 3.53, 3.42 (3 agricultural soils: Houston clay loam at pH 7.5, Muskingum silt loam at pH 5.8, Sassafras sandy loam at pH 5.6, Reinert 1989)

4.38	(organic carbon, Wauchope et al. 1991)
3.43–3.69	(Montgomery 1993)

Environmental Fate Rate Constants, k, or Half-Lives, $t_{½}$:

Volatilization:

Photolysis: $t_{½}$ = 48 h for 0% of 168 μg/mL to degrade in distilled water under > 290 nm light (Rueppel et al. 1977; quoted, Cessna & Muir 1991);

$t_{½}$ = 9 wk for > 90% of 2 μg/mL to degrade in distilled water under sunlight (Lund-Høie & Friestad 1986; quoted, Cessna & Muir 1991);

$t_{½}$ = 4.0 d and 3–4 wk for aqueous solutions of 1.0 and 2000 ppm under indoor UV light (Lund-Høie & Friestad 1986; quoted, Montgomery 1993).

Oxidation:

k(aq.) = 7.3×10^8 M^{-1} s^{-1} for the reaction (photo-Fenton with reference to glycolic acid) with hydroxyl radical in aqueous solutions at pH 3.8 and at 24 ± 1°C (Buxton et al. 1988; quoted, Faust & Hoigné 1990; Haag & Yao 1992)

k(aq.) = $(0.027–8.2) \times 10^3$ M^{-1} s^{-1} for direct reaction with ozone in water at pH 1.8–7.0 and 22 ± 2°C, with a half-life of 4.0 s at pH 7 (Yao & Haag 1991).

k(aq.) = $(1.8 \pm 0.5) \times 10^8$ M^{-1} s^{-1} for the reaction (photo-Fenton with reference to glycolic acid) with hydroxyl radical in aqueous solutions at pH 3.8 and at 24 ± 1°C (Haag & Yao 1992).

Hydrolysis: $t_{½}$ = 7 d for 10 μg/mL to hydrolyze in sterile water + soil (Rueppel et al. 1977; quoted, Muir 1991);

$t_{½}$ = 32 d for 25 and 250 μg/mL to hydrolyze in sterile distilled water at pH 3, 6 and 9 in the dark at 5 and 35°C (Ghassemi et al. 1981; quoted, Muir 1991)

Biodegradation: $t_{½}$ < 28 d for 10 μg/mL to biodegrade in soil-water suspension (Rueppel et al. 1977; quoted, Muir 1991);

$t_{½}$ > 9 wk for 2 μg/mL to biodegrade in polluted lake water (Rueppel et al. 1977; quoted, Muir 1991);

rate constant k = 0.1 d^{-1} from soil incubation die-away studies (Rao & Davidson 1980; quoted, Scow 1982);

$t_{½}$ = 70 d in pond water at pH 7.2, $t_{½}$ = 63 d in swamp water at pH 6.3 and $t_{½}$ = 49 d in Sphagnum bog water at pH 4.2 (Ghassemi et al. 1981; quoted, Muir 1991).

Biotransformation:

Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants:

Half-Lives in the Environment:

Air:

Surface water: $t_{½}$ > 9 wk for 2 μg/mL to biodegrade in polluted lake water (Rueppel et al. 1977; quoted, Muir 1991);

$t_{½}$ = 70 d in pond water at pH 7.2, $t_{½}$ = 63 d in swamp water at pH 6.3 and $t_{½}$ = 49 d in Sphagnum bog water at pH 4.2 (Ghossemi et al. 1981; quoted, Muir 1991);

measured rate constant k = $(0.027 - 8.2) \times 10^3$ M^{-1} s^{-1} for direct reaction with ozone in water at pH 1.8–7.0 and 22 ± 2°C, with $t_{½}$ = 4.0 s at pH 7 (Yao & Haag 1991).

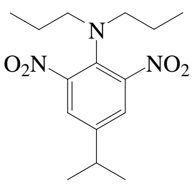
Ground water:

Sediment:

Soil: $t_{1/2}$ < 28 d for 10 μg/mL to biodegrade in soil-water suspension (Rueppel et al. 1977; quoted, Muir 1991);
estimated first-order $t_{1/2}$ = 7 d from biodegradation rate constant k = 0.1 d^{-1} from soil incubation die-away studies (Rao & davidson 1980; quoted, Scow 1982);
moderately persistent in soil with $t_{1/2}$ = 20–100 d (Willis & McDowell 1982);
average $t_{1/2}$ < 60 d (Hartley & Kidd 1987; Herbicide Handbook 1989; quoted, Montgomery 1993);
selected $t_{1/2}$ = 47 d (Wauchope et al. 1991; quoted, Dowd et al. 1993; Halfon et al. 1996).

Biota: average $t_{1/2}$ = 60 d in the forest (USDA 1989; quoted, Neary et al. 1993).

17.1.1.43 Isopropalin



Common Name: Isopropalin
Synonym: EL 179, Isopropaline, Isopropalin solution, Paarlan
Chemical Name: 4-isopropyl-2,6-dinitro-*N,N*-dipropylaniline; 4-(1-methylethyl)-2,6-dinitro-*N,N*-dipropylbenzenamine; 2,6-dinitro-*N,N*-dipropylcumidine
Uses: herbicide used pre-planting and incorporated with soil preparation to control broadleaf weeds and grasses in transplanted tobacco, and in direct-seeded tomatoes and capsicums.
CAS Registry No: 33820-53-0
Molecular Formula: $C_{15}H_{23}N_3O_4$
Molecular Weight: 309.362
Melting Point (°C): liquid
Boiling Point (°C):
Density (g/cm^3 at 20°C):
Molar Volume (cm^3/mol):

361.3	(calculated-Le Bas method at normal boiling point)

Dissociation Constant pK_a:
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
Entropy of Fusion, ΔS_{fus} (J/mol K):
Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F: 1.0

Water Solubility (g/m^3 or mg/L at 25°C or as indicated):

0.11	(Martin & Worthing 1977; Herbicide Handbook 1978)
1.10	(Ashton & Crafts 1981)
0.10	(Spencer 1982; Hartley & Kidd 1987; Budavari 1989; Milne 1955)
0.10	(Worthing & Walker 1987, Worthing & Hance 1991)
0.08	(Herbicide Handbook 1989)
0.10	(20–25°C, selected, Wauchope et al. 1992; Hornsby et al. 1996)
0.02	(predicted-AQUAFAC, Lee et al. 1996)

Vapor Pressure (Pa at 25°C or as indicated):

0.0019	(30°C, Ashton & Crafts 1981)
0.0019	(30°C, Hartley & Kidd 1987)
0.0040	(25.6°C, Herbicide Handbook 1989)
0.0012	(20–25°C, selected, Wauchope et al. 1992; Hornsby et al. 1996)

Henry's Law Constant (Pa·m^3/mol at 25°C):

5.34	(calculated-P/C, this work)

Octanol/Water Partition Coefficient, log K_{OW}:

Bioconcentration Factor, log BCF:

3.50	(calculated-S, Kenaga 1980; quoted, Isensee 1991)
3.88	(calculated-K_{OC}, Kenaga 1980)

Sorption Partition Coefficient, log K_{OC}:

4.88	(soil, Harvey 1974)
4.17	(soil, calculated-S as per Kenaga & Goring 1980, Kenaga 1980)
4.17–4.88	(soil, quoted values, Bottoni & Funari 1992)

4.00	(20–25°C, selected, Wauchope et al. 1992; Hornsby et al. 1996)
4.00	(selected, Lohninger 1994)
3.50	(soil, estimated-general model using molecular descriptors, Gramatica et al. 2000)

Environmental Fate Rate Constants, k, or Half-Lives, $t_{1/2}$:

Volatilization:

Photolysis: atmosphere photolysis $t_{1/2}$ = 288–864 h, based on observed photolysis on soil TLC plates under summer sunlight (Helling 1976; quoted, Howard et al. 1991) and adjusted for relative winter sunlight intensity (Lyman et al. 1982; quoted, Howard et al. 1991); aqueous photolysis $t_{1/2}$ = 288–864 h, based on observed photolysis on soil TLC plates under summer sunlight (Helling 1976; quoted, Howard et al. 1991) and adjusted for relative winter sunlight intensity (Lyman et al. 1982; quoted, Howard et al. 1991).

Oxidation: photooxidation $t_{1/2}$ = 0.743–74.3 h in air, based on estimated rate constant for the vapor-phase reaction with hydroxyl radicals in air (Atkinson 1987; quoted, Howard et al. 1991).

Hydrolysis:

Abiotic Transformation: Degradation by abiotic reductive transformations:

$k = 1.71\ M^{-1}\ s^{-1}$ in H_2S with (mecapto)juglone (hydroquinone moiety, an abiotic reductant found in natural systems) solution at pH 6.65 (Wang & Arnold 2003)

Aqueous solutions with surface-bound Fe(II) species and their furst-order rate constants as:

$k = 0.94 \times 10^{-3}\ h^{-1}$ at pH 6.5, $k = 0.36 \times 10^{-2}\ h^{-1}$ at pH 7.0, $k = 0.057\ h^{-1}$ at pH 7.4, and $k = 1.76\ h^{-1}$ at pH 7.8 for aqueous ferrous ion system;

$k = 0.297\ h^{-1}$ at pH 6.5, $k = 0.586\ h^{-1}$ at pH 6.7, $k = 1.28\ h^{-1}$ at pH 7.0, and $k = 6.90\ h^{-1}$ at pH 7.3 for Fe(II)/goethite system;

$k = 9.91 \times 10^{-3}\ h^{-1}$ at pH 6.5, $k = 8.45 \times 10^{-3}\ h^{-1}$ at pH 7.0, $k = 7.45 \times 10^{-3}\ h^{-1}$ at pH 7.4 and $k = 6.96 \times 10^{-2}\ h^{-1}$ at pH 7.8 for Fe(II)/clay system, all with total dissolved Fe(II) = 1 mM (Wang & Arnold 2003)

Biodegradation:

$t_{1/2}$(aq. aerobic) = 408–2520 h, based on aerobic soil die-away test data for one soil at 15°C and 30°C (Gingerich & Zimdahl 1976; quoted, Howard et al. 1991)

$t_{1/2}$(aq. anaerobic) = 96–360 h, based on anaerobic soil die-away test that tested one soil (Gingerich & Zimdahl 1976; quoted, Howard et al. 1991)

Biotransformation:

Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants:

Half-Lives in the Environment:

Air: $t_{1/2}$ = 0.743–74.3 h, based on estimated rate constant for the vapor-phase reaction with hydroxyl radicals in air (Atkinson 1987; quoted, Howard et al. 1991).

Surface water: $t_{1/2}$ = 288–864 h, based on observed photolysis on soil TLC plates under summer sunlight (Helling 1976; quoted, Howard et al. 1991) and adjusted for relative winter sunlight intensity (Lyman et al. 1982; quoted, Howard et al. 1991).

Ground water: $t_{1/2}$ = 96–5040 h, based on estimated unacclimated aqueous aerobic and anaerobic degradation half-lives (Howard et al. 1991)

reported $t_{1/2}$ < 180 d (Bottoni & Funari 1992)

Sediment:

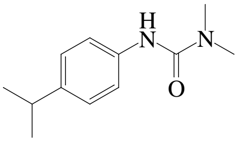
Soil: $t_{1/2}$ = 408–2520 h, based on aerobic soil die-away test data for one soil at 15°C and 30°C (Gingerich & Zimdahl 1976; quoted, Howard et al. 1991);

selected field $t_{1/2}$ = 100 d (Wauchope et al. 1992; Hornsby et al. 1996);

$t_{1/2}$ < 180 d (Bottoni & Funari 1992).

Biota:

17.1.1.44 Isoproturon



Common Name: Isoproturon
Synonym: Alon, Arelon, CGA 18731, Gramion, Graminon, Hoe 16410, Hytane, IP 50, IP flo, Tolkan
Chemical Name: 3-(4-isopropylphenyl)-1,1-dimethylurea; 3-*p*-cumenyl-l-1-dimethylurea
Uses: herbicide used for pre- and post-emergence control of annual grasses and broadleaf weeds in spring and winter wheat (except durum wheat), spring and winter barley, winter rye, and triticale.
CAS Registry No: 34123-59-6
Molecular Formula: $C_{12}H_{18}N_2O$
Molecular Weight: 206.284
Melting Point (°C):

155–156	(Worthing & Hance1991)
158	(Tomlin 1994)

Boiling Point (°C):
Density (g/cm^3 at 20°C):

1.16	(Hartley & Kidd 1987; Tomlin 1994)

Molar Volume (cm^3/mol):

259.1	(calculated-Le Bas method at normal boiling point)

Dissociation Constant pK_a:
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
Entropy of Fusion, ΔS_{fus} (J/mol K):
Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F:

Water Solubility (g/m^3 or mg/L at 25°C or as indicated):

60	(Martin & Worthing 1977)
70	(20°C, Spencer 1982)
72	(20°C, Hartley & Kidd 1987)
55	(Worthing & Walker 1987, Worthing & Hance 1991)
55.9	(Chaumat et al. 1991)
65	(22°C, Tomlin 1994; quoted, Otto et al. 1997)
65	(20°C, selected, Traub-Eberhard et al. 1994)

Vapor Pressure (Pa at 25°C or as indicated):

3.3×10^{-6}	(20°C, Spencer 1982; Hartley & Kidd 1987)
3.3×10^{-6}	(20°C, Worthing & Hance 1991)

3.3×10^{-6}, 3.15×10^{-2}, 0.172 (20, 77, 150°C, Tomlin 1994)

Henry's Law Constant (Pa·m^3/mol at 25°C):

1.05×10^{-5}	(calculated-P/C, Otto et al. 1997)
1.24×10^{-5}	(calculated-P/C, this work)

Octanol/Water Partition Coefficient, log K_{OW} at 25°C or as indicated:

2.87	(shake flask, Log P Database, Hansch & Leo 1987)
2.25	(Worthing & Hance 1991)
2.30	(shake flask, pH 7, Baker et al. 1992)
2.537	(calculated, Evelyne et al. 1992)
2.30	(Behrendt & Bruggemann 1993)
2.87	(recommended, Sangster 1993)
2.87	(recommended, Hansch et al. 1995)

2.50 (pH 7, 22°C, Tomlin 1994)
2.40 (quoted Pomona-database, Müller & Kördel 1996)

Bioconcentration Factor, log BCF:
1.79 (calculated-S, Kenaga 1980)
1.76, 1.82 (cuticle/water: tomato, pepper; Chaumat et al. 1991)
1.71, 1.90 (cuticle/water: box tree, pear; Chaumat et al. 1991)
1.52, 1.20 (cuticle/water: ivy, vanilla; Chaumat et al. 1991)
1.76, 1.82 (cuticle/water: tomato, pepper; Evelyne et al. 1992)

Sorption Partition Coefficient, log K_{OC}:
2.66 (soil, calculated-S, Kenaga 1980)
1.86 (soil, HPLC-screening method, mean value of different stationary and mobile phases, Kördel et al. 1993)
2.11 (soil, quoted from Kördel et al. 1993, Traub-Eberhard et al. 1994)
1.86; 2.40 (HPLC-screening method; calculated-PCKOC fragment method, Müller & Kördel 1996)
2.57, 1.71, 1.78, 1.73, 2.34 (first generation Eurosoils ES-1, ES-2, ES-3, ES-4, ES-5, shake flask/batch equilibrium-HPLC/UV, Gawlik et al. 1998, 1999)
1.86, 2.31; 2.81, 2.24, 2.83, 2.35, 1.93 (quoted lit., calculated-K_{OW}; HPLC-screening method with different LC-columns, Szabo et al. 1999)
2.155, 1.918, 1.790, 1.719, 2.367 (second generation Eurosoils ES-1, ES-2, ES-3, ES-4, ES-5, shake flask/batch equilibrium-HPLC/UV and HPLC-k′ correlation, Gawlik et al. 1999)
2.155, 1.918, 1.790, 1.719, 2.367 (second generation Eurosoils ES-1, ES-2, ES-3, ES-4, ES-5, shake flask/batch equilibrium-HPLC/UV and HPLC-k′ correlation, Gawlik et al. 2000)
1.78, 2.10 (Kishon river sediments, sorption isotherm, Chefetz et al. 2004)

Environmental Fate Rate Constants, k, or Half-Lives, $t_{1/2}$:
Volatilization:
Photolysis: atmosphere photolysis $t_{1/2}$ = 288–864 h, based on observed photolysis on soil TLC plates under summer sunlight (Helling 1976; quoted, Howard et al. 1991) and adjusted for relative winter sunlight intensity (Lyman et al. 1982; quoted, Howard et al. 1991);
aqueous photolysis $t_{1/2}$ = 288–864 h, based on observed photolysis on soil TLC plates under summer sunlight (Helling 1976; quoted, Howard et al. 1991) and adjusted for relative winter sunlight intensity (Lyman et al. 1982; quoted, Howard et al. 1991);
$t_{1/2}$ = 1.5 h for 215 µg/mL to degrade in distilled water under 254 nm light (Kulshrestha & Mukerjee 1986; quoted, Cessna & Muir 1991).
Oxidation: photooxidation $t_{1/2}$ = 0.743–74.3 h in air, based on estimated rate constant for the vapor-phase reaction with hydroxyl radicals in air (Atkinson 1987; quoted, Howard et al. 1991).
Hydrolysis:
Biodegradation: aqueous aerobic $t_{1/2}$ = 408–2520 h, based on aerobic soil die-away test data for one soil at 15°C and 30°C (Gingerich & Zimdahl 1976; quoted, Howard et al. 1991); aqueous anaerobic $t_{1/2}$ = 96–360 h, based on anaerobic soil die-away test which tested one soil (Gingerich & Zimdahl 1976; quoted, Howard et al. 1991)
Biotransformation: ~ 11% of a selection of 90 strains of micromycetes mostly isolated from soil-soil fungi, depleted over 50% of isoproturon (100 mg/L) in 5-d experiment (Vroumsia et al. 1996)
Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants:

Half-Lives in the Environment:
Air: $t_{1/2}$ = 0.743–74.3 h, based on estimated rate constant for the vapor-phase reaction with hydroxyl radicals in air (Atkinson 1987; quoted, Howard et al. 1991).
Surface water: $t_{1/2}$ = 288–864 h, based on observed photolysis on soil TLC plates under summer sunlight (Helling 1976; quoted, Howard et al. 1991) and adjusted for relative winter sunlight intensity (Lyman et al. 1982; quoted, Howard et al. 1991).
Groundwater: $t_{1/2}$ = 96–5040 h, based on estimated unacclimated aqueous aerobic and anaerobic degradation half-lives (Howard et al. 1991)
reported half-lives or persistence, $t_{1/2}$ = 12–29 and 60–120 d (Bottoni & Funari 1992)

Sediment:

Soil: $t_{1/2}$ = 408–2520 h, based on aerobic soil die-away test data for one soil at 15°C and 30°C (Gingerich & Zimdahl 1976; quoted, Howard et al. 1991);

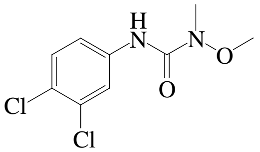
reported $t_{1/2}$ = 12–29 d and 60–120 d (Bottoni & Funari 1992);

$t_{1/2}$ = 15–21 d in sandy loam, $t_{1/2}$ = 11 d in silt loam at 20°C (Traub-Eberhard et al. 1994)

Degradation and mineralization $t_{1/2}$ = 16 d, 24 d and 34 d for pelosol, brown calcareous soil and brown acid soil, respectively, over 120 days under controlled laboratory conditions (Pieuchot et al. 1996)

estimated $t_{1/2}$ ~ 14.6 d under conventional tillage, $t_{1/2}$ = 7.99 d under ridge tillage and $t_{1/2}$ = 12.17 d with no tillage (Otto et al. 1997).

17.1.1.45 Linuron



Common Name: Linuron

Synonym: Afalon, Cephalon, Garnitan, Herbicide 326, Hoe 2810, Linex 4L, Linorox, Linurex, Lorox, Methoxydiuron, Premalin, Scarclex, Sinuron

Chemical Name: 3-(3,4-dichlorophenyl)-1-methoxy-1-methylurea; *N′*-(3,4-dichlorophenyl)-N-methoxy-*N*-methylurea

Uses: selective pre-emergence and post-emergence herbicide used on a wide variety of food crops to control many annual broadleaf and grass weeds.

CAS Registry No: 330-55-2

Molecular Formula: $C_9H_{10}Cl_2N_2O_2$

Molecular Weight: 249.093

Melting Point (°C):

93 (Lide 2003)

Boiling Point (°C):

Density (g/cm^3 at 20°C):

Molar Volume (cm^3/mol):

232.9 (calculated-Le Bas method at normal boiling point)

Dissociation Constant pK$_a$:

Enthalpy of Vaporization, ΔH_V (kJ/mol):

90.23 (Rordorf 1989)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

28.66 (DSC method, Plato & Glasgow 1969)

25.9 (Rordorf 1989)

Entropy of Fusion, ΔS_{fus} (J/mol K):

Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F: 0.215 (mp at 93°C)

Water Solubility (g/m^3 or mg/L at 25°C or as indicated):

75 (Woodford & Evans 1963; Bailey & White 1965; Hartley & Graham-Bryce 1980; Kenaga 1980; Kenaga & Goring 1980; Beste & Humburg 1983)

75 (Melnikov 1971; Spencer 1973, 1982; Wauchope 1978; Khan 1980; Weber et al. 1980; Ashton & Crafts 1981; Briggs 1981)

75 (Martin & Worthing 1977; Worthing & Walker 1983, 1987; Herbicide Handbook 1978,1989)

81 (Hartley & Kidd 1987; Milne 1995)

81 (24°C, Worthing & Hance 1991)

75 (20–25°C, selected, Wauchope et al. 1992; Hornsby et al. 1996)

75–81 (Montgomery 1993)

Vapor Pressure (Pa at 25°C or as indicated and reported temperature dependence equations):

0.00147 (20°C, Quellette & King 1977)

0.0012 (20°C, Hartley & Graham-Bryce 1980)

0.002 (24°C, Khan 1980)

0.002 (20–25°C, Weber et al. 1980)

0.002 (24°C, Hartley & Kidd 1987; Worthing & Hance 1991; Montgomery 1993)

0.0014 (20°C, selected, Suntio et al. 1988)

3.50×10^{-4}, 1.10×10^{-2}, 0.22, 2.90, 28.0 (25, 50, 70, 100, 125°C, gas saturation-GC, Rordorf 1989)

$\log (P_S/Pa) = 16.074 - 5824.2/(T/K)$; measured range 40.5–92 7°C (solid, gas saturation-GC, Rordorf 1989)

$\log (P_L/Pa) = 12.989 - 4713.7/(T/K)$; measured range 92.7–160°C (liquid, gas saturation-GC, Rordorf 1989)

0.0011 (20°C, selected, Taylor & Spencer 1990)

0.0023 (20–25°C, selected, Wauchope et al. 1992; Hornsby et al. 1996)

0.0027 (selected, Halfon et al. 1996)

Henry's Law Constant (Pa·m^3/mol at 25°C or as indicated):
0.0054 (20°C, calculated-P/C, Suntio et al. 1988)
0.004 (Taylor & Glotfelty 1988)
0.0062 (20–25°C, calculated-P/C, Montgomery 1993)
0.00465 (calculated-P/C, this work)

Octanol/Water Partition Coefficient, log K_{OW}:
2.19 (Briggs 1969)
3.20 (shake flask-UV, Erkell & Walum 1979)
2.76 (shake flask-UV, Briggs 1981)
3.11 (shake flask, Mitsutake et al. 1986)
2.48 (selected, Gerstl & Helling 1987)
3.00 (Worthing & Hance 1991; Milne 1995)
2.19, 3.00 (Montgomery 1993)
2.75 (RP-HPLC-RT correlation, Sicbaldi & Finizio 1993)
3.20 (recommended, Sangster 1993)
3.20 (recommended, Hansch et al. 1995)
3.18 (Pomona-database, Müller & Kördel 1996)
2.75 (RP-HPLC-RT correlation, Finizio et al. 1997)
2.72 (RP-HPLC-RT correlation, Yu et al. 1997)

Bioconcentration Factor, log BCF:
1.73 (calculated-S, Kenaga 1980; quoted, Isensee 1991)
1.68 (calculated-K_{OC}, Kenaga 1980)
1.73 (calculated, Pait et al. 1992)

Sorption Partition Coefficient, log K_{OC}:
2.91 (soil, Hamaker & Thompson 1972)
2.61 (soil, calculated-S as per Kenaga & Goring 1980, Kenaga 1980)
2.93 (average soils/sediments, Rao & Davidson 1980)
2.43 (soil, converted form reported K_{OM} multiplied by 1.724, Briggs 1981)
2.93, 2.80, 1.80 (estimated-S, calculated-S and mp, calculated-K_{OW}, Karickhoff 1981)
3.83 (Means & Wijayaratne 1982)
2.99, 2.58; 2.62, 2.80 (estimated-K_{OW}, S, Madhun et al. 1986)
2.76, 2.64 (quoted, calculated-MCI χ, Gerstl & Helling 1987)
2.94 (screening model calculations, Jury et al. 1987b)
2.61–2.91, 2.83, 2.93 (soil, quoted values, Bottoni & Funari 1992)
2.60 (soil, 20–25°C, selected, Wauchope et al. 1992;)
2.70–2.78 (Montgomery 1993)
2.59 (soil, HPLC-screening method, mean value from different stationary and mobile phases, Kördel et al. 1993, 1995a)
2.59 (soil, HPLC-screening method, Kördel et al. 1993, 1995b)
2.70 (soil, calculated-MCI $^1\chi$, Sabljic et al. 1995)
2.59; 2.54 (HPLC-screening method; calculated-PCKOC fragment method, Müller & Kördel 1996)
3.28, 2.39, 2.46, 2.29, 3.12 (first generation Eurosoils ES-1, ES2, ES-3, ES-4, ES-5, shake flask/batch equilibrium-HPLC/UV, Gawlik et al. 1998, 1999)
2.884, 2.58, 2.45, 1.33, 3.18 (second generation Eurosoils ES-1, ES2, ES-3, ES-4, ES-5, shake flask/batch equilibrium-HPLC/UV, Gawlik et al. 1999)
2.884, 2.578, 2.450, 2.336, 3.183 (second generation Eurosoils ES-1, ES-2, ES-3, ES-4, ES-5, shake flask/batch equilibrium-HPLC/UV and HPLC-k′ correlation, Gawlik et al. 2000)
2.70; 2.55, 2.61 (soil, quoted obs.; estimated-class-specific model, estimated-general model using molecular descriptors, Gramatica et al. 2000)
2.65, 2.64 (soils: organic carbon OC ≥ 0.1%, OC ≥ 0.5%, average, Delle Site 2001)

2.78 (average values for sediment OC≥ 0.5%, Delle Site 2001)

Environmental Fate Rate Constants, k, or Half-Lives, $t_{½}$:

Volatilization:

Photolysis: $t_{½}$ = 2 months for 31% of 55 μg mL^{-1} to degrade in distilled water under sunlight (Rosen et al. 1969; quoted, Cessna & Muir 1991);

$t_{½}$ = 2.25 h for 67–75% of 75 μg mL^{-1} to degrade in distilled water under 300 nm light (Tanaka et al. 1981; quoted, Cessna & Muir 1991);

atmosphere photolysis $t_{½}$ = 1344–4032 h, based on measured rate constant for summer sunlight photolysis in distilled water (Rosen et al. 1969; quoted, Howard et al. 1991) and adjusted to relative winter sunlight intensity (Lyman et al. 1982; quoted, Howard et al. 1991); aqueous photolysis $t_{½}$ = 1344–4032 h, based on measured rate constant for summer sunlight photolysis in distilled water (Rosen et al. 1969; quoted, Howard et al. 1991) and adjusted to relative winter sunlight intensity (Lyman et al. 1982; quoted, Howard et al. 1991).

Oxidation: photooxidation $t_{½}$ = 0.49–4.90 h in air, based on an estimated rate constant for the vapor-phase reaction with hydroxyl radicals in air (Atkinson 1987; quoted, Howard et al. 1991).

Hydrolysis: $t_{½}$ > 4 months for 4980 μg mL^{-1} to hydrolyze in phosphate buffer at pH 5–9 and 20°C (El-dib & Aly 1976; quoted, Muir 1991).

Biodegradation: $t_{½}$ = 78 d in soil (Moyer et al. 1972; quoted, Means et al. 1983),

$t_{½}$ = 87 d in soil (Hance 1974; quoted, Means et al. 1983),

$t_{½}$ = 58 and 180 d in soil (Urosol & Hance 1974; quoted, Means et al. 1983);

aqueous aerobic $t_{½}$ = 672–4272 h, based on soil die-away test data (Walker 1978; Walker & Zimdahl 1981; quoted, Howard et al. 1991);

rate constant k = 0.0096 d^{-1} by soil incubation die-away studies (Rao & Davidson 1980; quoted, Scow 1982);

aerobic $t_{½}$ ~ 40 d for 1 μg mL^{-1} to biodegrade in lake sediment and $t_{½}$ ~ 60 d for 4 μg mL^{-1} to biodegrade in lake sediment and water (Huber & Gemes 1981; quoted, Muir 1991);

aerobic $t_{½}$ ~ 20 d for 0.22 μg mL^{-1} to biodegrade in pond sediment plus aerobic salts medium of 34 g L^{-1} (Stepp et al. 1985; quoted, Muir 1991);

aqueous anaerobic $t_{½}$ = 2688–17088 h, based on estimated unacclimated aqueous aerobic biodegradation half-life (Howard et al. 1991)

degradation rate constant k = (3.48 ± 0.156) × 10^{-2} d^{-1} with $t_{½}$ = 19.9 d in control soil and k = (23.2 ± 2.07) × 10^{-2} d^{-1} with $t_{½}$ = 2.99 d in pretreated soil in the field; k = (3.73 ± 0.208) × 10^{-2} d^{-1} with $t_{½}$ = 18.6 d in control soil and k = (18.8 ± 2.76) × 10^{-2} d^{-1} with $t_{½}$ = 3.68 d in pretreated soil once only in the laboratory (Walker & Welch 1991)

Biotransformation:

Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants:

Half-Lives in the Environment:

Air: $t_{½}$ = 0.49–4.90 h, based on an estimated rate constant for the vapor-phase reaction with hydroxyl radicals in air (Atkinson 1987; quoted, Howard et al. 1991).

Surface water: $t_{½}$ = 672–4272 h, based on estimated unacclimated aqueous aerobic biodegradation half-life (Howard et al. 1991).

Ground water: $t_{½}$ = 1344–8544 h, based on estimated unacclimated aqueous aerobic biodegradation half-life (Howard et al. 1991)

reported half-lives or persistence, $t_{½}$ = 38–69 and 75 d (Bottoni & Funari 1992).

Sediment: degradation $t_{½}$ = 12 d in estuarine sediment (12‰) system (Cunningham et al. 1981; quoted, Means et al. 1983);

degradation $t_{½}$ = 6 d in estuarine sediment (18‰) system (Means et al. 1983).

Soil: estimated persistence of 4 months (Kearney et al. 1969; Edwards 1973; quoted, Morrill et al. 1982; Jury et al. 1987a);

$t_{½}$ = 672–4272 h, based on soil die-away test data (Walker 1978; Walker & Zimdahl 1981; quoted, Howard et al. 1991);

persistence of 4 months (Wauchope 1978);

correlated $t_{1/2}$ = 57 d at pH 5.1–5.8, $t_{1/2}$ = 22 d at pH 6.3–7.0 and $t_{1/2}$ = 19 d at pH 7.7–8.2 (Boddington Barn soil, Hance 1979) and $t_{1/2}$ = 67 d at pH 4.6–5.2, $t_{1/2}$ = 53 d at pH 5.3–6.1, and $t_{1/2}$ ~ 20 d at pH 6.3–8.0 (Triangle soil, Hance 1979);

estimated first-order $t_{1/2}$ = 72 d from biodegradation rate constant k = 0.0096 d^{-1} by soil incubation die-away studies (Rao & Davidson 1980; quoted, Scow 1982);

decomposition $t_{1/2}$ = 11 d in fresh soil and $t_{1/2}$ = 12 d in air dried soil both in polyethylene bags, $t_{1/2}$ = 49 d in undisturbed cores and $t_{1/2}$ = 40 d in perfusion (Hance & Haynes 1981);

moderately persistent in soil with $t_{1/2}$ = 20–100 d (Willis & McDowell 1982);

$t_{1/2}$ = 2 to 5 months under field conditions (Hartley & Kidd 1987; Herbicide Handbook 1989; quoted, Montgomery 1993);

$t_{1/2}$ = 75 d from screening model calculations (Jury 1987b);

$t_{1/2}$ = 60, 35, 35, 30 d in plots treated, i.e., repeated application of pesticide, for the first, second, third and fourth time, respectively, in the field; in the laboratory $t_{1/2}$ reduced from 19 d to 3–7 d in a single pretreatment in moist oil at 20°C (Walker & Welch 1991)

reported $t_{1/2}$ = 38–69 d and 75 d (Bottoni & Funari 1992);

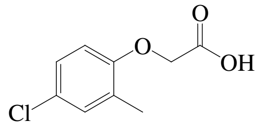
selected field $t_{1/2}$ = 60 d (Wauchope et al. 1992; quoted, Richards & Baker 1993; quoted, Halfon et al. 1996; Hornsby et al. 1996);

soil $t_{1/2}$ = 60 d (Pait et al. 1992);

soil $t_{1/2}$ = 29–67 d (Di Guardo et al. 1994).

Biota: biochemical $t_{1/2}$ = 75 d from screening model calculations (Jury et al. 1987b).

17.1.1.46 MCPA



Common Name: MCPA

Synonym: Agritox, Agroxohe, Agroxone, Anicon Kombi, Bordermaster, Chiptox, Chwastox, Cornox, Ded-weed, Dicopur-M, Dicotex, Dikotes, Emcepan, Empal, Hedapur M 52, Hederax M, Herbicide M, Hedonal, Hormotuho, Kilsem, Krezone, Legumex DB, Leuna M, Leyspray, Linormone, MCP, metaxon, Methoxone, Netazol, Okultin M, Phenoxylene Plus, Raphone, Razol dock killer, Rhomenc, Rhonox, Shamrox, Seppic MMD, Trasan, Ustinex, Vacate, Verdone, Weedar, Weed-rhap, Zelan

Chemical Name: (4-chloro-2-methylphenoxy)acetic acid; 4-chloro-*o*-tolyloxyacetic acid

Uses: systemic post-emergence herbicide to control annual and perennial weeds in cereals, rice, flax, vines, peas, potatoes, asparagus, grassland and turf.

CAS Registry No: 94-74-6

Molecular Formula: $C_9H_9ClO_3$

Molecular Weight: 200.618

Melting Point (°C):

120	(Montgomery 1993; Milne 1995; Lide 2003)

Boiling Point (°C):

Density (g/cm^3 at 20°C):

1.56	(25°C, Que Hee et al. 1981; Herbicide Handbook 1989; Montgomery 1993)

Molar Volume (cm^3/mol):

211.1	(calculated-Le Bas method at normal boiling point)

Dissociation Constant pK_a:

3.05	(potentiometric titration, Nelson & Faust 1969)
3.125	(Cessna & Grover 1978)
3.07	(Worthing & Hance 1991)
3.05–3.13	(Montgomery 1993)
3.12	(Hornsby et al. 1996)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

Entropy of Fusion, ΔS_{fus} (J/mol K):

Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F: 0.117 (mp at 120°C)

Water Solubility (g/m^3 or mg/L at 25°C or as indicated):

1605	(shake flask-UV, Leopold et al. 1960)
1605	(Bailey & White 1965)
< 1000	(Khan 1980)
630	(20°C, Melnikov 1971)
825	(Martin & Worthing 1977; Weber et al. 1980; Milne 1995)
1500	(selected, Seiber et al. 1986)
825	(room temp., Hartley & Kidd 1987; Worthing & Hance 1991)
817	(selected, Gerstl & Helling 1987)
835	(room temp., Worthing & Walker 1987)
730–825	(Montgomery 1993)

Vapor Pressure (Pa at 25°C or as indicated):

7.9×10^{-4}	(measured-volatilization rate, Seiber et al. 1986)
2.0×10^{-4}	(20°C, Hartley & Kidd 1987)
2.0×10^{-4}	(21°C, Worthing & Walker1987, 1991)
2.3×10^{-5}	(20°C, Tomlin 1994)
2.0×10^{-4}	(20°C, Milne 1995)
2.0×10^{-4}	(selected, Halfon et al. 1996)

Henry's Law Constant (Pa·m^3/mol at 25°C):

1.0×10^{-4} (calculated-P/C, Seiber et al. 1986)
4.86×10^{-4} (calculated-P/C as per Worthing & Walker 1987, Majewski & Capel 1995)
< 0.010 (estimated, Mabury & Crosby 1996)
2.5×10^{-4} (calculated-P/C, this work)

Octanol/Water Partition Coefficient, log K_{OW}:

2.69 (selected, Dao et al. 1983)
2.30 (RP-HPLC-k′ correlation, Braumann et al. 1983)
–1.41 (selected, Gerstl & Helling 1987)
–0.57 (shake flask-UV, pH 7, Stevens et al. 1988)
3.25 (countercurrent LC, Ilchmann et al. 1993)
1.37–1.43 (calculated, Montgomery 1993)
–0.57, 3.25 (quoted, Sangster 1993)
2.68 (MedChem Master file or ClogP program, Sabljic et al. 1995)

Bioconcentration Factor, log BCF:

1.15 (calculated-S, Kenaga 1980)

Sorption Partition Coefficient, log K_{OC}:

2.04 (soil, calculated-S, Kenaga 1980; quoted, Bottoni & Funari 1992)
1.95 (calculated-MCI χ, Gerstl & Helling 1987)
2.03–2.07 (calculated, Montgomery 1993)
1.73 (calculated-QSAR MCI $^1\chi$, Sabljic et al. 1995)
2.49; 1.58., 3.27, 3.17, 1.85, 2.19 (calculated-K_{OW}; HPLC-screening method with different LC-columns, Szabo et al. 1999)

Environmental Fate Rate Constants, k, or Half-Lives, $t_{1/2}$:

Volatilization: $k = 9.78 \times 10^{-7}$ h^{-1} at pH 3.5 (Seiber et al. 1986).

Photolysis: $t_{1/2}$ = 71 h for < 10% of 50 μg mL^{-1} to degrade in NaOH solution at pH 9.8 under > 290 nm light (Soderquist & Crosby 1975; quoted, Cessna & Muir 1991);

$t_{1/2}$ = 245 h for 17–98.5% of 9 μg mL^{-1} to degrade in distilled water under sunlight (Draper & Crosby 1984; quoted, Cessna & Muir 1991);

$t_{1/2}$ = 4.6 d for 14,700 μg mL^{-1} to degrade in droplets of spray solution suspended in air under sunlight (Freiberg & Crosby 1986; quoted, Cessna & Muir 1991).

Oxidation: degradation by ozone in dilute aqueous solutions (Benoit-Guyod et al. 1986) as follows:-

$t_{1/2}$ = 9.4 min - dark with O_3 in air; $t_{1/2}$ = 8.4 min - light with O_3 in air, $t_{1/2}$ = 500 min - light, air only, at initial pH of 3.55; MCPA concn of 224 μM L^{-1}, ozone input at 246 μM h^{-1};

$t_{1/2}$ = 10.4 min - dark with O_3 in air; $t_{1/2}$ = 9.0 min - light with O_3 in air, at initial pH of 8.0,

$t_{1/2}$ = 11.5 min - dark with O_3 in air; $t_{1/2}$ = 11.3 min - light with O_3 in air, at initial pH of 7.0,

$t_{1/2}$ = 8.4 min - dark with O_3 in air; $t_{1/2}$ = 9.4 min - light with O_3 in air, at initial pH of 7.0,

$t_{1/2}$ = 4.2 min - dark with O_3 in air; $t_{1/2}$ = 4.2 min - light with O_3 in air, $t_{1/2}$ = 150 min - light, air only, at initial pH of 8.0; MCPA concn of 5 μM L^{-1}, ozone input at 246 μM h^{-1};

$t_{1/2}$ = 176 min - dark with O_3 in air; $t_{1/2}$ = 63 min - light with O_3 in air, at initial pH of 8.0, MCPA concn of 224 μM L^{-1}, ozone input at 4.6 μM h^{-1};

$t_{1/2}$ = 300 min - dark with O_3 in air; $t_{1/2}$ = 162 min - light with O_3 in air, at initial pH of 8.0; MCPA concn of 224 μM L^{-1}, ozone input at 0.2 μM h^{-1} (Benoit-Guyod et al. 1986).

measured rate constant k_{OH}(aq.) = 1.70×10^9 M^{-1} s^{-1} for reaction with hydroxyl radical, in irradiated field water both in the laboratory and sunlit rice paddies (Mabury & Crosby 1996).

Hydrolysis:

Biodegradation: $t_{1/2}$ > 168 h for 1 μg mL^{-1} to degrade in activated sludge (Schmidt 1975; quoted, Muir 1991);

aerobic $t_{1/2}$ ~ 9 d for 1 μg mL^{-1} to degrade in natural water in absence of sunlight (Soderquist & Crosby 1975; quoted, Muir 1991);

$t_{1/2}$ > 12 d for 0.045–0.156 μg mL^{-1} to degrade in water after application to model crop and washoff (Virtanen et al. 1979; quoted, Muir 1991);

$t_{1/2}$ = 15–25 d for 10 μg mL^{-1} to degrade in flooded soils (Duah-Yentumi & Kuwatsuka 1980; quoted, Muir 1991);

first order microbial degradation k = 0.01393 d^{-1} with $t_{1/2}$ = 50 d at room temp, k = 0.01687 d^{-1} with $t_{1/2}$ = 41 d at 35°C in sandy clay soil from Finland; k = 0.02999 d^{-1} with $t_{1/2}$ = 23 d at room temp, k = 0.03397 d^{-1} with $t_{1/2}$ = 20 d at 35°C in sandy loam soil from Bangladesh (Sattar & Paasivirta 1980)

$t_{1/2}$ > 25 d for 10 μg mL^{-1} to degrade in flooded soils (Ursin 1985; quoted, Muir 1991).

Biotransformation:

Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants:

Half-Lives in the Environment:

Air:

Surface water: dissipation $t_{1/2}$ ~ 4 d in rice field; $t_{1/2}$ = 17 d in dilute aqueous solution under laboratory irradiation (Soderquist & Crosby 1975);

degradation $t_{1/2}$ = 4.2 - 300 min by ozone and light (UV > 300 nm) in dilute aqueous solution, depending on pH, concn of MCPA and ozone (shake flask-GC, Benoit-Guyod et al. 1986)

degraded rapidly with $t_{1/2}$ = 9 d in rice paddy water held under darkened conditions (Muir 1991)

field dissipation $t_{1/2}$ = 28.8 h in water (Mabury & Crosby 1996)

Ground water: reported $t_{1/2}$ < 7 and $t_{1/2}$ = 20–25 d (Bottoni & Funari 1992)

Sediment: $t_{1/2}$ = 80 to 400 d of MCPA at low concentrations in marine sediments (Muir 1991).

Soil: degradation $t_{1/2}$ = 50 d at room temp., $t_{1/2}$ = 41 d at 35°C in Finland sandy clay soil; degradation $t_{1/2}$ = 23 d at room temp., $t_{1/2}$ = 20 d at 35°C in Bangladesh loam soil from first-order rate constant obtained by linear regression (Sattar & Paasivirta 1980);

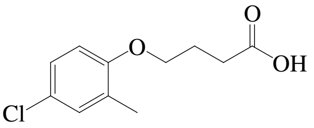
persistence of 3 months in soil (Edwards 1973; quoted, Morrill et al. 1982);

$t_{1/2}$ = 25 d in flooded soils (Muir 1991);

$t_{1/2}$ = 15 d (selected, Halfon et al. 1996).

Biota:

17.1.1.47 MCPB



Common Name: MCPB
Synonym: Bexane, Can-Trol, Legumex, Thistrol, Thitrol, Trifolex, Tropotox
Chemical Name: 4-(4-chloro-2-methylphenoxy)butanoic acid; 4-(4-chloro-2-methylphenoxy)-butyric acid
Uses: herbicide for post-emergence control of annual and perennial broadleaf weeds in cereals, clovers, sainfoin, groundnuts, peas, etc. and also used to control broadleaf and woody weeds in forestry.
CAS Registry No: 94-81-5
Molecular Formula: $C_{11}H_{13}ClO_3$
Molecular Weight: 228.672
Melting Point (°C):
100 (Hartley & Kidd 1987; Worthing & Hance 1991; Tomlin 1994; Milne 1995; Lide 2003)
Boiling Point (°C):
> 280 (Tomlin 1994)
Density (g/cm^3 at 22°C):
1.254 (Tomlin 1994)
Molar Volume (cm^3/mol):
255.5 (calculated-Le Bas method at normal boiling point)
Dissociation Constant pK_a:
4.80 (potentiometric titration, Nelson & Faust 1969)
4.84 (Worthing & Hance 1991; Tomlin 1994)
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
34.31 (DSC method, Plato 1972)
Entropy of Fusion, ΔS_{fus} (J/mol K):
Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F: 0.184 (mp at 100°C)

Water Solubility (g/m^3 or mg/L at 25°C or as indicated):
41 (shake flask-UV, Leopold et al. 1960)
44 (rm. temp., Melnikov 1971)
44 (Bailey & White 1965; Martin & Worthing 1977; Hartley & Kidd 1987)
44 (rm. temp., Worthing & Walker 1987, Worthing & Hance 1991; Tomlin 1994; Milne 1995)

Vapor Pressure (Pa at 25°C or as indicated):
5.77×10^{-5}, 9.83×10^{-5} (20, 25°C, Tomlin 1994)

Henry's Law Constant (Pa·m^3/mol at 25°C):
3.22×10^{-4} (calculated-P/C, this work)

Octanol/Water Partition Coefficient, log K_{OW}:
4.60 (selected, Dao et al. 1983)
3.53 (RP-HPLC-k′ correlation, Braumann et al. 1983)
3.473 (countercurrent LC, Ilchmann et al. 1993)
2.79 (Tomlin 1994)
3.43 (selected, Hansch et al. 1995)

Bioconcentration Factor, log BCF:
1.86 (calculated-S, Kenaga 1980)

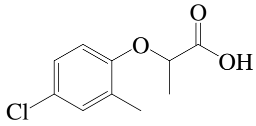
Sorption Partition Coefficient, log K_{OC}:
2.73 (soil, calculated-S, Kenaga 1980)

Environmental Fate Rate Constants, k, or Half-Lives, $t_{1/2}$:

Half-Lives in the Environment:

Soil: duration of residual activity in soil is ca. 3–4 months (Hartley & Kidd 1987; Tomlin 1994).

17.1.1.48 Mecoprop



Common Name: Mecoprop
Synonym: Compitox, Duplosan, Hedonal, Iso-Cornox, Kilprop, MCPP, Mecopex, Mepro, Methoxone, Propal
Chemical Name: (±)-2-(4-chloro-2-methylphenoxy)propanoic acid; (±)-2-(4-chloro-*o*-tolyl-oxy)propionic acid
Uses: herbicide for post-emergence control of broadleaf weeds in wheat, barley, rye, herbage seed crops, grassland, and under fruit trees and vines, etc.
CAS Registry No: 7085-19-0
Molecular Formula: $C_{10}H_{11}ClO_3$
Molecular Weight: 214.645
Melting Point (°C):

94–95	(Hartley & Kidd 1987; Herbicide Handbook 1989; Worthing & Hance 1991)

Boiling Point (°C):
Density (g/cm^3 at 20°C):
Molar Volume (cm^3/mol):

233.3	(calculated-Le Bas method at normal boiling point)

Dissociation Constant pK_a:

3.75	(Bailey & White 1965; quoted, Que Hee et al. 1981)
3.105	(Cessna & Grover 1978)
3.78	(Worthing & Hance 1991)
3.11	(Armbrust 2000)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

28.87	(DSC method, Plato 1972)

Entropy of Fusion, ΔS_{fus} (J/mol K):
Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F:

Water Solubility (g/m^3 or mg/L at 25°C or as indicated):

895	(Martin 1961; Bailey & White 1965)
891	(Bailey & White 1965)
620	(20°C, Melnikov 1971; Ashton & Crafts 1981; Herbicide Handbook 1989)
620	(Martin & Worthing 1977)
620	(20°C, Hartley & Kidd 1987; Worthing & Walker 1987, Worthing & Hance 1991)
734	(Tomlin 1994)

Vapor Pressure (Pa at 25°C or as indicated):

$< 1.0 \times 10^{-5}$	(20°C, Hartley & Kidd 1987)
3.10×10^{-4}	(20°C, Worthing & Hance 1991)
0.0	(selected, Halfon et al. 1996)

Henry's Law Constant (Pa·m^3/mol at 25°C):

7.43×10^{-5}	(calculated-P/C, this work)
1.11×10^{-5}	(quoted lit., Armbrust 2000)

Octanol/Water Partition Coefficient, log K_{OW}:

3.94	(selected, Dao et al. 1983)
2.83	(RP-HPLC-k′ correlation, Braumann et al. 1983)
0.10	(Worthing & Hance 1991)
0.09; 3.126	(quoted; countercurrent LC, Ilchmann et al. 1993)
3.13	(recommended, Hansch et al. 1995)

Bioconcentration Factor, log BCF:

1.20	(calculated-S, Kenaga 1980)

Sorption Partition Coefficient, log K_{OC}:

2.11	(soil, calculated, Kenaga 1980, quoted, Bottoni & Funari 1992)
1.30	(selected, Lohninger 1994)
1.30	(quoted lit., Armburst 2000)

Environmental Fate Rate Constants, k, or Half-Lives, $t_{1/2}$:

Volatilization:

Photolysis: photodegradation $t_{1/2}$ < 10 -15 d on 3 Spanish natural dry soils; $t_{1/2}$ = 15–50 d on 10% peat-amened dry soils; degradation $t_{1/2}$ ~ 2–5.5 d on moist soils at field capacity and saturated soils for degradation at 0,1 and 2 exposures days; and $t_{1/2}$ = 13–32 d on moist soils at field capacity and saturated soils for degradation at 2,4 and 10 exposure days (Romero et al. 1998)

Oxidation: photooxidation $t_{1/2}$ = 3.8–37.8 h in air, based on an estimated rate constant for the vapor-phase reaction with hydroxyl radicals in air (Atkinson 1987; quoted, Howard et al. 1991).

Hydrolysis: stable aqueous hydrolysis rate at pH 5, 7, pH 9; measured hydroxy radical rate constant for mecoprop $k = 9.0 \times 10^{12}\ M^{-1}\ h^{-1}$ (Armbrust 2000)

Biodegradation: aqueous aerobic $t_{1/2}$ = 168–240 h, based on aerobic soil grab sample data (Kirkland & Fryer 1972; Smith & Hayden 1981; quoted, Howard et al. 1991); aqueous anaerobic $t_{1/2}$ = 672–4320 h, based on anaerobic digest or sludge data (Battersby & Wilson 1989; quoted, Howard et al. 1991);

aerobic rate constant, $k = 2.89 \times 10^{-3}\ h^{-1}$ (Armbrust 2000).

Biotransformation:

Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants:

Half-Lives in the Environment:

Air: $t_{1/2}$ = 3.8–37.8 h, based on an estimated rate constant for the vapor-phase reaction with hydroxyl radicals in air (Atkinson 1987; quoted, Howard et al. 1991).

Surface water: $t_{1/2}$ = 168–240 h, based on estimated aqueous aerobic biodegradation half-life (Howard et al. 1991).

Groundwater: $t_{1/2}$ = 336–4320 h, based on estimated aqueous aerobic and anaerobic biodegradation half-lives (Howard et al. 1991)

reported $t_{1/2}$ = 8 d (Bottoni & Funari 1992).

Sediment:

Soil: $t_{1/2}$ = 168–240 h, based on aerobic soil grab sample data (Kirkland & Fryer 1972; Smith & Hayden 1981; quoted, Howard et al. 1991);

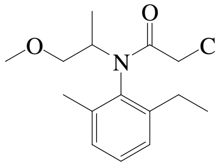
reported $t_{1/2}$ = 8 d (Bottoni & Funari 1992);

$t_{1/2}$ = 21 d (selected, Halfon et al. 1996)

photodegradation $t_{1/2}$ < 10 -15 d on 3 Spanish natural dry soils; $t_{1/2}$ = 15–50 d on 10% peat-amened dry soils; degradation $t_{1/2}$ ~ 2–5.5 d on moist soils at field capacity and saturated soils for degradation at 0,1 and 2 exposures days; and $t_{1/2}$ = 13–32 d on moist soils at field capacity and saturated soils for degradation at 2,4 and 10 exposure days (Romero et al. 1998).

Biota:

17.1.1.49 Metolachlor



Common Name: Metolachlor

Synonym: Bicep, CGA 24705, Codal, Cortoran multi, Dual, Metetilachlor, Milocep, Ontrack 8E, Pennant, Primagram, Primextra

Chemical Name: 2-chloro-6′-ethyl-*N*-(2-methoxy-1-methylethyl)acet-*o*-toluidide; 2-chloro-*N*-(2-ethyl-6-methylphenyl)-*N*-(2-methoxy-1-methylethyl)acetamide

Uses: pre-emergence herbicide to control most annual grasses and weeds in beans, chickpeas, corn, cotton, milo, okra, peanuts, peas, potatoes, sunflower, soybeans and some ornamentals.

CAS Registry No: 51218-45-2

Molecular Formula: $C_{15}H_{22}ClNO_2$

Molecular Weight: 283.795

Melting Point (°C): liquid

Boiling Point (°C):

100	(at 0.001 mmHg, Herbicide Handbook 1989; Budavari 1989; Worthing & Hance 1991; Montgomery 1993; Milne 1995)

Density (g/cm^3 at 20°C):

1.12	(Hartley & Kidd 1987; Worthing & Hance 1991; Montgomery 1993; Milne 1995)
1.085	(Herbicide Handbook 1989)

Molar Volume (cm^3/mol):

340.0	(calculated-Le Bas method at normal boiling point)
258.0	(calculated-density)

Dissociation Constant pK_a:

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

Entropy of Fusion, ΔS_{fus} (J/mol K):

Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F: 1.0

Water Solubility (g/m^3 or mg/L at 25°C or as indicated):

530	(Martin & Worthing 1977)
440	(selected, Ellgehausen et al. 1980)
520	(20°C, Ashton & Crafts 1981; Spencer 1982)
530	(shake flask-HPLC, Ellgehausen et al. 1981)
530	(20°C, Hartley & Kidd 1987; Herbicide Handbook 1989; Budavari 1989; Montgomery 1993)
530	(Hartley & Graham-Bryce 1980; Beste & Humburg 1983)
530	(20°C, Worthing & Walker 1987, Worthing & Hance 1991; Majewski & Capel 1995; Milne 1995)
488	(Tomlin 1994)
530	(20–25°C, selected, Hornsby et al. 1996)
531, 505	(supercooled liquid S_L: literature derived value LDV, final adjust value FAV, Muir et al. 2004)

Vapor Pressure (Pa at 25°C or as indicated and reported temperature dependence equations):

0.00170	(20°C, Hartley & Graham-Bryce 1980)
0.00173	(20°C, Ashton & Crafts 1981)
0.00173	(20°C, volatilization rate, Burkhard & Guth 1981)
0.00170	(20°C, Hartley & Kidd 1987)
0.00170	(20°C, Worthing & Walker 1987, Worthing & Hance 1991)
0.00173	(20°C, Herbicide Handbook 1989; Budavari 1989; Montgomery 1993)

4.20×10^{-3}, 6.60×10^{-2}, 0.70, 5.40, 33.0 (25, 50, 70, 100, 125°C, gas saturation-GC, Rordorf 1989)

$\log (P_L/Pa) = 13.115 - 4619.7/(T/K)$; measured range 32.5–140°C (gas saturation-GC, Rordorf 1989)

0.00420	(Tomlin 1994)

0.0023 (liquid P_L, GC-RT correlation; Donovan 1996)
0.00418 (selected, Halfon et al. 1996)
0.00418 (20–25°C, selected, Hornsby et al. 1996)
0.00239, 0.0024 (supercooled liquid P_L: literature derived value LDV, final adjust value FAV, Muir et al. 2004)

Henry's Law Constant (Pa·m^3/mol at 25°C or as indicated. Additional data at other temperatures designated * are complied at the end of this section):
0.00092 (Hartley & Graham-Bryce 1980)
0.00093 (20°C, volatilization rate, Burkhard & Guth 1981)
0.00091 (20°C, calculated-P/C as per Worthing & Walker 1987)
0.00093 (20°C, calculated-P/C, Montgomery 1993)
0.00082 (20°C, calculated-P/C, Majewski & Capel 1995)
0.00244 (calculated-P/C, Otto et al. 1997)
0.00782 (20°C, distilled water, wetted wall column-GC, Rice et al. 1997b)
0.00110 (calculated-P/C, this work)
0.00238* (20°C, gas stripping-GC/MS, measured range 283.05–299.45 K, Feigenbrugel et al. 2004)
$H'/(M\ atm^{-1}) = (3.0 \pm 0.4) \times 10^{-11} \exp[(10200 \pm 1000)/(T/K)]$; temp range 283–310 K (Arrhenius eq., gas stripping-GC/MS, Feigenbrugel et al. 2004)
0.0014. 0.0014 (literature derived value LDV, final adjust value FAV, Muir et al. 2004)

Octanol/Water Partition Coefficient, log K_{OW}:
3.13 (shake flask-HPLC, Ellgehausen et al. 1980; Geyer et al. 1991)
3.28 (shake flask-HPLC, Ellgehausen et al. 1981)
3.45 (Worthing & Hance 1991)
2.93, 3.45 (Montgomery 1993)
3.13, 3.28 (quoted, Sangster et al. 1993)
2.90 (Tomlin 1994)
3.45 (Milne 1995)
3.31, 2.95 (selected, calculated-f const., Pinsuwan et al. 1995)
3.13 (recommended, Hansch et al. 1995)
2.60 (RP-HPLC-RT correlation using short ODP column, Donovan & Pescatore 2002)
3.10 (literature derived value LDV, Muir et al. 2004)

Octanol/Air Partition Coefficient, log K_{OA}:
9.37 (final adjust value FAV, Muir et al. 2004)

Bioconcentration Factor, log BCF:
1.813 (log BF-bioaccumulation of algae, Ellgehausen et al. 1980)
0.733 (log BF-bioaccumulation of daphnids, Ellgehausen et al. 1980; quoted, Geyer et al. 1991)
0.851 (log BF-bioaccumulation of catfish, Ellgehausen et al. 1980)
1.26 (calculated-S, Kenaga 1980)
1.15 (catfish *Ictalurus melas*, wet wt basis, Wang et al. 1996)

Sorption Partition Coefficient, log K_{OC}:
2.15 (soil, calculated-S, Kenaga 1980)
2.26 (soil, screening model calculations, Jury et al. 1987b)
2.00, 2.15, 2.28, 2.30 (soil, quoted values, Bottoni & Funari 1992)
2.46, 2.46 (soil, quoted exptl., calculated-MCI χ and fragment contribution, Meylan et al. 1992)
2.30 (20–25°C, selected, Wauchope et al. 1992; Hornsby et al. 1996)
2.08–2.49 (Montgomery 1993; Tomlin 1994)
2.46 (soil, calculated-MCI $^1\chi$, Sabljic et al. 1995)
2.43 (soil, estimated-general model using molecular descriptors, Gramatica et al. 2000)
2.28, 2.19, 2.69 (soils: organic carbon OC ≥ 0.1%, OC ≥ 0.5%, 0.1 ≤ OC < 0 .5%, average, Delle Site 2001)

Environmental Fate Rate Constants, k, or Half-Lives, $t_{1/2}$:
Volatilization:

Photolysis: under optimum exposure conditions to natural sunlight, $t_{½}$ ~ 8 d (Herbicide Handbook 1989).
Oxidation ; $k_{OH} = 5.6 \times 10^{-11}$ cm^3 molecule^{-1} s^{-1} at 298 K in gas phase with atmospheric lifetime of 0.9 h but reduced to 0.4 h at 283 K; log k_{OH}(aq.) = 1.2×10^{10} M^{-1} s^{-1} in aqueous phase (Feigenbrugel et al. 2004)
Hydrolysis: $t_{½} > 200$ d at 20°C and $1 \leq pH \leq 9$ (Montgomery 1993);
$t_{½}$(calc) > 200 d ($2 \leq pH \geq 10$) (Tomlin 1994).
Biodegradation: overall degradation rate constant k = 0.0154 h^{-1} with $t_{½}$ = 45.0 h in sewage sludge and rate constant k = 0.0460 d^{-1} with $t_{½}$ = 15.1 d in garden soil (Müller & Buser 1995).
Biotransformation:
Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants:
k_2 = 9.11 d^{-1} (catfish, Ellgehausen et al. 1980)
k_1 = 0.336 h^{-1}, k_2 = 0.024 h^{-1} (catfish *Ictalurus melas*, Wang et al. 1996)

Half-Lives in the Environment:
Air:
Surface water:
Ground water: reported $t_{½}$ = 20, 30, 42, and 47–107 d (Bottoni & Funari 1992)
degradation time 500–1000 d (Tomlin 1994).
Sediment:
Soil: $t_{½}$ = 15–38 d in clay loam soils and $t_{½}$ = 33–100 d in sandy loam soils (Zimdahl & Clark 1982; quoted, Montgomery 1993);
$t_{½}$ = 42 d from field $t_{½}$ = 3–4 wk by using lysimeters (Bowman 1990);
$t_{½}$(calc) = 80, 99 and 142 d for the disappearance from upper 15 cm on an Ontario clay loam soil while the decline was followed for 332, 364 and 370 d, respectively, in 1987, 1988 and 1989 (Frank et al. 1991);
$t_{½}$ ~ 6 d in soil (Worthing & Hance 1991; quoted, Montgomery 1993);
reported $t_{½}$ = 20, 30, 42, 47–107 d (Bottoni & Funari 1992)
field $t_{½}$ = 90 d at 20–25°C (selected, Wauchope et al. 1992; quoted, Richards & Baker 1993; Halfon et al. 1996; Hornsby et al. 1996);
soil $t_{½}$ = 40 d (Pait et al. 1992);
soil $t_{½}$ = 28–46 d (Di Guardo et al. 1994);
$t_{½}$ ~ 30 d (Tomlin 1994);
degradation $t_{½}$ = 15.1 d in garden soil (Müller & Buser 1995);
$t_{½}$ ~ 28.3 d under conventional tillage, $t_{½}$ ~ 25.61 d under ridge tillage and $t_{½}$ ~ 8.63 d with no tillage (Otto et al. 1997).
Biota: $t_{½}$ = 1.15 d in catfish (Ellgehausen et al. 1980);
biochemical $t_{½}$ = 42 d from screening model calculations (Jury et al. 1987b).

TABLE 17.1.1.49.1
Reported Henry's law constants of metolachlor at various temperatures

Feigenbrugel et al. 2004			
gas stripping-GC/MS			
t/°C	H/(Pa m^3/mol)	t/°C	H/(Pa m^3/mol)
283.05	5.39×10^{-4}	293.25	2.262×10^{-3}
283.15	6.34×10^{-4}	297.55	3.099×10^{-3}
283.25	8.126×10^{-4}	298.05	4.053×10^{-3}
283.65	8.465×10^{-4}	298.15	4.757×10^{-3}
285.55	8.01×10^{-4}	298.15	4.312×10^{-3}
287.55	1.088×10^{-3}	299.45	4.170×10^{-3}
289.45	1.193×10^{-3}		
291.55	1.419×10^{-3}	ln H′= A – B/(T/K)	
293.05	2.702×10^{-3}		H′/(M/atm)
293.05	2.471×10^{-3}	A	−24.2298
293.15	2.282×10^{-3}	B	10200
293.15	2.227×10^{-3}		

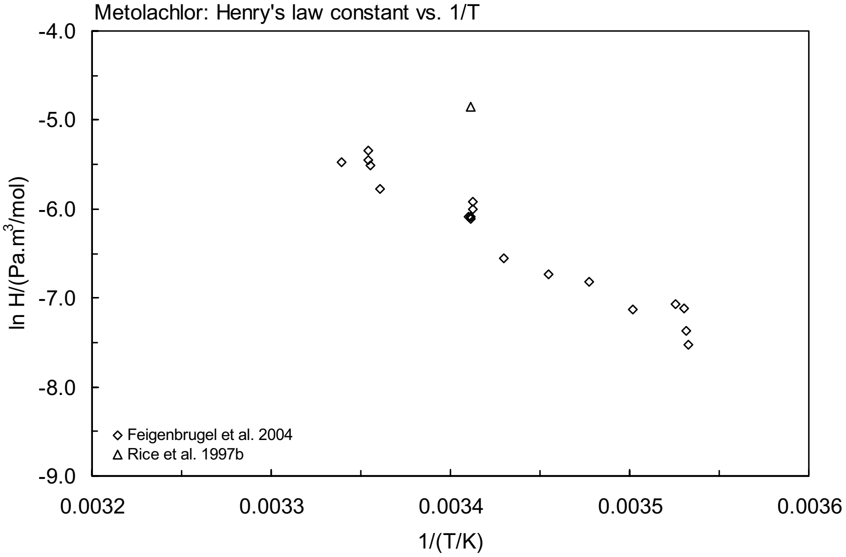
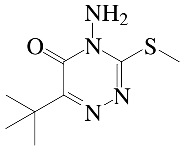


FIGURE 17.1.1.49.1 Logarithm of Henry's law constant versus reciprocal temperature for metolachlor.

17.1.1.50 Metribuzin



Common Name: Metribuzin
Synonym: Metribuzine, Lexone, Preview, Sencor, Sencoral, Sencorer, Sencorex
Chemical Name: 4-amino-6-(t-butyl)-3-(methylthio)-1,2,4-triazin-5-(4*H*)-one
CAS Registry No: 21087-64-9
Uses: herbicide
Molecular Formula: $C_8H_{14}N_4OS$
Molecular Weight: 214.288
Melting Point (°C):

126	(Lide 2003)

Boiling Point (°C): 132.2 Pa (Tomlin 1994)
Density (g/cm³ at 20°C):

1.31	(Hartley & Kidd 1987; Montgomery 1993; Tomlin 1994)
1.28	(Herbicide Handbook 1989)

Dissociation Constant pK_b:

13.0	(Wauchope et al. 1992; Hornsby et al. 1996)
1.0	(pK_a, Montgomery 1993)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

Entropy of Fusion, ΔS_{fus} (J/mol K):

Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F: 0.102 (mp at 126°C)

Water Solubility (g/m³ or mg/L at 25°C or as indicated):

1220	(Kenaga & Goring 1980; Kenaga 1980b; Verschueren 1983)
1200	(20°C, Spencer 1982; Worthing & Walker 1983, 1987; Hartley & Kidd 1987)
1220	(Herbicide Handbook 1989)
1050	(20°C, Montgomery 1993; Tomlin 1994)
1220	(20–25°C, selected, Wauchope et al. 1992; Hornsby et al. 1996)
1065	(20–25°C, reported as 4.97E + 01 mol/m³, Majewski & Capel 1995)

Vapor Pressure (Pa at 25°C or as indicated):

$< 1.3 \times 10^{-3}$	(20°C, Worthing 1983, 1987; Hartley & Kidd 1987; Tomlin 1994)
$< 1.3 \times 10^{-3}$; 2.67×10^{-2}	(20°C; 60°C, Herbicide Handbook 1989)
5.8×10^{-5}	(20°C, Montgomery 1993)
$< 1.3 \times 10^{-3}$	(20–25°C, Wauchope et al. 1992; Hornsby et al. 1996)
5.89×10^{-4}	(20–25°C, Majewski & Capel 1995)

Henry's Law Constant (Pa·m³/mol at 25°C):

$< 1.3 \times 10^{-3}$	(Spencer 1982; Worthing 1987; Hartley & Kidd 1987)
1.21×10^{-5}	(calculated-P/C, Montgomery 1993)
1.18×10^{-5}	(calculated-P/C, Majewski & Capel 1995)

Octanol/Water Partition Coefficient, log K_{OW}:

1.60, 1.70	(quoted, Montgomery 1993)
1.58	(pH 5.6, Tomlin 1994)
1.70	(LOGPSTAR or CLOGP data, Sabljic et al. 1995)

Octanol/Air Partition Coefficient, log K_{OA}:

Bioconcentration Factor, log BCF or log K_B:

2.46, 1.48, < 1.30 (algae, activated sludge, fish in 3-d testing, Korte et al. 1978)
1.77, 1.75 (*Chlorella*, calculated-solubility, Geyer et al. 1981)
1.77, 1.48, 1.04 (algae, activated sludge, *Golden orfe*, Geyer et al. 1982)
1.04, 0.602 (calculated-solubility, calculated-K_{OW}, Kenaga 1980a)
1.48, 1.78, 1.0 (activated sludge, algae, *Golden ide*, Freitag et al. 1985)

Sorption Partition Coefficient, log K_{OC}:

1.98 (soil, Kenaga & Goring 1980)
1.98; 1.94 (quoted, calculated-K_{OW}, Kenaga 1980b)
0.954–2.72 (soil, literature range, Wauchope et al. 1992)
1.80 (soil, estimated, Wauchope et al. 1992; Hornsby et al. 1996)
1.94–1.98, 2.18 (soil, Bottoni & Funari 1992)
1.80–2.72 (soil, Montgomery 1993)
1.78 (soil, Senseman et al. 1997)
1.71 (soil, calculated-MCI $^1\chi$, Sabljic et al. 1995)
1.71; 1.68, 1.33 (soil, quoted obs.; estimated-class-specific model, estimated-general model using molecular descriptors, Gramatica et al. 2000)
2.05, 2.06, 2.04 (soils: organic carbon OC ≥ 0.1%, OC ≥ 0.5%, 0.1 ≤ OC < 0.5%, average, Delle Site 2001)

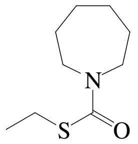
Environmental Fate Rate Constants, k, or Half-Lives, $t_{1/2}$:

Volatilization:
Photolysis: photodecomposition in water is very rapid with $t_{1/2}$ < 1 d; on soil surface under natural sunlight conditions, $t_{1/2}$ = 14–25 d (Tomlin 1994).
Oxidation:
Hydrolysis: $t_{1/2}$ ~ 1 wk in pond water (Hartley & Kidd 1987; Montgomery 1993).
Biodegradation: under goes microbial degradation in moist soil (Worthing 1987)
Biotransformation:
Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants:

Half-Lives in the Environment:

Air:
Surface water: hydrolysis $t_{1/2}$ ~ 1 wk in pond water (Hartley & Kidd 1987; Montgomery 1993; Tomlin 1994);
stable to dilute acids and alkalis, $t_{1/2}$ = 6.7 h at pH 1.2 and 37°C; $t_{1/2}$ = 569 h at pH 4, $t_{1/2}$ = 47 d at pH 7 and $t_{1/2}$ = 191 h at pH 9 for 70°C (Tomlin 1994).
Ground water: reported half-life or persistence $t_{1/2}$ = 4–25, 17–301 and 56 d (Bottoni & Funari 1992).
Sediment:
Soil: undergoes microbial degradation in moist soil (Worthing 1983, 1987);
half-life varies with soil types, $t_{1/2}$ ~ 90–115 d for Red River, Almasippi, and Stockton soils the 3 times this period for Newdale soil for normal application rates (Verschueren 1983);
$t_{1/2}$ ~ 1–2 months in soil (Hartley & Kidd 1987; Tomlin 1994);
$t_{1/2}$ ~ 30–60 d in various soil types varies greatly with climatic conditions, during the growing season (Herbicide Handbook 1989);
$t_{1/2}$ = 9–12 d irrespective of the number of previous treatments in the field; $t_{1/2}$ = 25–40 d irrespective of the pretreatment history of the soil at 20°C in the laboratory (Walker & Welch 1992)
reported $t_{1/2}$ = 23–120 d and the recommended field $t_{1/2}$ = 40 d (Wauchope et al. 1992; Hornsby et al. 1996; quoted, Senseman et al. 1997);
half-lives of in two surface soil microcosms under nitrate, $t_{1/2}$ = 157 d and non-nitrate, $t_{1/2}$ = 187 and 349 d in reducing culture conditions at 16.4°C (Pavel et al. 1999).
Biota: in mammals, following oral administration, 90% elimination within 96 h (Hartley & Kidd 1987).

17.1.1.51 Molinate



Common Name: Molinate
Synonym: Felan, Higalnate, Hydram, Jalan, Molmate, Ordram, Stauffer R 4572, Sakkimok, Yalan, Yulan
Chemical Name: 1*H*-azepine-1-carbothioic acid, hexahydro, *S*-ethyl ester; ethyl 1-hexa-methyleneiminecarbothioate
Uses: selective herbicide to control the germination of annual grasses and broadleaf weeds in rice crops.
CAS Registry No: 2212-67-1
Molecular Formula: $C_9H_{17}NOS$
Molecular Weight: 187.302
Melting Point (°C): < 25 (Montgomery 1993)
Boiling Point (°C):

202	(at 10 mmHg, Hartley & Kidd 1987; Herbicide Handbook 1989; Worthing & Hance 1991; Milne 1995)
117	(at 10 mmHg, Montgomery 1993)

Density (g/cm^3 at 20°C):

1.064	(Hartley & Kidd 1987)
1.0643	(Herbicide Handbook 1989; Montgomery 1993)
1.063	(Worthing & Hance 1991; Milne 1995)

Molar Volume (cm^3/mol):

220.6	(calculated-Le Bas method at normal boiling point)
176.1	(calculated-density)

Dissociation Constant pK_a:
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
Entropy of Fusion, ΔS_{fus} (J/mol K):
Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F: 1.0

Water Solubility (g/m^3 or mg/L at 25°C or as indicated):

880	(20°C, Weber 1972; Hartley & Kidd 1987; Worthing & Walker 1987; Worthing & Hance 1991)
800	(Martin & Worthing 1977)
800–912	(Weber et al. 1980)
912	(21°C, Spencer 1982)
800	(20°C, Herbicide Handbook 1983, 1989)
870	(Kanazawa 1989)
970	(20–25°C, selected, Wauchope et al. 1992; Hornsby et al. 1996; Armbrust 2000)
880	(20°C, Montgomery 1993; Tomlin 1994; Milne 1995)

Vapor Pressure (Pa at 25°C or as indicated):

0.748	(20°C, Weber 1972; Worthing & Walker 1987)
0.746	(20°C, Khan 1980)
0.185	(20°C, GC-RT correlation, Kim 1985)
0.413	(Seiber et al. 1986, 1989)
0.746	(Hartley & Kidd 1987; Montgomery 1993; Tomlin 1994)
0.746	(Herbicide Handbook 1989; Worthing & Hance 1991)
0.746	(20–25°C, selected, Wauchope et al. 1992)

Henry's Law Constant (Pa·m^3/mol at 25°C or as indicated):

0.097	(calculated-P/C, Seiber et al. 1986, 1989)
0.314	(20°C, calculated-P/C, Suntio et al. 1988)
0.159	(20°C, calculated-P/C as per Worthing & Walker 1987;)
0.159	(20°C, calculated-P/C, Muir 1991)

0.095 (20°C, calculated-P/C, Sagebiel et al. 1992)
0.460 (20°C, gas-stripping method, Sagebiel et al. 1992)
0.390 (20°C, headspace-GC method, Sagebiel et al. 1992)
0.162 (calculated-P/C, Montgomery 1993)
0.145 (calculated-P/C, this work)
0.132 (quoted lit., Armbrust 2000)
0.397 (20°C, selected from literature experimentally measured data, Staudinger & Roberts 2001)
$\log K_{AW} = 6.527 - 3024/(T/K)$ (van't Hoff eq. derived from literature data, Staudinger & Roberts 2001)

Octanol/Water Partition Coefficient, $\log K_{OW}$:

3.21 (shake flask-GC, Kanazawa 1981)
2.88 (Worthing & Hance 1991; Tomlin 1994)
2.88 (Montgomery 1993)
3.13 (RP-HPLC-RT correlation, Saito et al. 1993)
3.26 (RP-HPLC-RT correlation, Sicbaldi & Finizio 1993)
3.21 (recommended, Sangster 1993)
2.88 (Milne 1995)
3.21 (recommended, Hansch et al. 1995)
3.25 (RP-HPLC-RT correlation, Finizio et al. 1997)

Bioconcentration Factor, log BCF:

1.15 (calculated-S, Kenaga 1980; quoted, Pait et al. 1992)
1.41 (*Peudorasbora parva,* Kanazawa 1981)

Sorption Partition Coefficient, $\log K_{OC}$:

2.04 (soil, calculated-S, Kenaga 1980)
1.92 (average of 2 soils, Kanazawa 1989)
1.92, 2.04 (soil, quoted values, Bottoni & Funari 1992)
1.92, 2.46 (soil, quoted exptl., calculated-MCI χ and fragments contribution, Meylan et al. 1992)
2.28 (soil, 20–25°C, selected, Wauchope et al. 1992; Hornsby et al. 1996)
1.93–1.97 (Montgomery 1993)
2.28 (selected, Lohninger 1994)
1.92 (soil, calculated-MCI ${}^1\chi$, Sabljic et al. 1995)
2.07 (soil, quoted lit., Armbrust 2000)
1.92; 2.31, 1.86 (soil, quoted exptl.; estimated-class specific model, estimated-general model using molecular descriptors, Gramatica et al. 2000)

Environmental Fate Rate Constants, k, or Half-Lives, $t_{1/2}$:

Volatilization: $k = 0.0150\ h^{-1}$ (average of 2 runs, Seiber et al. 1986); 1.1 kg ha^{-1} (1st 4 day) from flooded rice fields (Seiber et al. 1986; Seiber & McChesney 1987);
estimated $t_{1/2}$ = 43 d from 1 m depth of water at 20°C (Muir 1991).

Photolysis: $t_{1/2}$ = 7–10 d for 8–10 μg mL^{-1} to degrade in distilled water under > 290 nm light (Soderquist et al. 1977; quoted, Cessna & Muir 1991);
$t_{1/2}$ = 96 h for < 5% of 0.2 μg mL^{-1} to degrade in distilled water under sunlight (Deuel et al. 1978; quoted, Cessna & Muir 1991);
$t_{1/2}$ = 245 h for 2–54% of 10 μg mL^{-1} to degrade in distilled water under sunlight (Draper & Crosby 1984; quoted, Cessna & Muir 1991).

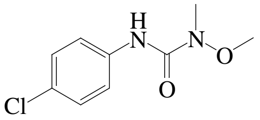
Oxidation: calculated life-time of 6 h for the vapor-phase reaction with OH radicals in the troposphere (Atkinson et al. 1992; Kwok et al. 1992);
measured rate constant for reaction with hydroxyl radical, $k(aq.) = 0.85 \times 10^9\ M^{-1}\cdot s^{-1}$ in irradiated field water both in the laboratory and sunlit rice paddies (Mabury & Crosby 1996);
measured hydroxy radical reaction rate constant for molinate $k = 7.7 \times 10^{12}\ M^{-1}\ h^{-1}$ (Armbrust 2000).

Hydrolysis: $t_{1/2}$ > 10 d in aqueous buffer at pH 5–9 in the dark (Soderquist et al. 1977; quoted, Muir 1991); stable aqueous hydrolysis rate at pH 5, 7, 9 (Armbrust 2000).

Biodegradation: $t_{½}$ ~16 d for 0.2 µg mL^{-1} to biodegrade in flooded soils (Deuel et al. 1978; quoted, Muir 1991);
$t_{½}$ = 10 wk for 4.2 µg mL^{-1} to biodegrade in flooded soil and $t_{½}$ < 2 wk in water both at 21–26°C (Thomas & Holt 1980; quoted, Muir 1991);
aerobic rate constant, $k = 2.22 \times 10^{-3}$ h^{-1} (Armbrust 2000).
Biotransformation:
Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants:

Half-Lives in the Environment:
Air: calculated lifetime of 6 h for the vapor-phase reaction with OH radicals in the troposphere (Atkinson et al. 1992; Kwok et al. 1992).
Surface water: $t_{½}$ = 84 h from dissipation from flooded rice fields (Seiber & McChesney 1987; quoted, Seiber et al. 1989).
Ground water: reported half-lives or persistence, $t_{½}$ = 3–14, 8–25 and 40–160 d (Bottoni & Funari 1992)
Sediment:
Soil: persistence of 2 months in soil (Wauchope 1978);
$t_{½}$ ~ 3 wk in moist loam soils at 21–27°C (Herbicide Handbook 1989);
selected field $t_{½}$ = 21 d (Wauchope et al. 1992; quoted, Halfon et al. 1996; Hornsby et al. 1996);
soil $t_{½}$ = 21 d (Pait et al. 1992);
reported $t_{½}$ = 3–14 d, 8–25 d and 40–160 d (Bottoni & Funari 1992).
Biota:

17.1.1.52 Monolinuron



Common Name: Monolinuron
Synonym: Afesin, Aresin, Arresin, Hoe 02747
Chemical Name: 3-(4-chlorophenyl)-1-methoxy-1-methylurea; *N'*-(4-chlorophenyl)-*N*-methoxy-*N*-methylurea
Uses: herbicide for pre- or post-emergence control of annual broadleaf weeds and annual grasses in asparagus, berry fruit, cereals, maize, field beans, vines, leeks, onions, potatoes, herbs, lucerne, flowers, ornamental shrubs and trees, etc.
CAS Registry No: 1746-81-2
Molecular Formula: $C_9H_{11}ClN_2O_2$
Molecular Weight: 214.648
Melting Point (°C):

77	(Lide 2003)

Boiling Point (°C):
Density (g/cm^3 at 20°C):
Molar Volume (cm^3/mol):

224.0	(calculated-Le Bas method at normal boiling point)

Dissociation Constant pK_a:
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
Entropy of Fusion, ΔS_{fus} (J/mol K):
Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F: 0.309 (mp at 77°C)

Water Solubility (g/m^3 or mg/L at 25°C or as indicated):

735	(20°C, Melnikov 1971)
735	(Spencer 1973, 1982)
580	(Martin & Worthing 1977; Khan 1980)
735	(Worthing & Walker 1983, 1987, Hartley & Kidd 1987; Worthing & Hance 1991; Tomlin 1994)
735	(20–25°C, selected, Augustijn-Beckers et al. 1994; Hornsby et al. 1996)

Vapor Pressure (Pa at 25°C or as indicated):

0.02	(22°C, Khan 1980; Hartley & Kidd 1987)
0.0015	(20°C, Spencer 1982)
6.40	(65°C, Worthing & Hance 1991)
0.02	(20–25°C, selected, Augustijn-Beckers et al. 1994; Hornsby et al. 1996)
0.0013, 0.10	(20°C, 50°C, Tomlin 1994)

Henry's Law Constant (Pa·m^3/mol at 25°C):

0.0058	(calculated-P/C, this work)

Octanol/Water Partition Coefficient, log K_{OW}:

1.60	(Briggs 1969)
2.30	(shake flask-UV, Briggs 1981)
1.60	(selected, Dao et al. 1983)
1.99	(RP-HPLC-k' correlation, Braumann et al. 1983)
2.22	(shake flask, Mitsutake et al.1986)
2.20	(Worthing & Hance 1991; Tomlin 1994)
2.16	(RP-HPLC-RT correlation, Sicbaldi & Finizio 1993)
2.30	(recommended, Sangster 1993)
2.30	(recommended, Hansch et al. 1995)
2.31	(Pomona-database, Müller & Kördel 1996)

2.16 (RP-HPLC-RT correlation, Finizio et al. 1997)

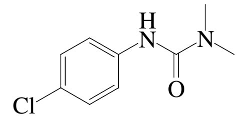
Bioconcentration Factor, log BCF:
1.23; 1.00 (calculated-S, calculated-K_{OC}, Kenaga 1980)
1.85 (activated sludge, Freitag et al. 1982, 1984, 1985)
1.52, < 1.0 (algae, golden orfe, Freitag et al. 1982)
1.60, 1.30 (algae, golden ide, Freitag et al. 1985)

Sorption Partition Coefficient, log K_{OC}:
2.30 (soil, Hamaker & Thompson 1972)
2.11 (soil, calculated-S as per Kenaga & Goring 1980, Kenaga 1980)
1.60 (reported as log K_{OM}, Briggs 1981)
2.36, 2.08, 1.21 (estimated-S, calculated-S and mp, calculated-K_{OW}, Karickhoff 1981)
2.40–2.70 (soil, Worthing & Hance 1991)
2.26–2.30, 2.40–2.70 (soil, quoted values, Bottoni & Funari 1992)
1.78 (soil, HPLC-screening method, mean value of different stationary and mobile phases, Kördel et al. 1993, 1995b)
2.30 (20–25°C, estimated, Augustijn-Beckers et al. 1994; Hornsby et al. 1996)
2.10 (soil, calculated-MCI $^1\chi$, Sabljic et al. 1995)
1.78; 2.33 (HPLC-screening method; calculated-PCKOC fragment method, Müller & Kördel 1996)
2.44, 1.50, 1.71, 1.754, 2.45 (first generation Eurosoils ES-1, ES2, ES-3, ES-4, ES-5, shake flask/batch equilibrium-HPLC/UV, Gawlik et al. 1998, 1999)
2.05, 1.72, 1.695, 1.825, 2.407 (second generation Eurosoils ES-1, ES2, ES-3, ES-4, ES-5, shake flask/batch equilibrium-HPLC/UV, Gawlik et al. 1999)
2.050, 1.721, 1.695, 1.825, 2.407 (second generation Eurosoils ES-1, ES-2, ES-3, ES-4, ES-5, shake flask-batch equilibrium-HPLC/UV and HPLC-k′ correlation, Gawlik et al. 2000)
2.10; 2.04, 2.31 (soil, quoted obs.; estimated-class-specific model, estimated-general model using molecular descriptors, Gramatica et al. 2000)
1.88, 1.88 (soils: organic carbon OC ≥ 0.1%, OC ≥ 0.5%, average, Delle Site 2001)

Environmental Fate Rate Constants, k, or Half-Lives, $t_{1/2}$:
Photolysis: $t_{1/2}$ = 23 h for 66% of 286 μg/mL to degrade in distilled water under > 300 nm light (Kotzias et al. 1974; quoted, Cessna & Muir 1991).

Half-Lives in the Environment:
Air:
Surface water:
Ground water: reported half-lives or persistence, $t_{1/2}$ = 45–60 d (Bottoni & Funari 1992)
Sediment:
Soil: reported $t_{1/2}$ = 45–60 d (Worthing & Hance 1991);
estimated field $t_{1/2}$ = 60 d (Augustijn-Beckers et al. 1994; Hornsby et al. 1996).
Biota:

17.1.1.53 Monuron



Common Name: Monuron
Synonym: Chlorfenidim, CMU, Karmex, Lirobetarex, Monurex, Monurox, Rosuran, Telvar, Urox
Chemical Name: *N*′-(4-chlorophenyl)-*N*-*N*-dimethylurea; 1,1-dimethyl-3-(*p*-chlorophenyl)urea
Uses: herbicide; also as sugar cane flowering suppressant.
CAS Registry No: 150-68-5
Molecular Formula: $C_9H_{11}ClN_2O$
Molecular Weight: 198.648
Melting Point (°C):
170.5 (Kühne et al. 1995; Lide 2003)
Boiling Point (°C):
185–200 (decomposes, Montgomery 1993)
Density (g/cm^3 at 20°C):
1.27 (Spencer 1982; Hartley & Kidd 1987; Montgomery 1993)
Molar Volume (cm^3/mol):
202.9 (calculated-Le Bas method at normal boiling point)
173.0 (modified Le Bas method, Spurlock & Biggar 1994a)
Dissociation Constant pK_a:
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
Entropy of Fusion, ΔS_{fus} (J/mol K):
Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F: 0.0374 (mp at 170.5°C)

Water Solubility (g/m^3 or mg/L at 25°C or as indicated):
203 (Freed 1966)
230 (Günther et al. 1968; Sanborn et al. 1977; Khan 1980; Ashton & Crafts 1981)
262 (shake flask-UV, Hurle & Freed 1972)
230 (20°C, Weber 1972; Worthing & Walker 1987)
230 (Martin & Worthing 1977; Hartley & Kidd 1987)
200 (shake flask-HPLC, Ellgehausen et al. 1981)
200 (20°C, selected, Suntio et al. 1988)
275 (Spurlock 1992; Spurlock & Biggar 1994b)
230 (at pH 6.26, Montgomery 1993)
230 (20–25°C, selected, Augustijn-Beckers et al. 1994; Hornsby et al. 1996)

Vapor Pressure (Pa at 25°C or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):
7.60×10^{-5}, 1.2×10^{-5} (25, 27°C, Nex & Swezey 1954)
6.67×10^{-5} (Bailey & White 1965)
6.72×10^{-5} (20°C, Weber 1972; Worthing & Walker 1987)
6.67×10^{-5} (Ashton & Crafts 1973, 1981; Khan 1980)
5.33×10^{-5}* (30.35°C, Knudsen effusion, measured range 303.5–379.1 K, Wiedemann 1972)
log (P/mmHg) = 13.3052 – 5988.39/(T/K); temp range 303.5–379.1 K (Antoine eq., effusion, Wiedemann 1972)
6.70×10^{-5} (OECD 1981)
2.30×10^{-5} (calculated, Jury et al. 1983)
6.00×10^{-5} (Hartley & Kidd 1987)
6.67×10^{-5} (Budavari 1989)
2.30×10^{-5} (selected, Taylor & Spencer 1990)
6.00×10^{-5} (20°C, Montgomery 1993)
6.67×10^{-5} (20–25°C, selected, Augustijn-Beckers et al. 1994; Hornsby et al. 1996)

Henry's Law Constant (Pa·m^3/mol at 25°C or as indicated):
5.80×10^{-5} (20°C, volatilization rate, Burkhard & Guth 1981)
1.88×10^{-5} (calculated-P/C, Jury et al. 1984, 1987a; Jury & Ghodrati 1989)
3.00×10^{-3} (20°C, calculated-P/C, Suntio et al. 1988)
1.91×10^{-5} (calculated-P/C, Taylor & Glotfelty 1988)
5.60×10^{-5} (20°C, calculated-P/C, Muir 1991)
3.00×10^{-3} (20°C, calculated-P/C, Montgomery 1993)
6.60×10^{-5} (calculated-P/C, this work)

Octanol/Water Partition Coefficient, log K_{OW}:
1.46 (Briggs 1969)
1.66 (calculated-fragment const., Rekker 1977)
1.80 (shake flask-UV, Erkell & Walum 1979)
2.08 (selected, Ellgehausen et al. 1980; Geyer et al. 1991)
2.12 (Rao & Davidson 1980)
1.98 (shake flask-UV, Briggs 1981)
2.08 (shake flask, Ellgehausen et al. 1980)
1.66 (shake flask, Ellgehausen et al. 1981)
1.86 (selected, Dao et al. 1983; Gerstl & Helling 1987)
1.91 (RP-HPLC-k′ correlation Braumann et al. 1983)
1.80 (selected, Suntio et al. 1988)
2.12 (shake flask-HPLC, Spurlock 1992; Spurlock & Biggar 1994b)
1.46, 2.12 (Montgomery 1993)
1.86 (RP-HPLC-RT correlation, Sicbaldi & Finizio 1993)
1.94 (recommended, Sangster 1993)
1.89; 1.88 (shake flask-UV; RP-HPLC-k′ correlation, Liu & Qian 1995)
1.94 (recommended, Hansch et al. 1995)
1.99 (Pomona-database, Müller & Kördel 1996)
1.86 (RP-HPLC-RT correlation, Finizio et al. 1997)

Bioconcentration Factor, log BCF:
1.786 (log BF bioaccumulation factor for algae, Ellgehausen et al. 1980)
0.32 (log BF bioaccumulation factor for daphnids, Ellgehausen et al. 1980)
0.245 (log BF bioaccumulation factor for daphnids, Ellgehausen et al. 1980)
1.46 (calculated-S, Kenaga 1980)
0.699 (calculated-K_{OC}, Kenaga 1980)
0.0 (*Triaenodes tardus*, Belluck & Felsot 1981)
1.58, 1.67 (cuticle/water: tomato, pepper; Evelyne et al. 1992)

Sorption Partition Coefficient, log K_{OC}:
2.00 (soil, Hamaker & Thompson 1972)
2.34 (soil, calculated-S as per Kenaga & Goring 1980, Kenaga 1980)
2.26 (av. of 18 soils, Rao & Davidson 1980)
1.70 (soil, converted from reported K_{OM}, multiplied by 1,724, Briggs 1981)
2.58, 1.51 (estimated-S, calculated-S and mp, Karickhoff 1981)
1.07, 1.73 2.58 (estimated-K_{OW}, Karickhoff 1981)
2.03, 1.85; 2.17, 1.52 (estimated-K_{OW}s; solubilities, Madhun et al. 1986)
1.99; 2.12 (quoted; calculated-MCI χ, Gerstl & Helling 1987)
2.26 (screening model calculations, Jury et al. 1987a,b; Jury & Ghoodrati 1989)
1.99, 2.33 (Montgomery 1993)
2.18 (20–25°C, estimated, Augustijn-Beckers et al. 1994; Hornsby et al. 1996)
1.99 (soil, HPLC-screening method, mean value from different stationary and mobile phases, Kördel et al. 1993, 1995a,b)
2.29 (calculated-K_{OW}, Liu & Qian 1995)
1.95 (soil, calculated-MCI $^1\chi$, Sabljic et al. 1995)

1.99; 1.92 (HPLC-screening method; calculated-PCKOC fragment method, Müller & Kördel 1996)
2.58, 1.77, 1.85, 1.77, 2.41 (first generation Eurosoils ES-1, ES2, ES-3, ES-4, ES-5, shake flask/batch equilibrium-HPLC/UV, Gawlik et al. 1998, 1999)
2.14, 2.018, 1.79, 1.764, 2.243 (second generation Eurosoils ES-1, ES2, ES-3, ES-4, ES-5, shake flask/batch equilibrium-HPLC/UV, Gawlik et al. 1999)
2.141, 2.018, 1.793, 1.764, 2.243 (second generation Eurosoils ES-1, ES-2, ES-3, ES-4, ES-5, shake flask/batch equilibrium-HPLC/UV and HPLC-k′ correlation, Gawlik et al. 2000)
1.95; 1.96, 2.13 (soil, quoted obs.; estimated-class-specific model, estimated-general model using molecular descriptors, Gramatica et al. 2000)
1.80, 1.80 (soils: organic carbon OC ≥ 0.1%, OC ≥ 0.5%, average, Delle Site 2001)

Environmental Fate Rate Constants, k, or Half-Lives, $t_{½}$:
Volatilization:
Photolysis: $t_{½}$ = 14 d for 6% of 200 μg mL^{-1} to degrade in distilled water under sunlight (Crosby & Tang 1969; quoted, Cessna & Muir 1991);
$t_{½}$ = 2.25 h for 44% of 200 μg mL^{-1} to degrade in distilled water under 300 nm light (Tanaka et al. 1977; quoted, Cessna & Muir 1991);
$t_{½}$ = 2.25 s for 75% of 100 μg mL^{-1} to degrade in 0.2% Triton X-100 aqueous solution under 300 nm light (Tanaka et al. 1981; quoted, Cessna & Muir 1991);
$t_{½}$ = 2.25 h for > 70% of 200 μg mL^{-1} to degrade in aqueous solutions of nonionic surfactants at concns. in excess of critical micelle concn. under 300 nm light (Tanaka et al. 1979; quoted, Cessna & Muir 1991);
$t_{½}$ = 45 h for 69% of 165 μg mL^{-1} to degrade in distilled water under > 280 nm light (Tanaka et al. 1982; quoted, Cessna & Muir 1991).
Oxidation:
Hydrolysis: $t_{½}$ > 4 months for 3974 μg mL^{-1} to hydrolyze in phosphate buffer at pH 5–9 and 20°C (El-Dib & Aly 1976; quoted, Muir 1991).
Biodegradation: aerobic $t_{½}$ ~ 7 d for 0.01 μg mL^{-1} to biodegrade in river water (Eichelberger & Lichtenberg 1971; quoted, Muir 1991);
$t_{½}$ = 166 d for a 100 d leaching and screening test in 0–10 cm depth of soil (Jury et al. 1983, 1984, 1987a,b; Jury & Ghodrati 1989);
aerobic $t_{½}$ ~ 10–15 d for 0.0005–10 μg mL^{-1} to biodegrade in filtered sewage water at 20°C (Wang et al. 1985; quoted, Muir 1991).
Biotransformation:
Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants:
$k_2 = 21.05\ d^{-1}$ (catfish, Ellgehausen et al. 1980)

Half-Lives in the Environment:
Air:
Surface water: persistence of up to 8 wk in river water (Eichelberger & Lichtenberg 1971).
Ground water:
Sediment:
Soil: $t_{½}$ = 5.0 months at 15°C and 4.1 months at 30°C in soils (Freed & Haque 1973);
reported $t_{½}$ = 166 d from screening model calculations (Jury et al. 1987a,b; Jury & Ghodrati 1989; quoted, Montgomery 1993);
estimated field $t_{½}$ = 170 d (Augustijn-Beckers et al. 1994; Hornsby et al. 1996).
Biota: $t_{½}$ = 0.45 d in catfish (Ellgehausen et al. 1980);
biochemical $t_{½}$ = 166 d from screening model calculations (Jury et al. 1987a,b; Jury & Ghodrati 1989).

TABLE 17.1.1.53.1
Reported vapor pressures of monuron at various temperatures

Wiedemann 1972			
Knudsen effusion			
T/K	P/Pa	T/K	P/Pa
303.5	5.33×10^{-5}	358.7	0.0536
316.0	2.44×10^{-4}	360.2	0.0561
329.8	2.16×10^{-3}	379.1	0.399
330.6	1.53×10^{-3}		
330.6	2.22×10^{-3}	$\log P = A - B/(T/K)$	
338.8	7.05×10^{-3}		P/mmHg
341.4	9.45×10^{-3}	A	13.3952
345.7	0.0105	B	5988.39
349.5	0.0204		
357.0	0.0529	$\Delta H_{subl}/(\text{kJ mol}^{-1}) = 114.6$	

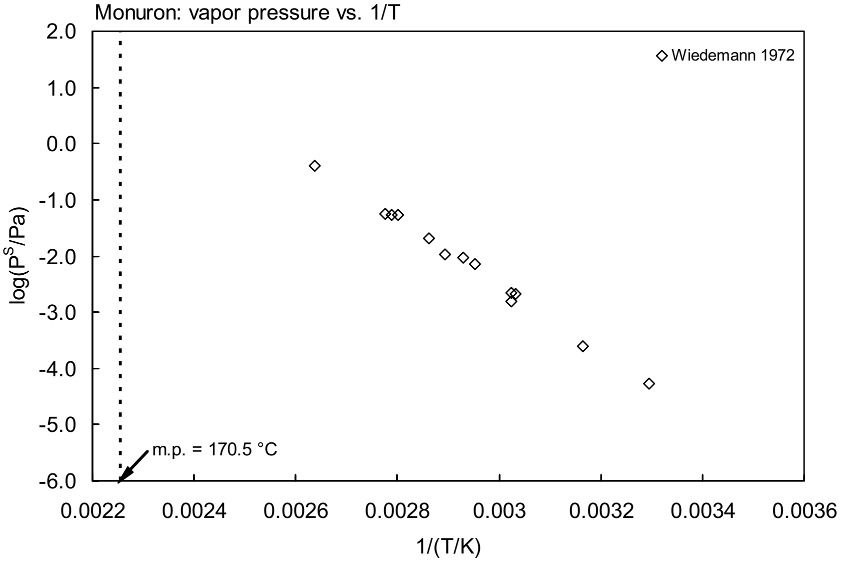
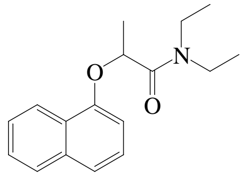


FIGURE 17.1.1.53.1 Logarithm of vapor pressure versus reciprocal temperature for monuron.

17.1.1.54 Napropamide



Common Name: Napropamide
Synonym: Devrinol
Chemical Name: 2-(α-naphthloxy)-*N*,*N*-diethylpropionamide
CAS Registry No: 15299-99-7
Uses: herbicide
Molecular Formula: $C_{17}H_{21}NO_2$
Molecular Weight: 271.355
Melting Point (°C):

75	(Worthing & Walker 1987; Lide 2003)

Density (g/cm^3 at 20°C):
Molar Volume (cm^3/mol):
Dissociation Constant pK_a:

2.93	(Woodburn et al. 1993)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
Entropy of Fusion, ΔS_{fus} (J/mol K):
Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F: 0.323 (mp at 75°C)

Water Solubility (g/m^3 or mg/L at 25°C or as indicated):

69	(shake flask-LSC or GC, Gerstl & Mingelgrin 1984)
73	(20°C, Spencer 1982; Hartley & Kidd 1987; Worthing & Walker 1987; Herbicide Handbook 1989; Montgomery 1993; Tomlin 1994)
74	(20–25°C, selected, Wauchope et al. 1992; Hornsby et al. 1996)

Vapor Pressure (Pa at 25°C or as indicated):

2.67×10^{-4}	(Spencer 1982)
5.3×10^{-4}	(Herbicide Handbook 1989)
5.3×10^{-4}	(Hartley & Kidd 1987; Worthing & Walker 1987; Montgomery 1993; Tomlin 1994)
2.27×10^{-5}	(20–25°C, selected, Wauchope et al. 1992; Hornsby et al. 1996)
1.67×10^{-3}	(20–25°C, Majewski & Capel 1995)

Henry's Law Constant (Pa·m^3/mol at 25°C or as indicated):

0.00294	(calculated-P/C, Montgomery 1993)
0.00197	(20–25°C, Majewski & Capel 1995)

Octanol/Water Partition Coefficient, log K_{OW}:

3.08	(shake flask-GC or LSC, Gerstl & Mingelgrin 1984)
3.36	(Montgomery 1993)
3.30	(Tomlin 1994)
3.36	(recommended, Hansch et al. 1995)

Octanol/Air Partition Coefficient, log K_{OA}:

Bioconcentration Factor, log BCF or log K_B:

Sorption Partition Coefficient, log K_{OC}:

2.04–3.09	(various soils, Mingelgrin & Gestl 1983)
2.82, 3.56	(soil: quoted, calculated-MCI χ, Gerstl & Helling 1987)

2.62 (soil, average of log K_{OC} values, Gerstl 1990)
3.52–4.29; 3.72 at pH 2, 3.35 at pH 6 (Dead sea sediment, Gestl & Kilger 1990)
2.62–3.54; 3.54 at pH 2, 3.40 at pH 6 (Kinnert F sediment, Gestl & Kilger 1990)
2.71–3.62; 3.62 at pH 2, 3.27 at pH 6 (Kinnert G sediment, Gestl & Kilger 1990)
2.40–3.31; 3.31 at pH 2, 3.20 at pH 5 (Oxford soil, Gestl & Kilger 1990)
2.39–3.15; 3.15 at pH 2, 2.88 at pH 6 (Malkiya soil, Gestl & Kilger 1990)
2.28–3.29; 3.29 at pH 2, 3.09 at pH 5 (Neve Ya'ar soil, Gestl & Kilger 1990)
2.85 (soil, Wauchope et al. 1992; Hornsby et al. 1996)
2.29–3.99 (soil/sediment, literature range, Montgomery 1993)
2.83 (soil, Montgomery 1993)
2.62 (soil, calculated-MCI χ, Sabljic et al. 1995)
2.58, 2.58, 2.61 (soils: organic carbon OC $\geq$ 0.1%, OC $\geq$ 0.5%, 0.1 $\leq$ OC < 0.5%, average, Delle Site 2001)
2.80 (sediment: organic carbon OC $\geq$ 0.5%, average, Delle Site 2001)

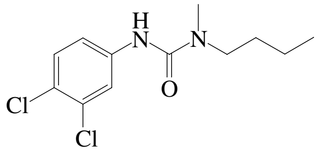
Environmental Fate Rate Constants, k, or Half-Lives, $t_{½}$:

Volatilization: very little loss occurred by volatilization from soil surface (Herbicide Handbook 1989).
Photolysis: under condition of high sunlight intensity in the summer, $t_{½}$ ~ 4 d on the soil surface (Herbicide Handbook 1989);
decomposed by sunlight, $t_{½}$ = 25.7 min. (Tomlin 1994).
Oxidation:
Hydrolysis: stable to hydrolysis between pH 4 and 10 at 40°C (Hartley & Kidd 1987; Worthing 1987; Tomlin 1994).
Biodegradation: slowly broken down by microorganisms in soil, in pure culture, a soil fungus metabolizes rapidly with $t_{½}$ = 2 wk (Herbicide Handbook 1989).
Biotransformation: rapidly metabolized in plants to water-soluble metabolites (Tomlin 1994).
Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants:

Half-Lives in the Environment:

Air:
Surface water:
Ground water: decomposed by sunlight, $t_{½}$ = 25.7 min. (Montgomery 1993; Tomlin 1994).
Sediment:
Soil: $t_{½}$ ~ 55 d in the plots treated for the first time whereas $t_{½}$ = 6–12 d in pre-treated plots that had previously been sprayed with napropamide in the field; $t_{½}$ = 25–40 d irrespective of the pre-treatment history of the soil in the laboratory at 20°C (Walker & Welch 1992)
$t_{½}$ ~ 8–12 wk (Hartley & Kidd 1987; Tomlin 1994);
field $t_{½}$ = 70 d (Wauchope et al. 1992; Hornsby et al. 1996);
moist loam or sandy-loam soils at 79–90°C, $t_{½}$ = 8–12 wk (Montgomery 1993).
Biota: rapidly metabolized in plants to water-soluble metabolites (Tomlin 1994).

17.1.1.55 Neburon



Common Name: Neburon
Synonym: Kloben, Neburea, Neburex
Chemical Name: 1-butyl-3-(3,4-dichlorophenyl)-1-methylurea; *N*-butyl-*N′*(3,4-dichloro-phenyl)-*N*-methylurea
Uses: pre-emergence herbicide to control grasses and broadleaf weeds in peas, beans, lucerne, garlic, beets, cereals, strawberries, ornamentals and forestry.
CAS Registry No: 555-37-3
Molecular Formula: $C_{12}H_{16}Cl_2N_2O$
Molecular Weight: 275.174
Melting Point (°C):
102–103 (Khan 1980; Spencer 1982; Worthing & Hance 1991; Tomlin 1994)
101.5–103 (Montgomery 1993)
Boiling Point (°C):
Density (g/cm^3 at 20°C):
Molar Volume (cm^3/mol):
236.0 (modified Le Bas method at normal boiling point, Spurlock & Biggar 1994a)
Dissociation Constant pK_a:
Enthalpy of Vaporization, ΔH_V (kJ/mol):
96.91 (Rordorf 1989)
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
29.71 (DSC method, Plato & Glasgow 1969)
26.9 (Rordorf 1989)
Entropy of Fusion, ΔS_{fus} (J/mol K):
Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F:

Water Solubility (g/m^3 or mg/L at 25°C or as indicated):
4.8 (24°C, Bailey & White 1965; Melnikov 1971)
4.8 (Martin & Worthing 1977)
4.8 (28°C, Khan 1980)
5.0 (Hartley & Kidd 1987; Tomlin 1994)
4.8 (24°C, Worthing & Walker 1987, Worthing & Hance 1991; Montgomery 1993)
5.2 (Spurlock 1992; Spurlock & Biggar 1994b)
5.0 (20–25°C, selected, Augustijn-Beckers et al. 1994; selected, Hornsby et al. 1996)
4.67, 9.99 (quoted, calculated-group contribution fragmentation method, Kühne et al. 1995)

Vapor Pressure (Pa at 25°C or as indicated and reported temperature dependence equations):
6.30×10^{-6}, 4.10×10^{-4}, 0.015, 0.33, 4.90 (25, 50, 70, 100, 125°C, gas saturation-GC, Rordorf 1989)
$\log (P_S/Pa) = 18.272 - 6999.1/(T/K)$; measured range 50–103°C (solid, gas saturation-GC, Rordorf 1989)
$\log (P_L/Pa) = 13.285 - 5062.2/(T/K)$; measured range 105–140°C (liquid, gas saturation-GC, Rordorf 1989)

Henry's Law Constant (Pa·m^3/mol at 25°C):

Octanol/Water Partition Coefficient, log K_{OW}:
4.59 (selected, Dao et al. 1983; Gerstl & Helling 1987)
4.31 (RP-HPLC-k′ correlation, Braumann et al. 1983)
4.22 (Spurlock 1992; Spurlock & Biggar 1994b)
3.80 (selected, Sangster 1993)
3.80 (calculated, Montgomery 1993)

4.10 (shake flask-UV, Liu & Qian 1995)
3.99 (RP-HPLC-k′ correlation, Liu & Qian 1995)
3.80 (recommended, Hansch et al. 1995)
3.40, 4.02, 4.13 (RP-HPLC-RT correlation, CLOGP, calculated-S, Finizio et al. 1997)

Bioconcentration Factor, log BCF:

2.41 (calculated-S, Kenaga 1980; quoted, Isensee 1991)
1.85, 2.18 (calculated-S, K_{OC}, Kenaga 1980)

Sorption Partition Coefficient, log K_{OC}:

3.36 (soil, Hamaker & Thompson 1972)
3.26, 2.72 (soil, calculated-S, Kenaga 1980)
3.49 (average of soils/sediments, Rao & Davidson 1980)
3.36, 3.23 (quoted, calculated-MCI χ, Gerstl & Helling 1987)
2.95 (soil, calculated-χ and fragment contribution, Meylan et al. 1992)
3.49 (Montgomery 1993)
3.40 (20–25°C, selected, Augustijn-Beckers et al. 1994; Hornsby et al. 1996)
3.40 (selected, Lohninger 1994)
3.60 (calculated-K_{OW}, Liu & Qian 1995)
3.140 (soil, calculated-MCI $^1\chi$, Sabljic et al. 1995)
3.40; 2.86, 2.69 (soil, quoted exptl.; estimated-class-specific model, estimated-general model using molecular descriptors, Gramatica et al. 2000)

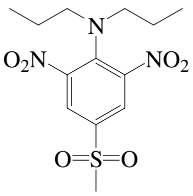
Environmental Fate Rate Constants, k, or Half-Lives, $t_{½}$:

Hydrolysis: $t_{½} > 4$ months for 5500 μg/mL to hydrolyze in phosphate buffer at pH 5–9 and 20°C (El-dib & Aly 1976; quoted, Muir 1991).

Half-Lives in the Environment:

Soil: residual activity in soil is limited to approximately 3–4 months (Hartley & Kidd 1987; quoted, Montgomery 1993);
selected field $t_{½} = 120$ d (Augustijn-Beckers et al. 1994; Hornsby et al. 1996).

17.1.1.56 Nitralin



Common Name: Nitralin
Synonym: Planavin
Chemical Name: 4-(methylsulfonyl)-2,6-dinitro-*N*,*N*-dipropylbenzamine
CAS Registry No: 4726-14-1
Uses: herbicide
Molecular Formula: $C_{13}H_{19}N_3O_6S$
Molecular Weight: 345.371
Melting Point (°C):
150 (Lide 2003)
Boiling Point (°C):
Density (g/cm^3 at 20°C): 1.39 (Hartley & Kidd 1987)
Molar Volume (cm^3/mol):
Dissociation Constant pK$_a$:
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
Entropy of Fusion, ΔS_{fus} (J/mol K):
Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F: 0.0594 (mp at 150°C)

Water Solubility (g/m^3 or mg/L at 25°C):
0.60 (Melnikov 1971; Kenaga & Goring 1980; Kenaga 1980b; Isensee 1991)
0.60 (Ashton & Crafts 1981; Hartley & Kidd 1987; Worthing & Walker 1987)

Vapor Pressure (Pa at 25°C):
0.240 (Ashton & Crafts 1981)
2.0×10^{-5} (Hartley & Kidd 1987)

Henry's Law Constant (Pa·m^3/mol):

Octanol/Water Partition Coefficient, log K_{OW}:
6.73 (calculated-MCI χ, Patil 1994)
2.81 (LOGPSTAR or CLOGP data, Sabljic et al. 1995)

Octanol/Air Partition Coefficient, log K_{OA}:

Bioconcentration Factor, log BCF or log K_B:
2.90, 1.76 (calculated-solubility, K_{OW}, Kenaga 1980b)

Sorption Partition Coefficient, log K_{OC}:
2.98 (Kenaga & Goring 1980)
3.76 (calculated, Kenaga 1980a)
2.92 (soil, calculated-MCI χ, Sabljic et al. 1995)
2.92; 3.28 (soil, quoted obs.; estimated-general model using molecular descriptors, Gramatica et al. 2000)

Environmental Fate Rate Constants, k, or Half-Lives, $t_{½}$:
Biotransformation: Degradation by abiotic reductive transformations:
k = 3.44 M^{-1} s^{-1} in H_2S with (mecapto)juglone (hydroquinone moiety, an abiotic reductant found in natural systems) solution at pH 6.65 (Wang & Arnold 2003)
Aqueous solutions with surface-bound Fe(II) species and their furst-order rate constants as:

$k = 0.44 \times 10^{-3}$ h^{-1} at pH 6.5, $k = 0.68 \times 10^{-2}$ h^{-1} at pH 7.0, $k = 0.133$ h^{-1} at pH 7.4, and $k = 1.96$ h^{-1} at pH 7.8 for aqueous ferrous ion system;

$k = 0.580$ h^{-1} at pH 6.5, $k = 1.15$ h^{-1} at pH 6.7, $k = 6.06$ h^{-1} at pH 7.0, and $k = 20.9$ h^{-1} at pH 7.3 for Fe(II)/goethite system;

$k = 2.54 \times 10^{-3}$ h^{-1} at pH 6.5, $k = 1.83 \times 10^{-3}$ h^{-1} at pH 7.0, $k = 4.13 \times 10^{-3}$ h^{-1} at pH 7.4 and $k = 7.70 \times 10^{-3}$ h^{-1} at pH 7.8 for Fe(II)/clay system, all with total dissolved Fe(II) = 1 mM(Wang & Arnold 2003)

Half-Lives in the Environment:

Air:

Surface water:

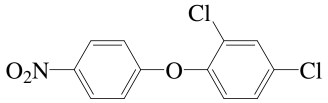
Ground water:

Sediment:

Soil: $t_{½} \sim 30–54$ d in dry soil (Hartley & Kidd 1987)

Biota: in mammals, following oral administration, degradation and elimination occur within a few days (Hartley & Kidd 1987).

17.1.1.57 Nitrofen



Common Name: Nitrofen
Synonym: nitrophen Tok, Tokkron
Chemical Name: 2,4-dichloro-1-(4-nitrophenoxy)benzene
CAS Registry No: 1836-75-5
Uses: herbicide
Molecular Formula: $C_{12}H_7Cl_2NO_3$
Molecular Weight: 284.095
Melting Point (°C):
  70 (Lide 2003)
Boiling Point (°C):
  180–190/0.25 mmHg (Hartley & Kidd 1987)
Density (g/cm^3 at 20°C):
Molar Volume (cm^3/mol):
Dissociation Constant pK_a:
Enthalpy of Vaporization, ΔH_V (kJ/mol):
  93.66 (Rordorf 1989)
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
  22,7 (Rordorf 1989)
Entropy of Fusion, ΔS_{fus} (J/mol K):
Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F: 0.362 (mp at 70°C)

Water Solubility (g/m^3 or mg/L at 25°C or as indicated):
  1.0 (Kenaga 1980b)
  ~1.0 (Spencer 1982)
  0.7–1.2 (22°C, Worthing 1987)
  ~1 (room temp., Hartley & Kidd 1987)
  1.0 (20–25°C, selected, Augustijn-Beckers et al. 1994; Hornsby et a;. 1996)

Vapor Pressure (Pa at 25°C or as indicated and reported temperature dependence equations.):
  1.07×10^{-3} (40°C, Spencer 1982)
  1.06×10^{-3} (40°C, Worthing 1987; Hartley & Kidd 1987)
  1.30×10^{-4}, 4.50×10^{-3}, 0.091, 1.20, 12.0 (25, 50, 70, 100, 125°C, gas saturation-GC, Rordorf 1989)
  $\log (P_S/Pa) = 15.867 - 5886.5/(T/K)$; measured range 50–70.2°C (solid, gas saturation-GC, Rordorf 1989)
  $\log (P_L/Pa) = 13.022 - 4892.8/(T/K)$; measured range 72.7–140°C (liquid, gas saturation-GC, Rordorf 1989)
  1.33×10^{-5} (20–25°C, selected, Augustijn-Beckers et al. 1994; Hornsby et al. 1996)

Henry's Law Constant (Pa·m^3/mol):

Octanol/Water Partition Coefficient, $\log K_{OW}$:
  3.09 (Rao & Davidson 1980)

Octanol/Air Partition Coefficient, $\log K_{OA}$:

Bioconcentration Factor, log BCF or $\log K_B$:
  2.79 (fish, Kenaga 1980b)

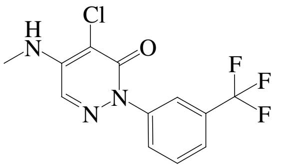
Sorption Partition Coefficient, $\log K_{OC}$:
  3.64 (soil, calculated, Kenaga 1980b)
  3.01, 3.64, 4.18, 4.05 (quoted literature values, Augustijn-Beckers et al. 1994)
  4.0 (soil, Augustijn-Beckers et al. 1994; Hornsby et al. 1996)

Environmental Fate Rate Constants, k, or Half-Lives, $t_{½}$:

Half-Lives in the Environment:

Soil: reported field $t_{½}$ = 3 to 25 d and the recommended field $t_{½}$ = 30 d (Augustijn-Beckers et al. 1994; Hornsby et al. 1996).

17.1.1.58 Norflurazon



Common Name: Norflurazon
Synonym: Zorial, Solicam, Evital, Telok
Chemical Name: 4-chloro-5-(methylamino)-2[3-(trifluoromethyl)phenyl]-3-(2*H*)-pyridazinone
CAS Registry No: 27314-13-2
Uses: herbicide
Molecular Formula: $C_{12}H_9ClF_3N_3O$
Molecular Weight: 303.666
Melting Point (°C):

184	(Lide 2003)

Boiling Point (°C):
Density (g/cm^3 at 20°C):
Molar Volume (cm^3/mol):
Dissociation Constant pK_a:
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
Entropy of Fusion, ΔS_{fus} (J/mol K):
Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F: 0.0275 (mp at 184°C)

Water Solubility (g/m^3 or mg/L at 25°C or as indicated):

28	(Kenaga & Goring 1980; Kenaga 1980b; Gerstl & Helling 1987; Isensee 1991)
28	(Ashton & Crafts 1981; Worthing & Walker 1987; Herbicide Handbook 1989; Tomlin 1994)
40	(Spencer 1982)
28	(23°C, Hartley & Kidd 1987)
28	(20–25°C, selected, Wauchope et al. 1992; Hornsby et al. 1996; quoted, Senseman et al. 1997)

Vapor Pressure (Pa at 25°C or as indicated):

2.7×10^{-6}	(20°C, Ashton & Crafts 1981; Spencer 1982)
2.8×10^{-6}	(20°C, Worthing & Walker 1987; Tomlin 1994)
2.7×10^{-6}, 3.3×10^{-5}, 3.3×10^{-4}, 1.6×10^{-3}, 1.3×10^{-2}	(20, 40, 60, 80, 100°C, Herbicide Handbook 1989)
9.24×10^{-5}	(20–25°C, Majewski & Capel 1995)

Henry's Law Constant (Pa·m^3/mol at 25°C or as indicated):

3.04×10^{-5}	(20–25°C, Majewski & Capel 1995)

Octanol/Water Partition Coefficient, log K_{OW}:

2.30	(22°C, shake flask-UV, Braumann & Grimme 1981)
2.52	(shake flask, Takahashi et al. 1993)
2.45	(pH 6.5, Tomlin 1994)
2.30	(recommended, Hansch et al. 1995)
2.30	(LOGPSTAR or CLOGP data, Sabljic et al. 1995)
2.60	(RP-HPLC-RT correlation using short ODP column, Donovan & Pescatore 2002)

Octanol/Air Partition Coefficient, log K_{OA}:

Bioconcentration Factor, log BCF or log K_B:

1.97	(fish, calculated-solubility, Kenaga 1980b; Isensee 1991)

Sorption Partition Coefficient, log K_{OC}:

3.28	(soil, Kenaga & Goring 1980)
2.85	(calculated-solubility, Kenaga 1980b)
3.28, 3.07	(soil: quoted, calculated-MCI χ, Gerstl & Helling 1987)
2.85	(soil, Wauchope et al. 1992; Hornsby et al. 1996)
3.02, 2.64, 3.02, 2.46 2.59	(sandy loam, Mississippi loam, Mississippi sediment, Keaton sandy loam, Biggs clay, Tomlin 1994)
3.75	(calculated-MCI χ, Meylan et al. 1992)
3.28	(soil, calculated-MCI χ, Sabljic et al. 1995)
2.78	(soil, Senseman et al. 1997)

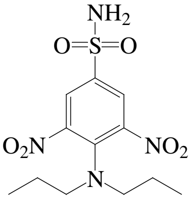
Environmental Fate Rate Constants, or Half-Lives, $t_{½}$:

Volatilization: dissipated in soil by photodegradation and volatilization, $t_{½}$ = 45–180 d (Tomlin 1994)
Photolysis: rapidly degraded by sunlight (Worthing 1987; Tomlin 1994)
 dissipated in soil by photodegradation and volatilization, $t_{½}$ = 45–180 d (Tomlin 1994)
Oxidation:
Hydrolysis:
Biodegradation:
Biotransformation:
Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants:

Half-Lives in the Environment:

Air:
Surface water: $t_{½}$ = 3.4 and 1.9 d reported in the absence and presence of 20 ppm H_2O_2 (quoted, Massad et al. 2004)
Ground water:
Sediment:
Soil: the average $t_{½}$ = 45–130 d residues in soil from the Delta and Southeast depending on clay and organic content (Herbicide Handbook 1989)
 field $t_{½}$ ~ 30 d (estimated, Wauchope et al. 1992; Hornsby et al. 1996)
 dissipated in soil by photodegradation and volatilization, $t_{½}$ = 45–180 d (Tomlin 1994)
 soil $t_{½}$ = 90 d (Senseman et al. 1997)
Biota:

17.1.1.59 Oryzalin



Common Name: Oryzalin
Synonym: Dirimal, EL 119, Rycelan, Rycelon, Ryzelan, Surflan
Chemical Name: 4-(dipropylamino)-3,5-dinitrobenzene-sulfonamide; 3,5-dinitro-*N*⁴, *N*⁴-dipropylsulfanilamide
Uses: herbicide for pre-emergence control of many annual grasses and broadleaf weeds in cotton, fruit trees, vines, nut trees, soybeans, groundnuts, oilseed rape, sunflowers, lucerne, peas, sweet potatoes, mint, ornamentals and also used in noncrop areas.
CAS Registry No: 19044-88-3
Molecular Formula: $C_{12}H_{18}N_4O_6S$
Molecular Weight: 346.359
Melting Point (°C):

141	(Lide 2003)

Boiling Point (°C): 265 (dec. Tomlin 1994)
Density (g/cm³ at 20°C):
Molar Volume (cm³/mol):

351.1	(calculated-Le Bas method at normal boiling point)

Dissociation Constant pK_a:

9.40	(Worthing & Hance 1991; Tomlin 1994)
8.60	(Wauchope et al. 1992; Hornsby et al. 1996)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
Entropy of Fusion, ΔS_{fus} (J/mol K):
Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F: 0.0728 (mp at 141°C)

Water Solubility (g/m³ or mg/L at 25°C or as indicated):

2.4	(Martin & Worthing 1977; Spencer 1982; Ashton & Crafts 1981)
2.6	(Weber et al. 1980)
2.5	(Hartley & Kidd 1987; Budavari 1989; Milne 1995)
2.4	(Worthing & Walker 1987, Worthing & Hance 1991)
2.6	(Herbicide Handbook 1989; Tomlin 1994)
2.5	(20–25°C, selected, Wauchope et al. 1992; Hornsby et al. 1996)
3.5	(calculated-group contribution fragmentation method, Kühne et al. 1995)

Vapor Pressure (Pa at 25°C or as indicated):

$< 1.33 \times 10^{-5}$	(30°C, Ashton & Crafts 1981)
$< 1.30 \times 10^{-5}$	(30°C, Hartley & Kidd 1987)
$< 1.33 \times 10^{-6}$	(Herbicide Handbook 1989; Tomlin 1994)
$< 1.33 \times 10^{-5}$	(30°C, Budavari 1989)
$< 1.30 \times 10^{-6}$	(Worthing & Hance 1991)
$< 1.30 \times 10^{-6}$	(20–25°C, selected, Wauchope et al. 1992; Hornsby et al. 1996)

Henry's Law Constant (Pa·m³/mol at 25°C):

0.000188	(calculated-P/C, this work)

Octanol/Water Partition Coefficient, log K_{OW}:

4.13	(selected, Dao et al. 1983)
3.73	(Worthing & Hance 1991)

3.72	(pH 7, Tomlin 1994)
3.73	(Milne 1995)
3.73	(selected, Hansch et al. 1995)
2.79	(MedChem master file or ClogP program, Sabljic et al. 1995)

Bioconcentration Factor, log BCF:

2.58	(calculated-S, Kenaga 1980)

Sorption Partition Coefficient, log K_{OC}:

3.43	(soil, calculated-S, Kenaga 1980)
2.78	(soil, 20–25°C, selected, Wauchope et al. 1992; Hornsby et al. 1996)
2.78	(estimated-chemical structure, Lohninger 1994)
2.85–3.04	(Tomlin 1994)
3.40	(quoted or calculated-QSAR MCI $^1\chi$, Sabljic et al. 1995)
3.40; 3.18	(soil, quoted obs.; estimated-general model using molecular descriptors, Gramatica et al. 2000)

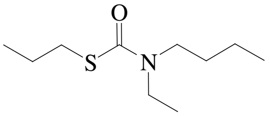
Environmental Fate Rate Constants, k, or Half-Lives, $t_{1/2}$:

Biodegradation: in soil, microbial degradation occurs rapidly, $t_{1/2}$ = 2.1 months for aerobic and $t_{1/2}$ = 10 d for anaerobic metabolism (Tomlin 1994).

Half-Lives in the Environment:

Soil: selected field $t_{1/2}$ = 20 d (Wauchope et al. 1992; Hornsby et al. 1996);
$t_{1/2}$ = 2.1 months for aerobic degradation and $t_{1/2}$ = 10 d for anaerobic degradation (Tomlin 1994).

17.1.1.60 Pebulate



Common Name: Pebulate
Synonym: PEBC, R-2061, Stauffer 2061, Tillam, Timmam-6-E
Chemical Name: *S*-propyl butylethyl(thiocarbamate); *S*-propyl butylethylcarbamothioate
Uses: selective pre-emergence herbicide to control annual grasses and broadleaf weeds in tomatoes, sugar beet, and tobacco.
CAS Registry No: 1114-71-2
Molecular Formula: $C_{10}H_{21}NOS$
Molecular Weight: 203.345
Melting Point (°C): liquid
Boiling Point (°C):

142	(at 20 mmHg, Hartley & Kidd 1987; Budavari 1989; Montgomery 1993; Milne 1995)
142	(at 21 mmHg, Herbicide Handbook 1989)

Density (g/cm^3 at 20°C):

0.956	(Hartley & Kidd 1987; Worthing & Hance 1991; Tomlin 1994; Milne 1995)
0.9555	(Herbicide Handbook 1989; Montgomery 1993)

Molar Volume (cm^3/mol):

258.7	(calculated-Le Bas method at normal boiling point)

Dissociation Constant pK_a:
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
Entropy of Fusion, ΔS_{fus} (J/mol K):
Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F: 1.0

Water Solubility (g/m^3 or mg/L at 25°C or as indicated):

92	(21°C, Woodford & Evans 1963)
92	(21°C, Spencer 1973, 1982)
60	(Herbicide Handbook 1978, 1989; quoted, Kenaga 1980; Kenaga & Goring 1980)
60	(Ashton & Crafts 1973, 1981)
60	(20°C, Khan 1980; Hartley & Kidd 1987; Tomlin 1994; Montgomery 1993; Milne 1995)
60	(20°C, Worthing & Walker 1987, Worthing & Hance 1991)
100	(20–25°C, selected, Wauchope et al. 1992; Hornsby et al. 1996)

Vapor Pressure (Pa at 25°C or as indicated):

4.67	(Ashton & Crafts 1973, 1981; Herbicide Handbook 1989)
3.60	(20°C, Hartley& Graham-Bryce 1980)
9.06	(30°C, Khan 1980)
0.216	(20°C, GC-RT correlation, Kim 1985)
9.00	(30°C, Hartley & Kidd 1987; Tomlin 1994)
3.50	(20°C, selected, Suntio et al. 1988)
4.70	(Worthing & Hance 1991; Tomlin 1994)
1.186	(20–25°C, selected, Wauchope et al. 1992; Hornsby et al. 1996)
9.064	(20°C, Montgomery 1993)

Henry's Law Constant (Pa·m^3/mol at 25°C or as indicated):

11.67	(20°C, calculated-P/C, Suntio et al. 1988)
11.65	(20°C, calculated-P/C, Montgomery 1993)

Octanol/Water Partition Coefficient, log K_{OW}:

3.78	(selected, Magee 1991)
3.84	(Worthing & Hance 1991; Montgomery 1993; Milne 1995)

3.83 (Tomlin 1994)
3.84 (selected, Hansch et al. 1995)
4.19, 3.74, 3.27 (RP-HPLC, CLOGP, calculated-S, Finizio et al. 1997)

Bioconcentration Factor, log BCF:

1.79 (calculated-S, Kenaga 1980)
1.54 (calculated-K_{OC}, Kenaga 1980)

Sorption Partition Coefficient, log K_{OC}:

2.80 (soil, Hamaker & Thompson 1972)
2.66 (soil, calculated-S as per Kenaga & Goring 1980, Kenaga 1980)
2.80 (reported as log K_{OM}, Magee 1991)
2.65 (estimated as log K_{OM}, Magee 1991)
2.63 (soil, 20–25°C, selected, Wauchope et al. 1992; Hornsby et al. 1996)
2.80 (Montgomery 1993)
2.63 (selected, Lohninger 1994)
2.80 (quoted or calculated-QSAR MCI $^1\chi$, Sabljic et al. 1995)
2.48, 2.10 (soil, estimated-class-specific model, estimated-general model using molecular descriptors, Gramatica et al. 2000)

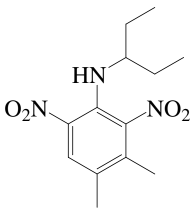
Environmental Fate Rate Constants, k, or Half-Lives, $t_{1/2}$:

Biodegradation: in soil, microbial degradation $t_{1/2}$ = 2–3 wk (Tomlin 1994).

Half-Lives in the Environment:

Air:
Surface water: $t_{1/2}$ = 11 d, at pH 4 and pH 10, $t_{1/2}$ = 12 d at pH 7 (40°C, Tomlin 1994).
Ground water:
Sediment:
Soil: $t_{1/2}$ ~ 2 wk in moist loam soil at 21–27°C (Herbicide Handbook 1989; Montgomery 1993);
selected field $t_{1/2}$ = 14 d (Wauchope et al. 1992; Hornsby et al. 1996);
$t_{1/2}$ = 2–3 wk (Tomlin 1994);.
Biota:

17.1.1.61 Pendimethalin



Common Name: Pendimethalin
Synonym: penoxalin
Chemical Name: *N*-(1-ethylpropyl-3,4-dimethyl-2,6-dinitrobenzenamine
CAS Registry No: 40487-42-1
Uses: herbicide
Molecular Formula: $C_{13}H_{19}N_3O_4$
Molecular Weight: 281.308
Melting Point (°C):

56	(Lide 2003)

Boiling Point (°C):

330	(Ashton & Crafts 1981; Herbicide Handbook 1989)
decomposes on heating (Hartley & Kidd 1987; Tomlin 1994)	

Density (g/cm^3 at 25°C):

1.19	(Ashton & Crafts 1981; Montgomery 19993; Tomlin 1994)
1.12	(Hartley & Kidd 1987)
1.17	(Herbicide Handbook 1989)

Molar Volume (cm^3/mol):
Dissociation Constant pK$_a$:
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
Entropy of Fusion, ΔS_{fus} (J/mol K):
Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F: 0.496 (mp at 56°C)

Water Solubility (g/m^3 or mg/L at 25°C or as indicated):

0.50	(23°C, Ashton & Crafts 1981)
0.30	(20°C, Hartley & Kidd 1987; Worthing & Walker 1987; Montgomery 1993; Tomlin 1994)
0.275	(Herbicide Handbook 1989)
0.275	(20–25°C, selected, Wauchope et al. 1992; Hornsby et al. 1996)
0.61	(20–25°C, Majewski & Capel 1995)

Vapor Pressure (Pa at 25°C or as indicated):

0.004	(Ashton & Crafts 1981; Herbicide Handbook 1989)
0.004	(Hartley & Kidd 1987; Worthing & Walker 1987; Tomlin 1994)
1.25×10^{-3}	(20–25°C, selected, Wauchope et al. 1992; Hornsby et al. 1996)
0.004	(Montgomery 1993)
8.16×10^{-3}	(20–25°C, Majewski & Capel 1995)
0.00123; 0.00776 (liquid P_L, GC-RT correlation; quoted lit., Donovan 1996)	

Henry's Law Constant (Pa·m^3/mol at 25°C or as indicated):

0.0867	(Montgomery 1993)
3.75	(20–25, calculated-P/C, Majewski & Capel 1995)

Octanol/Water Partition Coefficient, log K_{OW}:

5.18	(Montgomery 1993)
5.18	(Tomlin 1994)
5.24	(RP-HPLC-RT correlation using short ODP column, Donovan & Pescatore 2002)

Octanol/Air Partition Coefficient, log K_{OA}:

Bioconcentration Factor, log BCF or log K_B:

Sorption Partition Coefficient, log K_{OC}:

2.95 (soil, Wauchope et al. 1992; Hornsby et al. 1996)
4.20 (soil, Bottoni & Funari 1992)
4.14, 4.47 (loam, pH 7, pH 6.5, quoted, Montgomery 1993)
3.81 (sand, pH 7.6, Montgomery 1993)
4.07, 4.14 (sandy loam pH 6.4, silty loam, pH 7.0, Montgomery 1993)
1.48–2.93 (soil, Montgomery 1993)
3.70 (soil, Senseman et al. 1997)
3.14 (soil, estimated-general model using molecular descriptors, Gramatica et al. 2000)

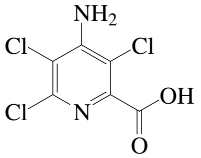
Environmental Fate Rate Constants, k, or Half-Lives, $t_{1/2}$:

Volatilization:
Photolysis: slowly decomposed by light (Hartley & Kidd 1987; Tomlin 1994).
Oxidation:
Hydrolysis: $t_{1/2}$ < 21 d (Montgomery 1993).
Biodegradation: observed $t_{1/2}$ = 33 d, 45 d, 52 d and 67 d in flooded and nonflooded conditions in nonsterile and sterile soils, respectively, in the study of degradation of pendimethalin under the influence of soil moisture and microbial activity in a sandy loam soil, in both nonsterile nonflooded and flooded soil, degradation followed first-order kinetics. (Kulshrestha & Singh 1992; quoted, Montgomery 1993).
Biotransformation: Degradation by abiotic reductive transformations:
$k = 1.25\ M^{-1}\ s^{-1}$ in H_2S with (mecapto)juglone (hydroquinone moiety, an abiotic reductant found in natural systems) solution at pH 6.65 (Wang & Arnold 2003)
Aqueous solutions with surface-bound Fe(II) species and their first-order rate constants as:
$k = 0.50 \times 10^{-3}\ h^{-1}$ at pH 6.5, $k = 0.27 \times 10^{-2}\ h^{-1}$ at pH 7.0, $k = 0.093\ h^{-1}$ at pH 7.4, and $k = 0.81\ h^{-1}$ at pH 7.8 for aqueous ferrous ion system;
$k = 0.216\ h^{-1}$ at pH 6.5, $k = 0.274\ h^{-1}$ at pH 6.7, $k = 0.918\ h^{-1}$ at pH 7.0, and $k = 2.10\ h^{-1}$ at pH 7.3 for Fe(II)/goethite system;
$k = 3.81 \times 10^{-3}\ h^{-1}$ at pH 6.5, $k = 2.66 \times 10^{-3}\ h^{-1}$ at pH 7.0, $k = 1.13 \times 10^{-2}\ h^{-1}$ at pH 7.4 and $k = 1.74 \times 10^{-2}\ h^{-1}$ at pH 7.8 for Fe(II)/clay system, all with total dissolved Fe(II) = 1 mM (Wang & Arnold 2003)
Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants:

Half-Lives in the Environment:

Air:
Surface water: $t_{1/2}$ < 21 d in water (Tomlin 1994).
Ground water: reported $t_{1/2}$ = 30–90 d (Bottoni & Funari 1992)
Sediment:
Soil: $t_{1/2}$ = 98 and 409 d at 30 and 10°C in a sandy loam soil with 75% moisture (Walker & Bond 1977)
$t_{1/2}$ = 4 d on Bosket silt loam, $t_{1/2}$ = 6 d on Sharkey clay for the first 3 to 5 days when sprayed onto soil surface, rate of loss much slower for the remainder of the 7- or 12-d sampling period with $t_{1/2}$ = 18 d on Bosket silt loam, $t_{1/2}$ = 27 d on Sharkey clay (Savage & Jordon 1980)
$t_{1/2}$ = 58–63 d in IARI sandy loam soil under Indian tropical climate (Kulshrestha & Yaduraju 1987)
$t_{1/2}$ = 30–90 d or persistence (Bottoni & Funari 1992)
$t_{1/2}$ = 66.9 d in sterile, $t_{1/2}$ = 52.2 d in nonsterile non-flooded sandy loam soil; $t_{1/2}$ = 44.9 d in sterile and 33.4 d in nonsterile flooded sandy loam soil in the study of degradation under the influence of soil moisture and microbial activity (Kulshrestha & Singh 1992; quoted, Montgomery 1993)
reported field $t_{1/2}$ = 8–480 d, recommended $t_{1/2}$ = 90 d (Wauchope et al 1992; Hornsby et al. 1996);
soil $t_{1/2}$ = 90 d (Senseman et al. 1997).
Biota: $t_{1/2}$ = 3–4 months (quoted, Hartley & Kidd 1987; Tomlin 1994)

17.1.1.62 Picloram



Common Name: Picloram
Synonym: Amdon, ATCP, Borolin, Grazon, K-Pin, Tordon
Chemical Name: 4-amino-3,5,6-trichloropicolinic acid; 4-amino-3,5,6-trichloro-2-pyridinecarboxylic acid
Uses: systemic herbicide to control most broadleaf weeds on grassland and noncropland.
CAS Registry No: 1918-02-1
Molecular Formula: $C_6H_3Cl_3N_2O_2$
Molecular Weight: 241.459
Melting Point (°C):

218.5	(Lide 2003)

Boiling Point (°C):
Density (g/cm^3 at 20°C):
Molar Volume (cm^3/mol):

204.2	(calculated-Le Bas method at normal boiling point, Suntio et al. 1988)

Dissociation Constant pK_a:

3.43, 3.42, 3.39, 3.36	(10, 20, 30. 40°C, Cheung & Biggar 1974)
1.90	(Weber et al. 1980; Willis & McDowell 1982)
3.60	(Windholz 1983; quoted, Howard 1991; Yao & Haag 1991; Haag & Yao 1992; Montgomery 1993)
2.3	(22°C, Worthing & Hance 1991; Montgomery 1993; Tomlin 1994)
1.94	(Hornsby et al. 1996)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
Entropy of Fusion, ΔS_{fus} (J/mol K):
Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F: 0.0126 (mp at 218.5°C)

Water Solubility (g/m^3 or mg/L at 25°C or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):

430	(Bailey & White 1965; Freed 1966; Khan 1980; Weber et al. 1980; Ashton & Crafts 1981; Spencer 1982)
546*	(20°C, shake flask-IR, measured range 10–40°C, pH 2.8, distilled water, Cheung & Biggar 1974)
73.65*	(20°C, shake flask-IR, measured range 10–40°C at pH 0.2, Cheung & Biggar 1974)
62.7*	(20°C, shake flask-IR, measured range 10v40°C at pH 1.1, Cheung & Biggar 1974)
137*	(20°C, shake flask-IR, measured range 10–40°C at pH 2.0, Cheung & Biggar 1974)
19560*	(20°C, shake flask-IR, measured range 10–40°C at pH 4.2, Cheung & Biggar 1974)
74593*	(20°C, shake flask-IR, measured range 10–40°C at pH 4.7, Cheung & Biggar 1974)
430	(Martin & Worthing 1977, Worthing & Hance 1991; quoted, Kenaga 1980; Kenaga & Goring 1980; Isensee 1991; Howard 1991)
430	(Hartley & Graham-Bryce 1980; Taylor & Glotfelty 1988)
430	(Hartley & Kidd 1987; Herbicide Handbook 1989; Tomlin 1994; Milne 1995)
400–430	(Montgomery 1993)

Vapor Pressure (Pa at 25°C or as indicated):

7.30×10^{-7}	(20°C, Hartley & Graham-Bryce 1980)
8.20×10^{-5}	(35°C, Khan 1980; Ashton & Crafts 1981; Hartley & Kidd 1987; Herbicide Handbook 1989)
8.26×10^{-5}	(20–25°C, Weber et al. 1980; Willis & McDowell 1982)
9.70×10^{-9}	(Dobbs & Cull 1982; quoted, Howard 1991)
7.30×10^{-6}	(20°C, quoted from Hartlet & Graham-Bryce 1980, Dobbs et al. 1984)
6.00×10^{-5}	(20°C, selected, Suntio et al. 1988)
1.40×10^{-4}	(45°C, Herbicide Handbook 1989)

4.50×10^{-8} (quoted, Nash 1989)
7.40×10^{-7} (20°C, selected, Taylor & Spencer 1990)
8.20×10^{-5} (35°C, Worthing & Hance 1991; Montgomery 1993; Tomlin 1994)

Henry's Law Constant (Pa m^3/mol at 25°C or as indicated):
3.40×10^{-5} (20°C, calculated-P/C, Suntio et al. 1988; quoted, Mabury & Crosby 1996)
4.20×10^{-7} (calculated-P/C, Taylor & Glotfelty 1988)
2.50×10^{-5} (calculated-P/C, Nash 1989)
4.10×10^{-6} (calculated-P/C, Howard 1991)
3.40×10^{-5} (20–35°C, calculated-P/C, Montgomery 1993)
3.17×10^{-5} (calculated-P/C, this work)

Octanol/Water Partition Coefficient, log K_{OW}:
0.30 (Kenaga 1975)
0.63 (selected, Dao et al. 1983)
0.30 (Hansch & Leo 1985; Hansch et al. 1995;)
–3.47 (selected, Gerstl & Helling 1987)
1.166 (calculated as per Broto et al. 1984, Karcher & Devillers 1990)
0.26, 0.30 (quoted, Sangster 1993)
1.87 (LOGPSTAR or CLOGP data, Sabljic et al. 1995)

Bioconcentration Factor, log BCF:
–1.70 (fish in static water, quoted from Dow Chemical data, Kenaga & Goring 1980)
1.30 (calculated-S, Kenaga 1980; quoted, Isensee 1991)
–0.222 (calculated-K_{OC}, Kenaga 1980)
0.0 (estimated-K_{OW}, Lyman et al. 1982; quoted, Howard 1991)
1.49 (fish in flowing water, Garten & Trabalka 1983; quoted, Howard 1991)

Sorption Partition Coefficient, log K_{OC}:
1.23 (soil, Hamaker & Thompson 1972)
1.10 (average in soil, Hamaker & Thompson 1972)
1.10 (average in soil, Reinhold et al. 1979)
1.23 (Kenaga & Goring 1980; quoted, Bahnick & Doucette 1988)
2.20 (soil, calculated-S as per Kenaga & Goring 1980, Kenaga 1980)
1.41 (av. of 26 soils, Rao & Davidson 1980)
1.40 (soil, Rao & Davidson 1982)
1.31, 1.05, 1.34, 1.0, 1.26. 1.10, 1.05 (Catlin soil, Commerce soil, Fargo soil, Holdredge soil, Norfolk soil, Kawkawlin soil, Walla-Walla soil, McCall & Agin 1985; quoted, Brusseau & Rao 1989)
2.11 (calculated-MCI χ, Gerstl & Helling 1987)
1.68 (screening model calculations, Jury et al. 1987b)
1.47 (calculated-MCI χ, Bahnick & Doucette 1988)
1.88 (Nash 1989)
1.23 (reported as log K_{OM}, Magee 1991)
1.20 (organic carbon, Wauchope et al. 1991)
1.11, 1.41, 1.68 (soil, quoted values, Bottoni & Funari 1992)
1.41 (Montgomery 1993)
1.30 (soil, calculated-QSAR MCI $^1\chi$, Sabljic et al. 1995)
1.55, 1.39, 2.38 (soils: organic carbon OC ≥ 0.1%, OC ≥ 0.5%, 0.1 ≤ OC < 0.5%, and pH 2.0–10.5, average, Delle Site 2001)
3.07, 2.96, 3.30 (soils: organic carbon OC ≥ 0.1%, OC ≥ 0.5%, 0.1 ≤ OC < 0.5%, and pH ≤ 2.0 undissociated, average, Delle Site 2001)
1.80, 1.76 (soils: organic carbon OC ≥ 0.1%, OC ≥ 0.5%, pH 4.2–5.9, average, Delle Site 2001)
1.12, 2.02, 1.93 (soils: organic carbon OC ≥ 0.1%, OC ≥ 0.5%, 0.1 ≤ OC < 0.5%, pH ≥ 6.0, dissociated, average, Delle Site 2001)

Environmental Fate Rate Constants, k, or Half-Lives, $t_{½}$:

Volatilization:

Photolysis: $t_{½}$ = 200 h for 40% of 4,840 μg/mL to degrade in dilute NaOH solution under sunlight (Hall et 1968; quoted, Cessna & Muir 1991);

$t_{½}$ = 2.3 d to 9.58 d direct photolysis by sunlight under various conditions, at depths of 2.54 cm-3.65 m at various times of the year; one result at 3.65 m during Sept.-Oct. gave $t_{½}$ = 41.3 d; distilled water and canal water gave essentially the same results in one set of experiments (Hedlund & Youngson 1972; quoted, Cessna & Muir 1991; Howard 1991);

$t_{½}$ = 72 h for 99% of 548 μg mL^{-1} to degrade in Na salt solution under 300–380 nm light (Mosier & Guenzi 1973; quoted, Cessna & Muir 1991);

$t_{½}$ = 0.5 h for 38% of 265 μg mL^{-1} to degrade in distilled water under 254 nm light (Glass 1975; quoted, Cessna & Muir 1991);

$t_{½}$ = 2.2 d for < 2.4 μg mL^{-1} L to degrade in distilled water under sunlight (Skurlatov et al. 1983; quoted, Cessna & Muir 1991);

$t_{½}$ = 16 h in surface water estimated from direct midday sunlight photolysis in mid-summer at 40°N (Zepp 1991).

Oxidation:

photooxidation: $t_{½}$ = 12.21 d in air, based on estimated rate constant for the reaction with photochemically produced hydroxyl radical in the atmosphere (GEMS 1986; quoted, Howard 1991)

k = 5.9×10^9 M^{-1} s^{-1} for the reaction (Fenton with reference to acetophenone) with hydroxyl radical in aqueous solutions at pH 2.1–3.7 and at 24 ± 1°C (Buxton et al. 1988; quoted, Haag & Yao 1992)

k(aq.) = (50–150) M^{-1} s^{-1} for direct reaction with ozone in water at pH 1.5–4.9 and 21 ± 1°C, with $t_{½}$ = 4.0 min at pH 7 (Yao & Haag 1991).

k(aq.) = $(3.4 \pm 0.3) \times 10^9$ M^{-1} s^{-1} for the reaction (Fenton with reference to acetophenone) with hydroxyl radicals in aqueous solutions at pH 2.1–3.7 and at 24 ± 1°C (Haag & Yao 1992)

k(aq.) = 1.3×10^9 M^{-1} s^{-1} for reaction with hydroxyl radical, in irradiated field water both in the laboratory and sunlit rice paddies (Mabury & Crosby 1996).

Hydrolysis:

Biodegradation: $t_{½}$ = 128–144 h in mixture of 5 g soil and 1–4 mL water, $t_{½}$ = 90–1000 h in mixture of 1 mL water with 0.25–10 g soil, (Hance 1969; quoted, Howard 1991);

$t_{½}$ > 15 months for 0.07, 0.72 and 10 μg mL^{-1} to biodegrade in groundwater (Weidner 1974; quoted, Muir 1991);

k = 0.0073 d^{-1} by soil incubation die-away test studies (Rao & Davidson 1980; quoted, Scow 1982);

biochemical $t_{½}$ = 100 d from screening model calculations (Jury et al. 1987b);

$t_{½}$ = 30–300 d, degraded slowly by soil microorganisms (Tomlin 1994).

Biotransformation:

Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants:

Half-Lives in the Environment:

Air: $t_{½}$ = 12.21 d, based on estimated rate constant for the vapor-phase reaction with photochemically produced hydroxyl radicals in the atmosphere (GEMS 1986; quoted, Howard 1991).

Surface water: $t_{½}$ = 2.6 d decomposed by UV irradiation (Tomlin 1994);

measured rate constant k = (50 - 150) M^{-1} s^{-1} for direct reaction with ozone in water at pH 1.5–4.9 and 21°C, with $t_{½}$ = 4.0 min at pH 7 (Yao & Haag 1991).

Ground water: $t_{½}$ > 15 months for 0.07, 0.72 and 10 μg/mL to biodegrade in ground water (Weidner 1974; quoted, Muir 1991);

measured rate constant k ≤ 0.005 M^{-1} s^{-1} for direct reaction with ozone in water at pH 2 and 21°C, with $t_{½}$ ≥ 80 d at pH 7 (Yao & Haag 1991)

reported $t_{½}$ = 30–330, 138, 180 and 206 d (Bottoni & Funari 1992).

Sediment:

Soil: estimated persistence of 18 months (Kearney et al. 1969; Edwards 1973; quoted, Morrill et al. 1982; Jury et al. 1987b);

persistent in soils with $t_{½}$ > 5 yr (Alexander 1973; quoted, Howard 1991);

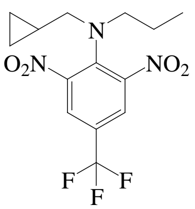
estimated first-order $t_{½}$ = 95 d in soil from biodegradation rate constant k = 0.0073 d^{-1} by soil incubation die-away test studies (Rao & Davidson 1980; quoted, Scow 1982);

persistent in soil with $t_{½} > 100$ d (Willis & McDowell 1982);
$t_{½} = 100$ d from screening model calculations (Jury et al. 1987b);
selected $t_{½} = 90$ d (Wauchope et al. 1991; quoted, Dowd et al. 1993);
reported $t_{½} = 30–330$ d, 18 d, 180 d and 206 d (Bottoni & Funari 1992);
$t_{½} = 3–330$ d (Tomlin 1994).
Biota: biochemical $t_{½} = 100$ d from screening model calculations (Jury et al. 1987b);
average $t_{½} = 60$ d in the forest (USDA 1989; quoted, Neary et al. 1993).

TABLE 17.1.1.62.1
Reported aqueous solubilities of picloram at various temperatures

	Cheung & Biggar 1974					
	shake flask-IR spec.					
t/°C	$S/g·m^{-3}$	$S/g·m^{-3}$	$S/g·m^{-3}$	$S/g·m^{-3}$	$S/g·m^{-3}$	$S/g·m^{-3}$
	pH 0.20	pH 1.10	pH 2.0	pH 2.8	pH 4.2	pH 4.7
10	43.95	39.12	89.11	475	22240	84446
20	73.65	62.78	136.92	545.74	19560	74953
30	119.5	108.9	205.3	683.4	21395	82248
40	214.9	199	316.3	704.5	21371	78240
$\Delta H_{sol}/(kJ\ mol^{-1})$	38.49	38.91	31.38	12.97	0	0

17.1.1.63 Profluralin



Common Name: Profluralin
Synonym: CGA 10832, Pregard, Tolban
Chemical Name: *N*-(cyclopropylmethyl)-2,6-dinitro-*N*-propyl-4-trifluoromethylaniline; N-(cyclopropylmethyl)-2,6-dinitro-*N*-propyl-4-(trifluoromethyl) benzenamine
Uses: herbicide for pre-planting by soil incorporation to control annual and perennial broadleaf and grass weeds in cotton, soybeans, brassicas, capsicums, tomatoes and other crops.
CAS Registry No: 26399-36-0
Molecular Formula: $C_{14}H_{16}F_3N_3O_4$
Molecular Weight: 347.290
Melting Point (°C):

34	(Lide 2003)

Boiling Point (°C):
Density (g/cm^3 at 20°C):

1.45	(25°C, Ashton & Crafts 1981)
1.38	(Hartley & Kidd 1987; Worthing & Hance 1991)

Molar Volume (cm^3/mol):

304.7	(calculated-Le Bas method at normal boiling point)

Dissociation Constant pK_a:
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
Entropy of Fusion, ΔS_{fus} (J/mol K):
Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F: 0.816 (mp at 34°C)

Water Solubility (g/m^3 or mg/L at 25°C or as indicated):

0.10	(20°C, Weber 1972)
0.10	(Spencer 1973, 1982; Wauchope 1978; Kenaga 1980)
0.10	(27°C, Ashton & Crafts 1973, 1981)
0.10	(shake flask-HPLC, Ellgehausen et al. 1981)
0.10	(20°C, Hartley & Kidd 1987; Milne 1995)
0.10	(20°C, Worthing & Walker 1987, Worthing & Hance 1991)
0.10	(20–25°C, selected, Augustijn-Beckers et al. 1994; Hornsby et al. 1996)

Vapor Pressure (Pa at 25°C or as indicated):

0.0092	(20°C, Weber 1972; Worthing & Walker 1987)
0.0092	(20°C, Ashton & Crafts 1973, 1981)
0.0084	(20°C, Hartley & Kidd 1987)
0.0084	(20°C, Worthing & Hance 1991)
0.0084	(20–25°C, selected, Augustijn-Beckers et al. 1994; Hornsby et al. 1996)

Henry's Law Constant (Pa·m^3/mol at 25°C or as indicated):

39.07	(20°C, calculated-P/C, Suntio et al. 1988)
31.91	(20°C, calculated-P/C, Muir 1991)

Octanol/Water Partition Coefficient, log K_{OW}:

5.16	(selected, Dao et al. 1983)
6.34	(shake flask-HPLC/UV, Ellgehausen et al. 1981)
6.34	(recommended, Sangster 1993)

4.46	(calculated-fragment const., Pinsuwan et al. 1995)
6.34	(recommended, Hansch et al. 1995)
5.08	(LOGPSTAR or CLOGP data, Sabljic et al. 1995)

Bioconcentration Factor, log BCF:

3.35	(calculated-S, Kenaga 1980; quoted, Isensee 1991)
2.83	(calculated-K_{OC}, Kenaga 1980)

Sorption Partition Coefficient, log K_{OC}:

3.93	(soil, exptl., Kenaga 1980)
4.19	(soil, calculated-S as per Kenaga & Goring 1980, Kenaga 1980)
3.83	(estimated as log K_{OM}, Magee 1991)
3.93	(soil, quoted exptl., Meylan et al. 1992)
4.26	(soil, calculated-MCI χ and fragment contribution, Meylan et al. 1992)
4.00	(20–25°C, estimated, Augustijn-Beckers et al. 1994; Hornsby et al. 1996)
4.16	(selected, Lohninger 1994)
4.01	(soil, calculated-QSAR MCI $^1\chi$, Sabljic et al. 1995)
3.87	(soil, estimated-general model using molecular descriptors, Gramatica et al. 2000)

Environmental Fate Rate Constants, k, or Half-Lives, $t_{1/2}$:

Volatilization: estimated $t_{1/2} \sim 1.2$ d from 1 m depth of water at 20°C (Muir 1991).

Photolysis:

Oxidation:

Hydrolysis:

Biodegradation: $t_{1/2} = 12$ d for 0.5 µg mL^{-1} to biodegrade in flooded soils at 20–42°C (Savage 1978; quoted, Muir 1991);

Degradation $t_{1/2} < 1$ month in three soils, Goldsborol loamy sand, Cecil loamy sand Drummer clay loam treated with 1 ppm profluralin) for 4 month under aerobic conditions, no degradation in sterile controls. (shake flask-TLC, Camper et al. 1980)

$t_{1/2} < 1$ month for 1 µg/mL to biodegrade in flooded soils at 25°C (derived from results of Camper et al. 1980, Muir 1991);

biodegradation $t_{1/2} < 20$ d in water and sediment with flooded soils and terrestrial-aquatic model ecosystems (Miur 1991).

Biotransformation:

Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants:

Half-Lives in the Environment:

Air:

Surface water: biodegradation $t_{1/2} < 20$ d in water and sediment with flooded soils and terrestrial-aquatic model ecosystems (Muir 1991).

Ground water:

Sediment: biodegradation $t_{1/2} < 20$ d in water and sediment with flooded soils and terrestrial-aquatic model ecosystems (Muir 1991).

Soil: $t_{1/2} = 12$ d for 0.5 µg mL^{-1} to biodegrade in flooded soils at 20–42°C (Savage 1978, Muir 1991)

persistence of 12 months in soil (Wauchope 1978);

aerobic and anaerobic degradation $t_{1/2} < 1$ month in 3 flooded soils at 25°C (Camper et al. 1980);

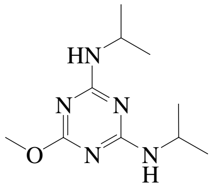
field studies, $t_{1/2} = 10.9$ wk - 1978 first study; $t_{1/2} = 10.1$ wk -1978 second study; $t_{1/2} = 11.5$ wk -1979, in a Crowley silt loam at Stuttgart, Arkansas (Brewer et al. 1982)

laboratory studies: $t_{1/2} = 19.9$ wk at 4°C, $t_{1/2} = 6.7$ wk at 25°C for soil of field capacity moisture (27% w/w for Crowley silt loam), $t_{1/2} = 20.4$ wk at 4°C, $t_{1/2} = 4.8$ wk at 25°C for flooded soils, Crowley silt loam; and $t_{1/2} = 25.8$ wk at 4°C, $t_{1/2} = 8.6$ wk at 25°C for soil of field capacity moisture (34% w/w for Sharkey silty clay), $t_{1/2} = 21.3$ wk at 4°C and $t_{1/2} = 6.2$ wk at 25°C for flooded soils, Sharkey silty clay (Brewer et al. 1982);

selected field $t_{1/2} = 110$ d (Augustijn-Beckers et al. 1994; Hornsby et al. 1996).

Biota:

17.1.1.64 Prometon



Common Name: Prometon

Synonym: G 31435, Gesafram, Gesagram, Methoxypropazine, Ontracic 800, Ontrack, Pramitol, Prometone

Chemical Name: 6-methoxy-*N,N′*-bis(methylethyl)-1,3,5-triazine-2,4-diamine; 2,4-bis(isopropylamino)-6-methoxy-1,3,5-triazine

Uses: nonselective pre-emergence and post-emergence herbicide to control most annual and broadleaf weeds, grasses, and brush weeds on noncropland.

CAS Registry No: 1610-18-0

Molecular Formula: $C_{10}H_{19}N_5O$

Molecular Weight: 225.291

Melting Point (°C):
91.5 (Lide 2003)

Boiling Point (°C):

Density (g/cm^3 at 20°C):
1.088 (Hartley & Kidd 1987; Worthing & Hance 1991; Montgomery 1993)

Molar Volume (cm^3/mol):
280.2 (calculated-Le Bas method at normal boiling point)

Dissociation Constant:
4.28 (pK_a, Weber 1970; quoted, Bintein & Devillers 1994)
4.30 (pK_a, 21°C, Worthing & Hance 1991; Montgomery 1993)
9.73 (pK_b, Wauchope et al. 1992; Hornsby et al. 1996)
9.7 (21°C, pK_b, Tomlin 1994)

Enthalpy of Vaporization, ΔH_V (kJ/mol):
90.77 (Rordorf 1989)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
22.175 (DSC method, Plato & Glasgow 1969)
21.6 (Rordorf 1989)

Entropy of Fusion, ΔS_{fus} (J/mol K):

Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F: 0.223 (mp at 91.5°C)

Water Solubility (g/m^3 or mg/L at 25°C or as indicated):
750 (20°C, Bailey & White 1965; Ashton & Crafts 1981; Herbicide Handbook 1989)
1000, 678, 669 (26°C, pH 3.0, 7.0, 10.0, shake flask-UV, Ward & Weber 1968)
750 (Martin & Worthing 1977; Herbicide Handbook 1978)
677 (Weber et al. 1980)
620 (20°C, Spencer 1982)
750 (20°C, Verschueren 1983)
750 (20°C, Hartley & Kidd 1987; Montgomery 1993)
620 (20°C, Worthing & Walker 1987, 1991; Tomlin 1994)
720 (20–25°C, selected, Wauchope et al. 1992; Hornsby et al. 1996)

Vapor Pressure (Pa at 25°C or as indicated and reported temperature dependence equations.):
3.07×10^{-4} (20°C, extrapolated-Antoine eq. from gas saturation-GC measurements, measured range 50–130°C, Friedrich & Stammbach 1964) (See figure at the end of this section.)
$\log (P/mmHg) = 11.911 - 4933/(T/K)$, temp range 50–130°C (gas saturation-GC, data presented in Antoine eq., Friedrich & Stammbach 1964)

0.00030 (20°C, Khan 1980)
0.00031 (20°C, Ashton & Crafts 1981; Worthing & Hance 1991)
0.00083 (Jury et al. 1984; selected, Spencer et al. 1988; Spencer & Cliath 1990; Taylor & Spencer 1990)
0.00031 (20°C, Hartley & Kidd 1987)
0.00031, 0.00105 (20°C, 30°C, Herbicide Handbook 1989)
1.0×10^{-3}, 3.30×10^{-2}, 0.65, 8.60, 82 (25, 50, 70, 100, 125°C, gas saturation-GC, Rordorf 1989)
$\log (P_S/Pa) = 16.525 - 5817.4/(T/K)$; measured range 32.1–89.3°C (gas saturation-GC, Rordorf 1989)
$\log (P_L/Pa) = 13.617 - 4741.7/(T/K)$; measured range 92.3–140°C (gas saturation-GC, Rordorf 1989)
0.00103 (20–25°C, selected, Wauchope et al. 1992; Hornsby et al. 1996)
0.00031 (20°C, Montgomery 1993)
0.000306 (20°C, Tomlin 1994)

Henry's Law Constant (Pa·m³/mol at 25°C or as indicated):
2.50×10^{-4} (calculated-P/C, Jury et al. 1984; Spencer et al. 1988; Spencer & Cliath 1990)
9.02×10^{-5} (20°C, calculated-P/C, Montgomery 1993)
9.01×10^{-5} (calculated-P/C, this work)

Octanol/Water Partition Coefficient, log K_{OW}:
1.94 (selected, Dao et al. 1983)
1.94 (Gerstl & Helling 1987)
2.99 (RP-HPLC-RT correlation, Finizio et al. 1991; quoted, Sangster 1993)
2.85 (selected, Magee 1991)
2.55 (shake flask-UV, Liu & Qian 1995)
2.69, 2.99 (Montgomery 1993)
2.99 (recommended, Hansch et al. 1995)
2.82 (RP-HPLC-RT correlation, Finizio et al. 1997)

Bioconcentration Factor, log BCF:
1.18 (calculated-S, Kenaga 1980; quoted, Isensee 1991)
1.28 (calculated-K_{OC}, Kenaga 1980)

Sorption Partition Coefficient, log K_{OC}:
2.54 (soil, Hamaker & Thompson 1972; Kenaga 1980; Kenaga & Goring 1980)
2.04 (soil, calculated-S as per Kenaga & Goring 1980, Kenaga 1980)
2.61 (Jury et al. 1984; quoted, Spencer & Cliath 1990)
2.40 (calculated-MCI χ, Gerstl & Helling)
2.48 (Spencer et al. 1988)
2.35 (estimated as log K_{OM}, Magee 1991)
2.20 (soil, calculated-MCI χ and fragment contribution, Meylan et al. 1992)
2.18 (soil, 20–25°C, selected, Wauchope et al. 1992; Hornsby et al. 1996)
1.92–2.24 (Montgomery 1993)
2.77 (selected, Lohninger 1994)
2.39 (calculated-K_{OW}, Liu & Qian 1995)
2.50 (soil, calculated-MCI $^1\chi$, Sabljic et al. 1995)
2.60; 2.70, 2.68 (soil, quoted obs.; estimated-class-specific model, estimated-general model using molecular descriptors, Gramatica et al. 2000)
2.47, 2.50 (soils: organic carbon OC ≥ 0.1%, OC ≥ 0.5%, pH 4.3–7.1, average, Delle Site 2001)
2.81, 2.65, 2.53 (soils with organic carbon OC ≥ 0.5% at: pH 4.3–4.9, pH 5.0–5.9, pH- 6.0, average, Delle Site 2001)

Environmental Fate Rate Constants, or Half-Lives, $t_{1/2}$:
Volatilization: estimated $t_{1/2}$ ~ 100 d (Spencer & Cliath 1990).
Photolysis: $t_{1/2}$ = 2.25 h for 1% of 100 μg mL⁻¹ to degrade in distilled water under 300 nm light (Tanaka et al. 1981; quoted, Cessna & Muir 1991).
Oxidation:

Hydrolysis:
Biodegradation:
Biotransformation:
Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants:

Half-Lives in the Environment:
Soil: selected field $t_{½}$ = 500 d (Wauchope et al. 1992; Hornsby et al. 1996).

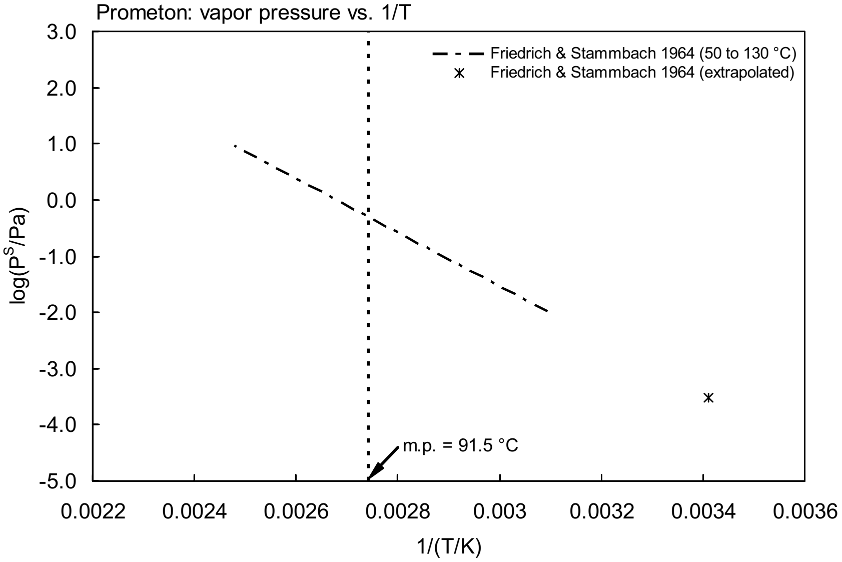
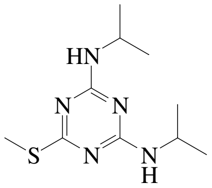


FIGURE 17.1.1.64.1 Logarithm of vapor pressure versus reciprocal temperature for prometon.

17.1.1.65 Prometryn



Common Name: Prometryn

Synonym: Caparol, Cotton-Pro, Gesagard, G-34161, Mercasin, Mercazin, Polisin, Primatol, Prometrex, Prometrin, Selectin, Sesagard, Uvon

Chemical Name: *N,N′*-bis(1-methylethyl)-6-(methylthio)-1,3,5-triazine-2,4-diamine; 2,4-bis(isopropylamino)-6-(methylthio)-1,3,5-triazine

Uses: selective herbicide to control many annual grass and broadleaf weeds in celery, cotton and peas.

CAS Registry No: 7287-19-6

Molecular Formula: $C_{10}H_{19}N_5S$

Molecular Weight: 241.357

Melting Point (°C):
119 (Lide 2003)

Boiling Point (°C):

Density (g/cm^3 at 20°C):
1.157 (Hartley & Kidd 1987; Worthing & Hance 1991; Montgomery 1993; Milne 1995)

Molar Volume (cm^3/mol):
299.7 (calculated-Le Bas method at normal boiling point)

Dissociation Constant:
4.05 (pK_a, Weber 1970; Pacakova et al. 1988; Somasundaram et al. 1991; Bintein & Devillers 1994)
4.10 (pK_a, 21°C, Weber et al. 1980; Willis & McDowell 1982; Worthing & Hance 1991)
9.95 (pK_b, Wauchope et al. 1992; Hornsby et al. 1996)
4.05 (pK_a, 21°C, Montgomery 1993)

Enthalpy of Vaporization, ΔH_V (kJ/mol):
96.43 (Rordorf 1989)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
26.36 (DSC method, Plato & Glasgow 1969)
25.4 (Rordorf 1989)

Entropy of Fusion, ΔS_{fus} (J/mol K):

Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F: 0.120 (mp at 119°C)

Water Solubility (g/m^3 or mg/L at 25°C or as indicated):
48 (20°C, Woodford & Evans 1963)
48 (20°C, Bailey & White 1965; Ashton & Crafts 1973, 1981; Khan 1980)
206, 40.3, 41.8 (26°C, shake flask-UV at pH 3.0, 7.0, 10.0, Ward & Weber 1968)
48 (Martin & Worthing 1977; Herbicide Handbook 1978)
40 (Weber et al. 1980)
48 (20°C, Hartley & Kidd 1987; Herbicide Handbook 1989; Montgomery 1993; Milne 1995)
33 (20°C, Worthing & Walker 1987, Worthing & Hance 1991)
33 (20–25°C, selected, Wauchope et al. 1992; Hornsby et al. 1996)
33 (Tomlin 1994; selected, Lohninger 1994)
241 (calculated-group contribution method, Kühne et al. 1995)

Vapor Pressure (Pa at 25°C or as indicated and reported temperature dependence equations.):
1.33×10^{-4} (20°C, extrapolated-Antoine eq. from gas saturation-GC measurements, measured range 50–130°C, Friedrich & Stammbach 1964) (See figure at the end of this section.)
$\log (P/\text{mmHg}) = 11.911 - 4933/(T/\text{K})$, temp range 50–130°C (gas saturation-GC, data presented in Antoine eq., Friedrich & Stammbach 1964)

0.00028 (from Friedrich & Stammbach 1964; Jury et al. 1983; 1984; Spencer & Cliath 1990)
0.00013 (20°C, Ashton & Crafts 1973, 1981)
0.00013 (20–25°C, Weber et al. 1980)
0.00028 (quoted, Jury et al. 1984; Spencer & Cliath 1990)
0.00013 (20°C, Hartley & Kidd 1987; Worthing & Hance 1991; Montgomery 1993)
0.00010 (20°C, selected, Suntio et al. 1988)
0.00013, 0.00053 (20, 30°C, Herbicide Handbook 1989)
1.60×10^{-4}, 6.70×10^{-3}, 0.16, 2.50, 28.0 (25, 50, 70, 100, 125°C, gas saturation-GC, Rordorf 1989)
$\log (P_S/Pa) = 17.063 - 6215.6/(T/K)$; measured range 32.4–117°C (gas saturation-GC, Rordorf 1989)
$\log (P_L/Pa) = 14.013 - 5037.2/(T/K)$; measured range 129–140°C (gas saturation-GC, Rordorf 1989)
0.00017 (20–25°C, selected, Wauchope et al. 1992; Hornsby et al. 1996)
0.000169 (Tomlin 1994)

Henry's Law Constant (Pa·m³/mol at 25°C or as indicated):
0.00139 (calculated-P/C, Jury et al. 1984; quoted, Spencer & Cliath 1990)
0.00139 (calculated-P/C, Jury et al. 1987a,b; Jury & Ghodrati 1989)
0.00050 (20°C, calculated-P/C, Suntio et al. 1988; quoted, Majewski & Capel 1995)
0.00050 (20°C, calculated-P/C, Montgomery 1993)

Octanol/Water Partition Coefficient, log K_{OW}:
2.99 (selected, Dao et al. 1983)
1.91 (RP-HPLC-k′ correlation, Braumann et al. 1983)
3.46 (selected, Yoshioka et al. 1986)
3.51 (shake flask, Mitsutake et al. 1986)
2.99 (Gerstl & Helling 1987)
3.34 (RP-HPLC-RT correlation, Finizio et al. 1991)
3.43 (selected, Magee 1991)
3.34 (Worthing & Hance 1991; Milne 1995)
3.34, 3.46 (Montgomery 1993)
3.51 (recommended, Sangster 1993)
2.93 (RP-HPLC-k′ correlation, Liu & Qian 1995)
3.51 (recommended, Hansch et al. 1995)
3.35 (Pomona-database, Müller & Kördel 1996)
3.25 (RP-HPLC-RT correlation, Finizio et al. 1997)
2.99 (RP-HPLC-RT correlation using short ODP column, Donovan & Pescatore 2002)

Bioconcentration Factor, log BCF:
1.85, 1.67 (calculated-S, K_{OC}, Kenaga 1980)

Sorption Partition Coefficient, log K_{OC}:
2.91 (soil, Hamaker & Thompson 1972; Kenaga 1980; Kenaga & Goring 1980)
2.72 (soil, calculated-S as per Kenaga & Goring 1980, Kenaga 1980)
2.79 (Rao & Davidson 1980)
3.17 (calculated-MCI χ, Gerstl & Helling)
2.78 (screening model calculations, Jury et al. 1987a,b; Jury & Ghodrati 1989)
2.75 (estimated as log K_{OM}, Magee 1991)
2.72–2.91, 2.79, 2.83 (soil, quoted values, Bottoni & Funari 1992)
2.60 (soil, 20–25°C, selected, Wauchope et al. 1992; Hornsby et al. 1996)
2.38 (soil, HPLC-screening method, mean value from different stationary and mobile phases, Kördel et al. 1993, 1995b)
2.28–2.79 (Montgomery 1993)
3.15 (estimated-chemical structure, Lohninger 1994)
2.60 (soil, Tomlin 1994)
2.63 (calculated-K_{OW}, Liu & Qian 1995)
2.85 (soil, calculated-QSAR MCI $^1\chi$, Sabljic et al. 1995)

2.38; 2.84 (HPLC-screening method; calculated-PCKOC fragment method, Müller & Kördel 1996)

3.54, 1.595, 1.968, 1.77, 2.67 (first generation Eurosoils ES-1, ES-2, ES-3, ES-4, ES-5, shake flask/batch equilibrium-HPLC/UV, Gawlik et al. 1998)

3.24, 2.16, 2.86, 2.59, 2.53 (calculated-K_{OW}; HPLC-screening method with different LC-columns, Szabo et al. 1999)

2.544, 2.635, 2.484, 1.816, 2.933 (second generation Eurosoils ES-1, ES-2, ES-3, ES-4, ES-5, shake flask/batch equilibrium-HPLC/UV and HPLC-k′ correlation, Gawlik et al. 2000)

2.85, 2.89 (soil, estimated-class-specific model, estimated-general model using molecular descriptors, Gramatica et al. 2000)

Environmental Fate Rate Constants, k, or Half-Lives, $t_{1/2}$:

Volatilization: $t_{1/2}$ = 60 d (Jury et al. 1984).

Photolysis:

Oxidation:

Hydrolysis: $t_{1/2}$ = 22 d in 0.1 N hydrochloric acid solution, $t_{1/2}$ = 500 yr at pH 7 in distilled water and $t_{1/2}$ = 30 yr in 0.01 sodium hydroxide solution all at 25°C (Montgomery 1993).

Biodegradation: $t_{1/2}$ = 60 d (Wauchope 1978);

$t_{1/2}$ = 60 d for a 100 d leaching and screening test in 0–10 cm depth of soil (Jury et al. 1987a,b; Jury & Ghodrati 1989);

soil microbial degradation $t_{1/2}$ = 70 d (Tomlin 1994).

Biotransformation:

Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants:

Half-Lives in the Environment:

Air:

Surface water: completely decomposed when exposed to UV light for 3 h (Montgomery 1993).

Ground water: reported half-lives or persistence, $t_{1/2}$ = 40–70, 60 and 94 d (Bottoni & Funari 1992)

Sediment:

Soil: estimated persistence of 3 months (Kearney et al. 1969; Edwards 1973; quoted, Morrill et al. 1982; Jury et al. 1987a,b; Jury & Ghodrati 1989);

$t_{1/2}$ ~ 6 months to biodegrade in flooded soils (Plimmer et al. 1970; quoted, Muir 1991);

persistence of 2 months in soil (Wauchope 1978);

reported $t_{1/2}$ = 40–70 d, 60 d and 94 d (Bottoni & Funari 1992);

selected field $t_{1/2}$ = 60 d (Wauchope et al. 1992; Hornsby et al. 1996);

$t_{1/2}$ = 70 d for microbial degradation in soil (Tomlin 1994).

Biota: biochemical $t_{1/2}$ = 60 d from screening model calculations (Jury et al. 1987a,b; Jury & Ghodrati 1989).

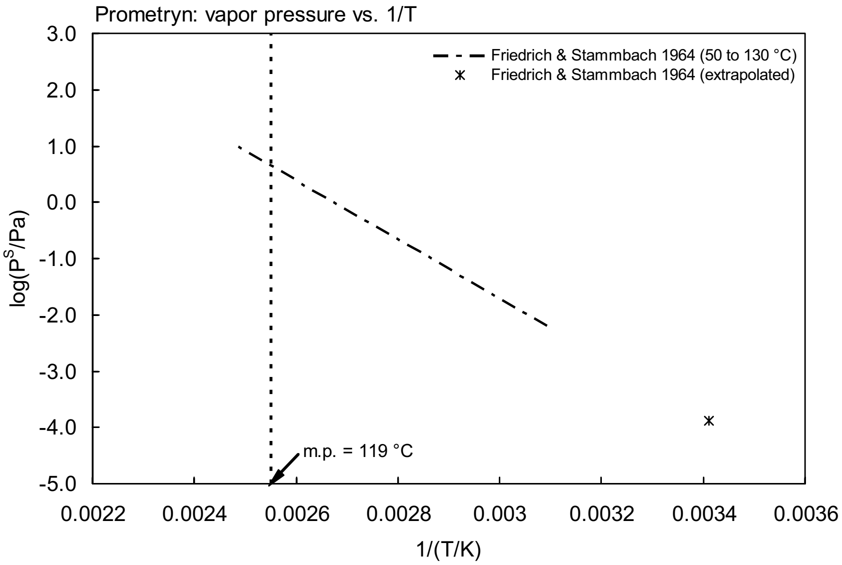
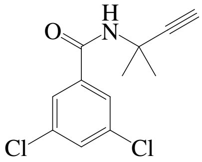


FIGURE 17.1.1.65.1 Logarithm of vapor pressure versus reciprocal temperature for prometryn.

17.1.1.66 Pronamide



Common Name: Pronamide
Synonym: Kerb, Promamide, Propyzamide, RH-315
Chemical Name: 3,5-dichloro-N-(1,1-dimethylpropynyl)benzamide
Uses: herbicide.
CAS Registry No: 23950-58-5
Molecular Formula: $C_{12}H_{11}Cl_2NO$
Molecular Weight: 256.127
Melting Point (°C):

155	(Lide 2003)

Boiling Point (°C): 321
Density (g/cm^3 at 20°C):
Molar Volume (cm^3/mol):

270.4	(calculated-Le Bas method at normal boiling point)

Dissociation Constant pK_a:
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
Entropy of Fusion, ΔS_{fus} (J/mol K):
Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F: 0.0530 (mp at 155°C)

Water Solubility (g/m^3 or mg/L at 25°C or as indicated):

15	(Martin & Worthing 1977; Herbicide Handbook 1978, 1983; Worthing & Walker 1987)
15	(15°C, Khan 1980)
15	(Ashton & Crafts 1981)
15	(24°C, Herbicide Handbook 1989)
15	(20–25°C, selected, Wauchope et al. 1992; Hornsby et al. 1996)
15	(Tomlin 1994; Milne 1995)

Vapor Pressure (Pa at 25°C or as indicated):

0.0113	(Khan 1980)
0.0113	(Ashton & Crafts 1981; Herbicide Handbook 1989)
0.0536	(Dixon & Rissman 1985; quoted, Howard 1991)
0.227	(Worthing & Walker 1987)
0.0113	(20–25°C, selected, Wauchope et al. 1992; Hornsby et al. 1996)
0.000058	(Tomlin 1994)

Henry's Law Constant (Pa·m^3/mol at 25°C):

0.912	(Dixon & Rissman 1985)
0.193	(calculated-P/C as per Worthing & Walker 1987, Majewski & Capel 1995)
0.188	(calculated-P/C, this work)

Octanol/Water Partition Coefficient, log K_{OW}:

3.26	(estimated, Lyman et al. 1982; quoted, Howard 1991)
3.36	(selected, Magee 1991)
3.26	(selected, Dao et al. 1983)
2.95	(estimated-QSAR and SPARC, Kollig et al. 1993)
3.09–3.28	(Tomlin 1994; Milne 1995)
3.87	(LOGPSTAR or CLOGP data, Sabljic et al. 1995)

Bioconcentration Factor, log BCF:

2.13	(calculated-S, Kenaga 1980)
1.00	(calculated-K_{OC}, Kenaga 1980)
2.25	(estimated-K_{OW}, Lyman et al. 1982; quoted, Howard 1991)
2.13	(estimated-S, Lyman et al. 1982; quoted, Howard 1991)

Sorption Partition Coefficient, log K_{OC}:

2.30	(soil, Leistra et al. 1974; Carlson et al.)
2.30	(measured for single soil, Kenaga 1980)
3.00	(soil, calculated-S as per Kenaga & Goring 1980, Kenaga 1980)
2.99	(soil, estimated-S, Lyman et al. 1982; quoted, Howard 1991)
2.30; 2.42	(reported as log K_{OM}, estimated as log K_{OM}, Magee 1991)
2.30; 3.20	(soil, quoted; calculated-MCI χ and fragment contribution, Meylan et al. 1992)
2.90	(soil, 20–25°C, selected, Wauchope et al. 1992; Hornsby et al. 1996)
2.63	(estimated-QSAR and SPARC, Kollig 1993)
2.54	(selected, Lohninger 1994)
2.31	(soil, calculated-QSAR MCI $^1\chi$, Sabljic et al. 1995)

Environmental Fate Rate Constants, k, or Half-Lives, $t_{1/2}$:

Volatilization: based on a Henry's law constant of 0.9118 Pa·m^3/mol, $t_{1/2}$ ~ 6.6 d from a river 1-m deep flowing 1 m/s with a wind velocity of 3 m/s (estimated, Lyman et al. 1982; quoted, Howard 1991).

Photolysis: degraded photolytically on soil thin films, $t_{1/2}$ = 13–57 d in artificial sunlight (Tomlin 1994).

Oxidation: photooxidation $t_{1/2}$ = 4.2 h in air, based on an estimated rate constant for the vapor-phase reaction with photochemically produced hydroxyl radicals in the atmosphere (Atkinson 1985; quoted, Howard 1991).

Hydrolysis: neutral hydrolysis rate constant $k < 1.5 \times 10^{-5}$ h^{-1} with a calculated $t_{1/2}$ > 700 d in neutral solution and with faster hydrolysis rates in acidic and basic solutions to be expected (Ellington et al. 1987, 1988; quoted, Howard 1991).

Biodegradation: depending on soil and climatic conditions, the degradation $t_{1/2}$ = 10 to 112 d, but a $t_{1/2}$ = 40 d may be more common under field conditions (Walker 1976,78; Zandvoort et al. 1979; quoted, Howard 1991).

Biotransformation: second-order rate constant $k = 5 \times 10^{-14}$ L/organisms·h with an estimated $t_{1/2}$ ~ 580 d for microbial degradation in natural water (Steen & Collette 1989; quoted, Howard 1991).

Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants:

Half-Lives in the Environment:

Air: $t_{1/2}$ = 4.2 h, based on an estimated rate constant for the vapor-phase reaction with photochemically produced hydroxyl radicals in the atmosphere (Atkinson 1985; quoted, Howard 1991).

Surface water:

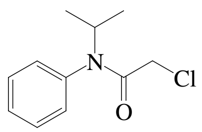
Ground water:

Sediment:

Soil: depending on soil and climatic conditions, the degradation $t_{1/2}$ = 10 to 112 d, but a $t_{1/2}$ = 40 d may be more common under field conditions (Walker 1976, 1978; Zandvoort et al. 1979; quoted, Howard 1991);
selected field $t_{1/2}$ = 60 d (Wauchope et al. 1992; Hornsby et al. 1996);
degraded photolytically on soil thin films, $t_{1/2}$ = 13–57 d in artificial sunlight (Tomlin 1994).

Biota:

17.1.1.67 Propachlor



Common Name: Propachlor
Synonym: Albrass, Bexton, CIPA, CP 31393, Niticid, Propachlore, Prolex, Ramrod, Satecid
Chemical Name: 2-chloro-*N*-(1-methylethyl)-*N*-phenylacetamide; 2-chloro-*N*-isopropyl-acetanilide
Uses: selective pre-emergence herbicide to control most annual grasses and some broadleaf weeds in brassicas, corn, cotton, flax, leeks, maize, milo, onions, peas, roses, ornamental trees and shrubs, soybeans, and sugar cane.
CAS Registry No: 1918-16-7
Molecular Formula: $C_{11}H_{14}ClNO$
Molecular Weight: 211.688
Melting Point (°C):
77 (Herbicide Handbook 1989; Worthing & Hance 1991; Tomlin 1994; Milne 1995; Lide 2003)
Boiling Point (°C):
110 (at 0.03 mmHg, Ashton & Crafts 1981; Hartley & Kidd 1987; Herbicide Handbook 1989; Worthing & Hance 1991; Montgomery 1993; Milne 1995)
Density (g/cm^3 at 20°C):
1.13 (25°C, Ashton & Crafts 1981)
1.242 (25°C, Hartley & Kidd 1987; Worthing & Hance 1991; Montgomery 1993; Tomlin 1994; Milne 1995)
1.134 (25°C, Herbicide Handbook 1989)
Molar Volume (cm^3/mol):
231.6 (calculated-Le Bas method at normal boiling point)
Dissociation Constant pK_a:
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
27.614 (DSC method, Plato 1972)
Entropy of Fusion, ΔS_{fus} (J/mol K):
Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F: 0.309 (mp at 77°C)

Water Solubility (g/m^3 or mg/L at 25°C or as indicated):
700 (Melnikov 1971; Khan 1980)
614 (20°C, Weber 1972)
693 (Spencer 1973, 1982)
580 (20°C, Ashton & Crafts 1973)
580 (Martin & Worthing 1977; Herbicide Handbook 1978)
839 (generator column-HPLC-RI, Swann et al. 1983)
2300 (HPLC-RT correlation, Swann et al. 1983)
613 (Hartley & Kidd 1987; Worthing & Walker 1987, Herbicide Handbook 1989 Worthing & Hance 1991; Tomlin 1994; Milne 1995)
613 (20–25°C, selected, Wauchope et al. 1992; Hornsby et al. 1996)
613–700 (Montgomery 1993)

Vapor Pressure (Pa at 25°C or as indicated):
0.032 (20–25°C, Weber et al. 1980)
0.0307 (24°C, Beestman & Demming 1974)
0.0307 (Ashton & Crafts 1981; Herbicide Handbook 1989)
0.03 (Hartley & Kidd 1987)
0.03 (20°C, selected, Suntio et al. 1988)
0.0306 (Worthing & Hance 1991; Tomlin 1994)

0.0307 (20–25°C, selected, Wauchope et al. 1992; Hornsby et al. 1996)
0.03 (Montgomery 1993)

Henry's Law Constant (Pa·m^3/mol at 25°C or as indicated):
0.011 (20°C, calculated-P/C, Suntio et al. 1988)
0.011 (20°C, calculated-P/C, Muir 1991)
0.011 (calculated-P/C, Montgomery 1993)

Octanol/Water Partition Coefficient, log K_{OW}:
2.75 (Leo et al. 1971)
1.61 (Rao & Davidson 1980)
2.80 (selected, Gerstl & Helling 1987)
2.18 (shake flask, Log P Database, Hansch & Leo 1987)
2.18 (selected, Magee 1991)
1.61 (Montgomery 1993)
2.18 (recommended, Sangster 1993)
1.62–2.30 (Tomlin 1994)
2.18 (recommended, Hansch et al. 1995)
2.36 (RP-HPLC-RT correlation, Finizio et al. 1997)
2.88 ± 0.17, 2.86 ± 0.12 (isocratic RP-HPLC-k′ correlation, gradient RP-HPLC-k′ correlation, Paschke et al. 2004)

Bioconcentration Factor, log BCF:
1.23 (calculated-S, Kenaga 1980)
1.15 (calculated-K_{OC}, Kenaga 1980)

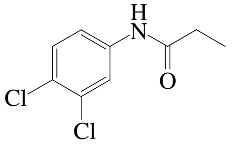
Sorption Partition Coefficient, log K_{OC}:
2.42 (soil, Beestman & Demming 1976; Kenaga 1980; Kenaga & Goring 1980)
2.11 (soil, calculated-S as per Kenaga & Goring 1980, Kenaga 1980)
2.43 (calculated-MCI χ, Gerstl & Helling 1987)
2.62 (screening model calculations, Jury et al. 1987b)
2.31 (estimated as log K_{OM}, Magee 1991)
2.45 (soil, calculated-MCI χ and fragment contribution, Meylan et al. 1992)
1.90 (soil, 20–25°C, selected, Wauchope et al. 1992; Hornsby et al. 1996)
2.07–2.11 (Montgomery 1993)
2.62 (estimated-chemical structure, Lohninger 1994)
2.42 (quoted or calculated-QSAR MCI $^1\chi$, Sabljic et al. 1995)
2.18 (soil, estimated-general model using molecular descriptors, Gramatica et al. 2000)

Environmental Fate Rate Constants, k, or Half-Lives, $t_{1/2}$:
Volatilization: estimated $t_{1/2}$ = 671 d from 1 m depth of water at 20°C (Muir 1991).
Photolysis: $t_{1/2}$ = 2.25 h in distilled water (Tanaka et al. 1981; quoted, Cessna & Muir 1991);
1 ppb contaminated water in the presence of TiO_2 and H_2O_2 completely photodegraded after 3 h by solar irradiation (Muszkat et al. 1992).
Oxidation:
Hydrolysis:
Biodegradation: $t_{1/2}$ µ10–14 d for 0.001–1.0 µg/mL to biodegrade in sewage effluent lake water (Novick & Alexander 1985; quoted, Muir 1991);
biochemical $t_{1/2}$ = 7 d from screening model calculations (Jury et al. 1987b).
Biotransformation: second-order microbial rate constant k = 1.1 × 10^{-9} L·organisms^{-1} h^{-1} (Steen & Collette 1989).
Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants:

Half-Lives in the Environment:
Air:
Surface water: $t_{1/2}$ ~ 10–14 d for 0.001–1.0 µg/mL to biodegrade in sewage effluent lake water (Novick & Alexander 1985; quoted, Muir 1991).

Ground water:
Sediment:
Soil: persistence of 2 months (Wauchope 1978);
  $t_{1/2}$ = 7 d from screening model calculations Jury et al. 1987b);
  persists in soil for 28–42 d (Worthing & Hance 1991);
  selected field $t_{1/2}$ = 6.3 d (Wauchope et al. 1992; Hornsby et al. 1996).
Biota: biochemical $t_{1/2}$ = 7 d from screening model calculations (Jury et al. 1987b).

17.1.1.68 Propanil



Common Name: Propanils

Synonym: Bay 30130, Chem rice, Crystal Propanil-4, DCPA, Dipram, DPA, DPA, Erban, Erbanil, Farmco propanil, FW-734, Grascide, Herbax technical, Prop-Job, Propanex, Propanid, Riselect, Rogue, Rosanil, S 10165, Stam F-34, Stampede, Stam Supernox, Strel, Supernox, Surcopur, Surpur, STAM, Synpran N, Vertac, Wham EZ

Chemical Name: *N*-(3,4-dichlorophenyl)propionamide; *N*-(3,4-dichlorophenyl)propanamide

Uses: selective emergence and post-emergence herbicide to control many grasses and broadleaf weeds in potatoes, rice and wheat.

CAS Registry No: 709-98-8

Molecular Formula: $C_9H_9Cl_2NO$

Molecular Weight: 218.079

Melting Point (°C):
- 92 (Lide 2003)

Boiling Point (°C):

Density (g/cm^3 at 20°C):
- 1.25 (25°C, Ashton & Crafts 1981; Hartley & Kidd 1987; Herbicide Handbook 1989; Montgomery 1993; Milne 1995)
- 1.41 (22°C, Tomlin 1994)

Molar Volume (cm^3/mol):
- 220.1 (calculated-Le Bas method at normal boiling point)

Dissociation Constant pK_a:

Enthalpy of Vaporization, ΔH_V (kJ/mol):
- 95.1 (Rordorf 1989)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
- 20.08 (DSC method, Plato & Glasgow 1969)
- 15.3 (Rordorf 1989)

Entropy of Fusion, ΔS_{fus} (J/mol K):

Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F: 0.220 (mp at 92°C)

Water Solubility (g/m^3 or mg/L at 25°C or as indicated):
- 225 (Woodford & Evans 1963; Khan 1980)
- 500 (Bailey & White 1965; Ashton & Crafts 1973; Herbicide Handbook 1989)
- 268 (Freed 1966)
- 225 (Martin & Worthing 1977; Worthing & Walker 1987; Herbicide Handbook 1983)
- 268–500 (Weber et al. 1980)
- 130 (20°C, Spencer 1982)
- 225 (Hartley & Kidd 1987; Milne 1995)
- 130 (20°C, Worthing & Hance 1991)
- 200 (20–25°C, selected, Wauchope et al. 1992; Hornsby et al. 1996)
- 130, 225 (20°C, 25°C, Montgomery 1993)
- 130 (Tomlin 1994)

Vapor Pressure (Pa at 25°C or as indicated and reported temperature dependence equations):
- 0.012 (60°C, Khan 1980)
- 0.012 (60°C, Verschueren 1983)
- 0.012 (60°C, Hartley & Kidd 1987)
- 0.005 (20°C, selected, Suntio et al. 1988)
- 2.50×10^{-4}, 7.20×10^{-3}, 0.130, 1.50, 13.0 (25, 50, 70, 100, 125°C, gas saturation-GC, Rordorf 1989)

$\log (P_S/Pa) = 15.201 - 5604.1/(T/K)$; measured range 36.4–92.6°C (gas saturation-GC, Rordorf 1989)
$\log (P_L/Pa) = 13.192 - 4863.1/(T/K)$; measured range 95.1–160°C (gas saturation-GC, Rordorf 1989)

2.60×10^{-5}	(20°C, Worthing & Hance 1991)
0.00533	(20–25°C, selected, Wauchope et al. 1992; Hornsby et al. 1996)
2.67×10^{-5}	(20°C, Montgomery 1993)

Henry's Law Constant ($Pa \cdot m^3/mol$ at 25°C or as indicated):

0.0036	(20°C, calculated-P/C, Suntio et al. 1988)
0.0036	(20°C, calculated-P/C, Montgomery 1993)
0.00545	(calculated-P/C, this work)

Octanol/Water Partition Coefficient, $\log K_{OW}$:

2.02	(Rao & Davidson 1980)
2.80	(20 ± 2°C, shake flask-UV, Briggs 1981)
3.12	(selected, Dao et al. 1983)
3.07	(shake flask, Log P Database, Hansch & Leo 1987)
2.99	(selected, Gerstl & Helling 1987)
2.29	(Worthing & Hance 1991; Milne 1995)
2.34	(quoted from Kenaga 1980, Bottoni & Funari 1992)
2.73	(RP-HPLC-RT correlation, Sicbaldi & Finizio 1993)
2.03, 2.29	(Montgomery 1993)
3.07	(recommended, Sangster 1993)
2.80	(RP-HPLC-RT correlation, Saito et al. 1993)
3.30	(Tomlin 199)
3.07	(selected, Hansch et al. 1995)
2.73	(RP-HPLC-RT correlation, Finizio et al. 1997)
3.21	(RP-HPLC-RT correlation using short ODP column, Donovan & Pescatore 2002)

Bioconcentration Factor, log BCF:

1.46	(calculated-S, Kenaga 1980)
1.34	(calculated, Pait et al. 1992)

Sorption Partition Coefficient, $\log K_{OC}$:

2.34	(calculated-S, Kenaga 1980)
2.23	(calculated-MCI χ, Gerstl & Helling 1987)
2.33	(selected, Trevisan et al. 1991)
2.19	(Montgomery 1993)
2.17	(soil, 20–25°C, selected, Wauchope et al. 1992; Hornsby et al. 1996)
2.38–2.90	(Tomlin 1994)

Environmental Fate Rate Constants, k, or Half-Lives, $t_{1/2}$:

Volatilization:

Photolysis: $t_{1/2}$ = 34 d for 82% of 200 μg/mL to degrade in distilled water under sunlight (Moilanen & Crosby 1972; quoted, Cessna & Grover 1991);
$t_{1/2}$ = 2.25 h for 37–51% of 100 μg mL^{-1} to degrade in distilled water under > 300 nm light (Tanaka et al. 1981; quoted, Cessna & Grover 1991);
$t_{1/2}$ = 245 h for 14–81% of 15 μg mL^{-1} to degrade in distilled water under sunlight (Draper & Crosby 1984; quoted, Cessna & Grover 1991);
photolysis $t_{1/2}$ = 12–13 h in water (Tomlin 1994).

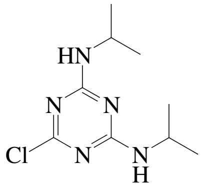
Oxidation: measured rate constant for reaction with hydroxyl radical, $k(aq.) = 1.60 \times 10^9\ M^{-1}\ s^{-1}$ in irradiated field water both in the laboratory and sunlit rice paddies (Mabury & Crosby 1996).

Hydrolysis: $t_{1/2}$ > 4 months for 4360 μg mL^{-1} to hydrolyze in phosphate buffers pH 5–9 at 20°C (El-dib & Aly 1976; quoted, Muir 1991);
hydrolysis $t_{1/2}$ >> 1 yr at pH 4, 7, 9 at 22°C (Tomlin 1994).

Biodegradation: $t_{1/2}$ = 1–2 d for 30 µg mL^{-1} to biodegrade in flooded soil at 30°C (Kuwatsuka 1972; quoted, Muir 1991);
$t_{1/2}$ ~ 10 d for 40 µg mL^{-1} to biodegrade in pond sediment (Stepp et al. 1985; quoted, Muir 1991).
Biotransformation: second-order microbial degradation rate constant k = 5×10^{-10} L·$organisms^{-1}$ h^{-1} (Steen & Collette 1989).
Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants:

Half-Lives in the Environment:
Air:
Surface water: hydrolysis $t_{1/2}$ >> 1 yr (pH 4, 7, 9) at 22°C and photolysis $t_{1/2}$ = 12–13 h in aqueous solution (Tomlin 1994).
Groundwater: reported $t_{1/2}$ < 5 d (Bottoni & Funari 1992)
Sediment: $t_{1/2}$ ~ 10 d for 40 µg mL^{-1} to biodegrade in pond sediment (Stepp et al. 1985; quoted, Muir 1991).
Soil: $t_{1/2}$ = 1–2 d for 30 µg mL^{-1} to biodegrade in flooded soil at 30°C (Kuwatsuka 1972; quoted, Muir 1991);
selected field $t_{1/2}$ = 1.0 d (Wauchope et al. 1992; Hornsby et al. 1996; quoted, Halfon et al. 1996);
soil $t_{1/2}$ = 15 d (Pait et al. 1992);
$t_{1/2}$ < 5 d (Bottoni & Funari 1992).
Biota:

17.1.1.69 Propazine



Common Name: Propazine

Synonym: G-30028, Geigy 30028, Gesamil, Maax, Milogard, Plantulin, Primatol P, Propasin, Prozinex

Chemical Name: 6-chloro-*N,N′*-bis(1-methylethyl)-1,3,5-triazine-2,4-diamine; 2-chloro-4,6-bis(isopropylamino)-1,3,5-triazine

Uses: selective pre-emergence herbicide to control annual grasses and broadleaf weeds in milo and sweet sorghum.

CAS Registry No: 139-40-2

Molecular Formula: $C_9H_{16}ClN_5$

Molecular Weight: 229.710

Melting Point (°C):
- 213 (Lide 2003)

Boiling Point (°C):

Density (g/cm^3 at 20°C):
- 1.162 (Hartley & Kidd 1987; Worthing & Hance 1991; Montgomery 1993; Tomlin 1994; Milne 1995)

Molar Volume (cm^3/mol):
- 272.8 (calculated-Le Bas method at normal boiling point)

Dissociation Constant:
- 1.85 (pK_a, Weber 1970; quoted, Bintein & Devillers 1994)
- 1.80 (pK_a, Weber et al. 1980; Willis & McDowell 1982)
- 1.85 (pK_a, Herbicide Handbook 1989)
- 1.70 (pK_a, 21°C, Worthing & Hance 1991)
- 12.15 (pK_b, Wauchope et al. 1992)
- 1.85 (pK_a, 22°C, Montgomery 1993)
- 12.3 (pK_b, 21°C, Tomlin 1994)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
- 41.84 (DSC method, Plato 1972)

Entropy of Fusion, ΔS_{fus} (J/mol K):

Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F: 0.0143 (mp at 213°C)

Water Solubility (g/m^3 or mg/L at 25°C or as indicated):
- 10 (Gysin 1962)
- 8.6 (20–22°C, Bailey & White 1965; Spencer 1973; Quellette & King 1977)
- 4.82, 4.60, 5.05 (26°C, shake flask-UV at pH 3.0, 7.0, 10.0, Ward & Weber 1968)
- 8.60 (Martin & Worthing 1977)
- 4.8–8.6 (Weber et al. 1980)
- 5.0 (20°C, Spencer 1982)
- 8.60 (20°C, Hartley & Kidd 1987; Herbicide Handbook 1989)
- 5.0 (20°C, Worthing & Walker 1987, Worthing & Hance 1991; Tomlin 1994; Milne 1995)
- 8.60 (20–25°C, selected, Wauchope et al. 1992; Hornsby et al. 1996)
- 8.50 (20°C, Montgomery 1993)

Vapor Pressure (Pa at 25°C or as indicated and reported temperature dependence equations):
- 3.87×10^{-6} (20°C, extrapolated-Antoine eq. from gas saturation-GC measurements, measured range 50–130°C, Friedrich & Stammbach 1964) (See figure at the end of this section.)
- $\log (P/mmHg) = 11.911 - 4933/(T/K)$, temp range 50–130°C (gas saturation-GC, data presented in graph and Antoine eq., Friedrich & Stammbach 1964)
- 3.90×10^{-6} (20°C, Quellette & King 1977)

4.00×10^{-6} (20–25°C, Weber et al. 1980)
3.90×10^{-6} (20°C, Ashton & Crafts 1981; Herbicide Handbook 1989)
4.00×10^{-6} (20°C, Hartley & Kidd 1987)
2.10×10^{-5} (30°C, Herbicide Handbook 1989)
3.90×10^{-6} (20°C, Worthing & Hance 1991; Montgomery 1993)
1.75×10^{-5} (20–25°C, selected, Wauchope et al. 1992; Hornsby et al. 1996)

Henry's Law Constant (Pa·m^3/mol at 25°C or as indicated):
1.00×10^{-4} (20°C, selected, Suntio et al. 1988; quoted, Majewski & Capel 1995)
1.00×10^{-3} (20°C, calculated-P/C, Montgomery 1993)
1.04×10^{-3} (calculated-P/C, this work)

Octanol/Water Partition Coefficient, log K_{OW}:
2.89 (Kenaga & goring 1980; Yoshioka et al. 1986)
2.94 (shake flask-GC or UV, Brown & Flagg 1981)
2.59 (RP-HPLC-k′ correlation, Braumann et al. 1983)
2.93 (shake flask, Biagi et al. 1991)
2.91 (RP-HPLC-RT correlation, Finizio et al. 1991)
2.91, 2.94 (Montgomery 1993)
2.77 (RP-HPLC-RT correlation, Sicbaldi & Finizio 1993)
2.93 (recommended, Sangster 1993; Hansch et al. 1995)
2.89 (shake flask-UV, Liu & Qian 1995)
3.13 (Pomona-database, Müller & Kördel 1996)
2.77 (RP-HPLC-RT correlation, Finizio et al. 1997)

Bioconcentration Factor, log BCF:
2.26 (calculated-S, Kenaga 1980)
0.903 (calculated-K_{OC}, Kenaga 1980)

Sorption Partition Coefficient, log K_{OC}:
2.20 (soil, Hamaker & Thompson 1972; Brown 1978; Kenaga 1980; Kenaga & Goring 1980; Sabljic 1987)
3.11 (soil, calculated-S per Kenaga & Goring 1980; Kenaga 1980)
2.56 (Georgia's Hickory Hill pond sediment, Brown & Flagg 1981)
2.78 (calculated-MCI χ, Gerstl & Helling 1987)
2.34 (estimated as log K_{OM}, Magee 1991)
2.18 (soil, quoted, Bottoni & Funari 1992)
2.19 (soil, 20–25°C, selected, Wauchope et al. 1992; Hornsby et al. 1996)
1.94 (soil, HPLC-screening method, mean value from different stationary and mobile phases, Kördel et al. 1993, 1995b)
1.69–2.56 (Montgomery 1993)
2.44 (selected, Lohninger 1994)
1.90, 2.0 (Tomlin 1994)
2.57 (calculated-K_{OW}, Liu & Qian 1995)
2.40 (soil, calculated-MCI $^1\chi$, Sabljic et al. 1995)
1.94; 2.55 (HPLC-screening method; calculated-PCKOC fragment method, Müller & Kördel 1996)
2.59, 1.93, 2.08, 1.95, 2.70 (first generation Eurosoils ES-1, ES-2, ES-3, ES-4, ES-5, shake flask/batch equilibrium-HPLC/UV, Gawlik et al. 1998, 1999)
2.18, 2.148, 2.10, 1.98, 2.58 (second generation Eurosoils ES-1, ES-2, ES-3, ES-4, ES-5, shake flask/batch equilibrium-HPLC/UV, Gawlik et al. 1999)
2.818, 2.148, 2.100, 1.977, 2.579 (second generation Eurosoils ES-1, ES-2, ES-3, ES-4, ES-5, shake flask/batch equilibrium-HPLC/UV and HPLC-k′ correlation, Gawlik et al. 2000)
2.40; 2.43, 2.84 (soil, quoted obs.; estimated-class-specific model, estimated-general model using molecular descriptors, Gramatica et al. 2000)
2.15, 2.17 (soils: organic carbon OC ≥ 0.1%, OC ≥ 0.5%, pH 3.2–7.4, average, Delle Site 2001)

2.29, 2.21, 2.03 (soil with organic carbon OC ≥ 0.5% at: pH 4.3–5.0, pH 5.1–5.0, pH ≥ 6.0, average, Delle Site 2001)

Environmental Fate Rate Constants, k, or Half-Lives, $t_{1/2}$:

Volatilization:

Photolysis: 1 ppb contaminated water in presence of TiO_2 and H_2O_2 completely photodegraded after 3.5 h by solar irradiation (Muszkat et al. 1992).

Oxidation:

Hydrolysis: calculated rate constant $k = 9.70 \times 10^{-6}\ s^{-1}$ with $t_{1/2}$ = 83 d at 20°C in a buffer at pH 5 (Burkhard & Guth 1981).

Biodegradation:

Biotransformation:

Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants:

Half-Lives in the Environment:

Air:

Surface water:

Ground water: reported half-lives or persistence, $t_{1/2}$ = 80–100 d (Bottoni & Funari 1992)

Sediment:

Soil: persistence of 18 months (Edwards 1973; quoted, Morrill et al. 1982);

persistence of 12 months in soil (Wauchope 1978);

$t_{1/2}$ = 62 d and 127 d in a Hatzenbühl soil at pH 4.8 and Neuhofen soil at pH 6.5 respectively at 22°C under laboratory conditions (Burkhard & Guth 1981; quoted, Montgomery 1993);

reported $t_{1/2}$ = 80–100 d (Bottoni & Funari 1992);

selected field $t_{1/2}$ = 135 d (Wauchope et al. 1992; Hornsby et al. 1996).

Biota:

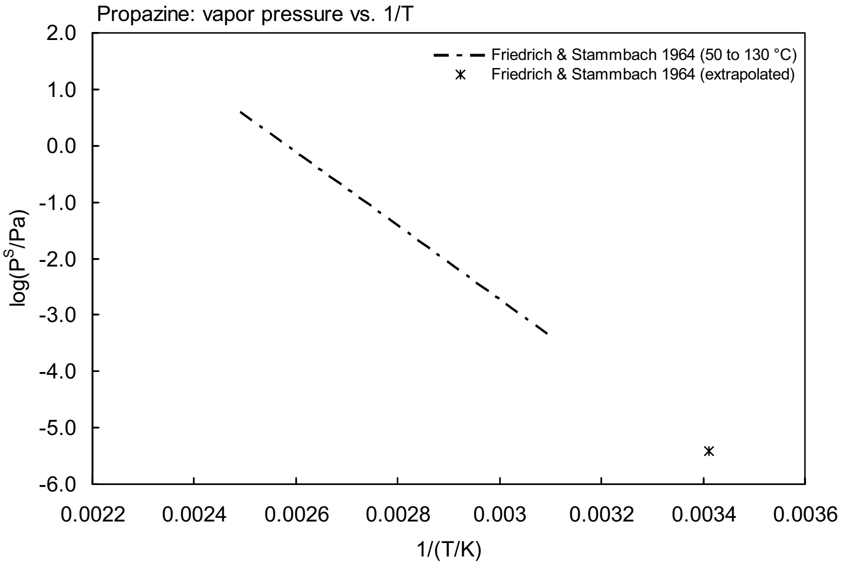
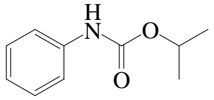


FIGURE 17.1.1.69.1 Logarithm of vapor pressure versus reciprocal temperature for propazine.

17.1.1.70 Propham



Common Name: Propham

Synonym: Agermin, Ban-Hoe, Beet-Kleen, Birgin, Chem-Hoe, Collavin, IFC, IFK, INPC, IPC

Chemical Name: carbanilate acid isopropyl ester; isopropyl carbanilate; isopropyl-N-phenyl carbamate; 1-methylethyl phenylcarbamate

Uses: pre-emergence and post-emergence herbicide to control annual grass weeds in peas, beans, sugar beet, lettuce, lucerne, clover, flax, sunflowers and lentils.

CAS Registry No: 122-42-9

Molecular Formula: $C_{10}H_{13}NO_2$

Molecular Weight: 179.2 16

Melting Point (°C):
90 (Lide 2003)

Boiling Point (°C):
> 150 (sublimes but decomposes, Montgomery 1993)

Density (g/cm^3 at 20°C):
1.09 (Spencer 1982; Tomlin 1994; Hartley & Kidd 1987; Milne 1995)
1.09 (30°C, Ashton & Crafts 1981; Herbicide Handbook 1989; Montgomery 1993)

Molar Volume (cm^3/mol):
213.6 (calculated-Le Bas method at normal boiling point)

Dissociation Constant pK$_a$:

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

Entropy of Fusion, ΔS_{fus} (J/mol K):

Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F: 0.230 (mp at 90°C)

Water Solubility (g/m^3 or mg/L at 25°C or as indicated):
100 (Freed 1953)
250 (Nex & Sweezey 1954; Ashton & Crafts 1981)
22.5–32 (Bailey & White 1965)
250 (20°C, Spencer 1973, 1982)
250 (Martin & Worthing 1977; Herbicide Handbook 1978, 1983, 1989; Hartley & Kidd 1987)
250–254 (Weber et al. 1980)
127 (selected, Gerstl & Helling 1987)
32–250 (20–25°C, Worthing & Hance 1991; Montgomery 1993)
250 (20–25°C, selected, Wauchope et al. 1992; Hornsby et al. 1996)
250 (20°C, Tomlin 1994; Milne 1995)

Vapor Pressure (Pa at 25°C or as indicated):
sublimes (rm. temp., Herbicide Handbook 1989)
sublimes (rm. temp., Montgomery 1993; Tomlin 1994)

Henry's Law Constant (Pa m^3/mol):

Octanol/Water Partition Coefficient, log K_{OW}:
2.60 (20 ± 2°C, shake flask-UV, Briggs 1981)
2.16 (selected, Dao et al. 1983; Gerstl & Helling 1987)
2.27 (shake flask, Mitsutake et al. 1986)
2.60 (recommended, Sangster 1993)

Bioconcentration Factor, log BCF:

1.43	(calculated-S, Kenaga 1980)
0.301	(calculated-K_{OC}, Kenaga 1980)

Sorption Partition Coefficient, log K_{OC}:

1.71	(Hamaker & Thompson 1972; Kenaga 1980; Kenaga & Goring 1980)
2.32	(soil, calculated-S as per Kenaga & Goring 1980, Kenaga 1980)
1.71	(20 ± 2°C, reported as log K_{OM}, Briggs 1981)
1.93	(calculated-MCI χ, Gerstl & Helling 1987)
2.30	(soil, 20–25°C, estimated, Wauchope et al. 1992; Hornsby et al. 1996)
1.71	(Montgomery 1993)
2.30	(estimated-chemical structure, Lohninger 1994)

Environmental Fate Rate Constants, or Half-Lives, $t_{½}$:

Volatilization:

Photolysis: direct $t_{½}$ = 254 d in clear water body near the surface for a mid-summer day at latitude 40° (Wolfe et al. 1978)

direct $t_{½}$ = 254 d in distilled water assuming for a mid-summer day at latitude 40°; $t_{½}$ = 2.25 h for 1% of 100 μg/ml to degrade in distilled water under 300 nm light (Tanaka et al. 1981; quoted, Cessna & Muir 1991).

Oxidation:

Hydrolysis: $t_{½}$ > 4 months for 3550 μg/mL to hydrolyze in phosphate buffer at pH 5–9 and 20°C (El-Dib & Aly 1976; quoted, Muir 1991)

k(alkaline) = 7.6×10^{-6} M^{-1} s^{-1} at 27°C, k = 5.6×10^{-5} M^{-1} s^{-1} at 50°C, k = 2.6×10^{-4} M^{-1} s^{-1} at 70°C; with $t_{½}$ > 1×10^4 d at pH 5, 7 and 9 (Wolfe et al. 1978)

Biodegradation: $t_{½}$ = 190 d by 1 mg/L fungus *Asperillus fumigaurs*, $t_{½}$ = 3.2 d by bacteria (Wolfe et al. 1978)

k = 1.5×10^{-4} L (mg M)$^{-1}$ h^{-1} with $t_{½}$ = 190 d for 2–25 μg/mL fungus *Aspergillus fumigatus*; k = 9×10^{-2} L (mg M)$^{-1}$ h^{-1} with $t_{½}$ = 3.2 d for bacteria *Pseudomonas striata* to biodegrade in stream water at pH 7 and 28°C (Muir 1991)

$t_{½}$ ~ 30–40 d for 1–0.0004 μg/mL to biodegrade in filtered sewage water at 20–22°C and $t_{½}$ ~ 20 to 50 d at 29°C in filtered lake water (Wang et al. 1984; quoted, Muir 1991)

$t_{½}$(aerobic) > 4 months for 6–7 μg/mL to biodegrade in river water at 25°C (Stepp et al. 1985; quoted, Muir 1991)

Biotransformation:

Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants:

Half-Lives in the Environment:

Air:

Surface water: hydrolysis $t_{½}$ > 1×10^4 d based on neutral and alkaline hydrolysis assuming pseudo-first order kinetics; direct photolysis $t_{½}$ = 254 d assuming a mid-summer day at altitude 40°, and biolysis $t_{½}$ = 190 d for 1 mg/L of fungus and $t_{½}$ = 3.2 d for bacteria at 28°C (Wolfe et al. 1978);

$t_{½}$ ~ 30–40 d for 1–0.0004 μg/mL to biodegrade in filtered sewage water at 20–22°C and $t_{½}$ ~ 20 to 50 d at 29°C in filtered lake water (Wang et al. 1984; quoted, Muir 1991);

aerobic $t_{½}$ > 4 months for 6–7 μg/mL to biodegrade in river water at 25°C (Stepp et al. 1985; quoted, Muir 1991).

Ground water:

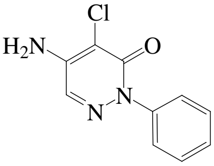
Sediment:

Soil: $t_{½}$ ~ 15 d in soil and $t_{½}$ = 5 d at 16 and 29°C (Hartley & Kidd 1987; Herbicide Handbook 1989; quoted, Montgomery 1993; Tomlin 1994);

selected field $t_{½}$ = 10 d (Wauchope et al. 1992; Hornsby et al. 1996).

Biota:

17.1.1.71 Pyrazon



Common Name: Pyrazon
Synonym: chloridazon, chloridazone, Blurex, Burex, Dazon, Phenosane, Piramin, Pyramin
Chemical Name: 5-amino-4-chloro-2-phenylpyridazin-3(2*H*)-one
Uses: as pre- and post-emergence herbicide to control of annual broadleaf weeds in sugar-beet, fodder beet and beet root; and also used in combination with other herbicides, etc.
CAS Registry No: 1698-60-8
Molecular Formula: $C_{10}H_8ClN_3O$
Molecular Weight: 221.643
Melting Point (°C):

205	(Lide 2003)

Boiling Point (°C):
Density (g/cm^3 at 20°C):

1.54	(Tomlin 1994)

Molar Volume (cm^3/mol):

205.7	(calculated-Le Bas method at normal boiling point)
143.9	(calculated-density)

Dissociation Constant pK_a:
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

26.59	(DSC method, Plato & Glasgow 1969)

Entropy of Fusion, ΔS_{fus} (J/mol K):
Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F: 0.0171 (mp at 205°C)

0.013	(20°C, Suntio et al. 1988)

Water Solubility (g/m^3 or mg/L at 25°C or as indicated):

400	(20°C, Ashton & Crafts 1973, 1981)
300	(20°C, Khan 1980)
400	(20°C, Spencer 1982)
400	(20°C, Worthing & Walker 1987; Hartley & Kidd 1987; Milne 1995)
360	(20°C, selected, Suntio et al. 1988)
400	(20–25°C, selected, Wauchope et al. 1992; Hornsby et al. 1996)
340	(20°C, Tomlin 1994)

Vapor Pressure (Pa at 25°C or as indicated):

9.86	(40°C, Ashton & Craft 1973; Spencer 1982)
< 0.00001	(20°C, Worthing & Walker 1987; Hartley & Kidd 1987; Tomlin 1994)
7.0	(20°C, estimated, Suntio et al. 1988)
6.67	(20–25°C, selected, Wauchope et al. 1992; Hornsby et al. 1996)

Henry's Law Constant (Pa·m^3/mol at 25°C or as indicated):

4.31	(20°C, calculated-P/C, Suntio et al. 1988)

Octanol/Water Partition Coefficient, log K_{OW}:

1.14	(22°C, shake flask-AS, Braumann & Grimme 1981; quoted, Sangster 1993)
1.50	(selected, Gerstl & Helling 1987)
1.12	(RP-HPLC-RT correlation, Sicbaldi & Finizio 1993)
1.19	(pH 7, Tomlin 1994)

2.20	(Milne 1995)
1.14	(recommended, Hansch et al. 1995)
1.12	(RP-HPLC-RT correlation, Finizio et al. 1997)

Bioconcentration Factor, log BCF:

1.32	(calculated-S per Kenaga 1980, this work)

Sorption Partition Coefficient, log K_{OC}:

2.12, 2.18	(selected, calculated-MCI χ, Gerstl & Helling 1987)
2.74	(soil, calculated-MCI and fragments contribution method, Meylan et al. 1992)
2.08	(soil, Wauchope et al. 1992; Hornsby et al. 1996)
1.95–2.53	(soil, Tomlin 1994)

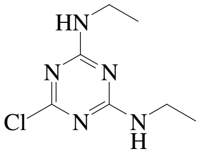
Environmental Fate Rate Constants, or Half-Lives:

Photolysis: $t_{1/2}$ = 150 h at pH 7 in simulated sunlight and $t_{1/2}$ = 47.7 h by 80000 lux, xenon lamp (Tomlin 1994).

Half-Lives in the Environment:

Soil: field $t_{1/2}$ = 21 d (Wauchope et al. 1992; Hornsby et al. 1996)

17.1.1.72 Simazine



Common Name: Simazine

Synonym: A 2079, Aktinit S, Amizine, Aquazine, Batazina, Bitemol, Cekusan, CAT, CET, DCT, Framed, G 27692, Gesapun, Gesaran, Gesatop, Herbazin, Herbex, Herboxy, Premazine, Primatol, Primcep, Princep, Printop, Radocon, Radokor, Simadex, Simanex, Sim-Trol, Tafazine, Weedex, Zeapur

Chemical Name: 6-chloro-*N,N′*-diethyl-1,3,5-triazine-2,4-diamine; 2-chloro-4,6-bis(ethyl-amino)-1,3,5-triazine

Uses: selective pre-emergence systemic herbicide to control many broadleaf weeds and annual grasses in deep-rooted fruit and vegetable crops.

CAS Registry No: 122-34-9

Molecular Formula: $C_7H_{12}ClN_5$

Molecular Weight: 201.657

Melting Point (°C):

226 (Lide 2003)

Boiling Point (°C):

Density (g/cm^3 at 20°C):

1.302 (Hartley & Kidd 1987; Milne 1995)
1.203 (Montgomery 1993)

Molar Volume (cm^3/mol):

228.4 (calculated-Le Bas method at normal boiling point)

Dissociation Constant:

1.65 (pK_a, Weber 1970; quoted, Bintein & Devillers 1994)
1.60 (pK_a, Weber et al. 1980; Willis & McDowell 1982)
1.70 (pK_a, 21°C, Worthing & Hance 1991; Montgomery 1993)
2.00 (pK_a, Yao & Haag 1991; Haag & Yao 1992)
12.35 (pK_b, Wauchope et al. 1992; Hornsby et al. 1996)
12.3 (pK_b, Tomlin 1994)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

43.932 (DSC method, Plato 1972)

Entropy of Fusion, ΔS_{fus} (J/mol K):

Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F: 0.0107 (mp at 226°C)

Water Solubility (g/m^3 or mg/L at 25°C or as indicated):

5.0 (Bailey & White 1965 Freed 1976; Wauchope 1978)
5.8, 5.0, 5.0 (26°C, shake flask-UV at pH 3.0, 7.0, 10.0, Ward & Weber 1968)
15.1 (26°C, Getzen & Ward 1971)
5.0 (20°C, Weber 1972; Spencer 1973; Khan 1980)
5.0 (20°C, Martin & Worthing 1977; Worthing & Walker 1987; Worthing & Hance 1991; Milne 1995)
3.5 (Herbicide Handbook 1978, 1989)
3.5 (20°C, Ashton & Crafts 1981; Hartley & Kidd 1987)
5.0, 3.50, 7.4(20°C, quoted, exptl., calculated-Parachor & mp, Briggs 1981)
6.2 (20–25°C, selected, Wauchope et al. 1992; Hornsby et al. 1996)
3.5–5.0 (20°C), Montgomery 1993)

Vapor Pressure (Pa at 25°C or as indicated and reported temperature dependence):

8.13×10^{-7} (20°C, extrapolated-Antoine eq. from gas saturation-GC measurements, measured range 50–130°C, Friedrich & Stammbach 1964) (See figure at the end of this section.)
$\log(P/mmHg) = 11.911 - 4933/(T/K)$, temp range 50–130°C (gas saturation-GC, data presented in graph and Antoine eq., Friedrich & Stammbach 1964)

8.10×10^{-7} (20°C, Weber 1972; Khan 1980; Ashton & Crafts 1981; Herbicide Handbook 1989)
2.00×10^{-6} (gas saturation, Spencer & Cliath 1974)
8.00×10^{-7} (20–25°C, Weber et al. 1980; Willis & McDowell 1982)
8.10×10^{-7} (20°C, Hartley & Kidd 1987; Worthing & Walker 1987; Worthing & Hance 1991; Montgomery 1993)
8.50×10^{-6} (20°C, selected, Suntio et al. 1988)
4.80×10^{-6} (30°C, Herbicide Handbook 1989)
2.95×10^{-6} (20–25°C, selected, Wauchope et al. 1992; Hornsby et al. 1996)
2.94×10^{-6} (OECD 104, Tomlin 1994)

Henry's Law Constant (Pa·m^3/mol at 25°C or as indicated):
8.40×10^{-5} (calculated-P/C, Jury et al. 1983, 1984, 1987a; Jury & Ghodrati 1989)
3.40×10^{-4} (20°C, calculated-P/C, Suntio et al. 1988)
8.40×10^{-5} (calculated-P/C, Taylor & Glotfelty 1988)
3.30×10^{-5} (20°C, calculated-P/C, Muir 1991)
3.40×10^{-4} (20°C, calculated-P/C, Montgomery 1993)

Octanol/Water Partition Coefficient, log K_{OW}:
2.19 (Kenaga & Goring 1980)
1.94 (Rao & Davidson 1980)
1.51 (shake flask-UV, Lord et al. 1980)
1.51 (20 ± 2°C, shake flask-UV, Briggs 1981)
2.16 (shake flask, Brown & Flagg 1981)
1.96, 2.06 (RP-HPLC-k′ correlation, McDuffie et al. 1981)
2.27 (selected, Dao et al. 1983; Gerstl & Helling 1987)
2.14 (shake flask, Mitsutake et al. 1986)
1.50 (Nicholls 1988)
2.18 (shake flask, Biagi et al. 1991)
2.26, 2.20 (RP-HPLC-RT correlation, calculated, Finizio et al. 1991)
1.96 (Worthing & Hance 1991; Milne 1995)
2.00 (shake flask, pH 7, Baker et al. 1992)
1.94–2.26 (Montgomery 1993)
2.07 (RP-HPLC-RT correlation, Sicbaldi & Finizio 1993)
2.18 (recommended, Sangster 1993)
2.10 (Tomlin 1994)
2.18 (shake flask-UV, Liu & Qian 1995)
2.18 (recommended, Hansch et al. 1995)
2.51 (Pomona-database, Müller & Kördel 1996)
2.07 (RP-HPLC-RT correlation, Finizio et al. 1997)
1.83 (RP-HPLC-RT correlation, Nakamura et al. 2001)
1.49 (RP-HPLC-RT correlation using short ODP column, Donovan & Pescatore 2002)

Bioconcentration Factor, log BCF:
2.48 (calculated-S, Kenaga 1980)
0.778 (calculated-K_{OC}, Kenaga 1980)
2.16 (earthworms, Lord et al. 1980)
0.699 (calculated-K_{OW}, Briggs 1981)

Sorption Partition Coefficient, log K_{OC}:
2.13 (soil, Hamaker & Thompson 1972; Brown 1978; Kenaga 1980; Kenaga & Goring 1980)
3.34 (soil, calculated-S as per Kenaga & Goring 1980, Kenaga 1980)
2.15 (av. soils/sediments, Rao & Davidson 1980)
1.68 (20 ± 2°C, K_{OM} multiplied by 1.724, Briggs 1981)
2.33 (Georgia's Hickory Hill pond sediment, Brown & Flagg 1981)
3.66, 2.53, 1.77 (estimated-S, calculated-S and mp, estimated-K_{OW}, Karickhoff 1981)
2.14 (soil average, Jury et al. 1983)

2.20, 2.15 (selected, calculated-MCI χ, Gerstl & Helling 1987)
2.15 (screening model calculations, Jury et al. 1987a,b; Jury & Ghodrati 1989)
1.60–2.20 (Carsel 1989)
1.92 (estimated as log K_{OM}, Magee 1991)
2.13–3.34, 2.15, 2.45, 2.70 (soil, quoted values, Bottoni & Funari 1992)
2.11 (soil, 20–25°C, selected, Wauchope et al. 1991, Hornsby et al. 1996)
3.02 (average of 12 soils, calculated-linearize Freundlich Isotherm, Sukop & Cogger 1992)
2.14 (Montgomery 1993)
1.78 (soil, HPLC-screening method, mean value from different stationary and mobile phases, Kördel et al. 1993, 1995b)
2.37 (selected, Lohninger 1994)
2.01–2.58 (Tomlin 1994)
2.18 (calculated-K_{OW}, Liu & Qian 1995)
2.10 (soil, calculated-MCI $^1\chi$, Sabljic et al. 1995)
1.79; 2.17 (HPLC-screening method; calculated-PCKOC fragment method, Müller & Kördel 1996)
3.07, 1.65, 1.68, 1.61, 2.48 (soil, first generation Eurosoils ES-1, ES-2, ES-3, ES-4, ES-5, shake flask/batch equilibrium-HPLC/UV, Gawlik et al. 1998, 1999)
2.625, 1.90, 1.69, 1.66, 2.382 (soil, second generation Eurosoils ES-1, ES-2, ES-3, ES-4, ES-5, shake flask/batch equilibrium-HPLC/UV, Gawlik et al. 1999)
2.625, 1.901, 1.689, 1.656, 2.382 (soil, second generation Eurosoils ES-1, ES-2, ES-3, ES-4, ES-5, shake flask/batch equilibrium-HPLC/UV and HPLC-k′ correlation, Gawlik et al. 2000)
2.10; 2.10, 2.47 (soil, quoted obs.; estimated-class-specific model, estimated-general model using molecular descriptors, Gramatica et al. 2000)
2.29, 2.29, 2.29 (soils: organic carbon OC ≥ 0.1%, OC ≥ 0.5%, 0.1 ≤ OC < 0.5%, pH 3.2–8.0, average, Delle Site 2001)
2.50, 2.34, 2.10 (soils with organic carbon OC ≥ 0.5% at: pH 3.2–5.0, pH 5.1–5.9, pH ≥ 6.0, average, Delle Site 2001)

Environmental Fate Rate Constants, k, or Half-Lives, $t_{1/2}$:

Volatilization: $t_{1/2}$ = 276 d (Jury et al. 1983; quoted, Grover 1991); measured rate constant k = 600 d^{-1} and estimated rate constant k = 1000 d^{-1} (Glotfelty et al. 1989).

Photolysis:

Oxidation:

k(aq.) = 5.9×10^9 M^{-1} s^{-1} for the reaction (photo-Fenton with reference to acetophenone) with hydroxyl radical in aqueous solutions at pH 3.5 and 24 ± 1°C (Buxton et al. 1988; quoted, Faust & Hoigné 1990; Haag & Yao 1992)

k(aq.) = (4.8 ± 0.2) M^{-1} s^{-1} for direct reaction with ozone in water at pH 4.3 and 23°C, with $t_{1/2}$ = 1.9 h at pH 7 (Yao & Haag 1991).

k(aq.) = $(2.8 \pm 0.2) \times 10^9$ M^{-1} s^{-1} for the reaction (photo-Fenton with reference to acetophenone) with hydroxyl radical in aqueous solutions at pH 3.5 and 24 ± 1°C (Haag & Yao 1992).

Hydrolysis: calculated rate constant k = 8.32×10^{-6} s^{-1} with $t_{1/2}$ = 96 d at 20°C in a buffer at pH 5 (Burkhard & Guth 1981).

Biodegradation: rate constant k = 0.014 d^{-1} by soil incubation die-away studies (Rao & Davidson 1980; quoted, Scow 1982);

$t_{1/2}$ = 8–27 d for 3 μg mL^{-1} to biodegrade in pond sediment/water and $t_{1/2}$ > 32 d in pond water both at 25°C (Tucker & Boyd 1981; quoted, Muir 1991);

$t_{1/2}$ = 75 d for a 100 d leaching and screening test in 0–10 cm depth of soil (Rao & Davidson 1980; quoted, Jury et al. 1983, 1984, 1987a,b; Jury & Ghodrati 1989; Grover 1991);

microbial degradation $t_{1/2}$ = 70–11 d in soil (Tomlin 1994).

Biotransformation:

Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants:

Half-Lives in the Environment:

Air:

Surface water: $t_{1/2}$ > 32 d for 3 μg mL^{-1} to biodegrade in pond water at 25°C (Tucker & Boyd 1981; quoted, Muir 1991);

$t_{1/2}$ = 1–4 wk in estuarine systems (Jones et al. 1982; quoted, Meakins et al. 1994);

$t_{1/2}$ ~ 30 d in ponds (Herbicide Handbook 1989);

measured rate constant k = (4.8 ± 0.2) M^{-1} s^{-1} for direct reaction with ozone in water at pH 4.3 and 23°C, with $t_{1/2}$ = 1.9 h at pH 7 (Yao & Haag 1991).

Ground water: reported half-lives or persistence, $t_{1/2}$ = 15–75, 46–174 and 56 d (Bottoni & Funari 1992)

Sediment: $t_{1/2}$ = 8–27 d for 3 μg mL^{-1} to biodegrade in pond sediment/water at 25°C (Tucker & Boyd 1981; quoted, Muir 1991).

Soil: estimated persistence of 12 months (Kearney et al. 1969; Edwards 1973; quoted, Morrill et al. 1982; Jury et al. 1987a);

persistence of 12 months (Wauchope 1978);

estimated first-order $t_{1/2}$ = 49.5 d from biodegradation rate constant k = 0.014 d^{-1} by soil incubation die-away studies (Rao & Davidson 1980; quoted, Scow 1982);

$t_{1/2}$ = 45 d in Hatzenbühl soil at pH 4.8 and $t_{1/2}$ = 100 d in Neuhofen soil at pH 6.5 both at 22°C, respectively, under lab. conditions (Burkhard & Guth 1981; quoted, Montgomery 1993);

$t_{1/2}$ = 1–6 months (Jones et al. 1982; quoted, Meakins et al. 1994);

$t_{1/2}$ = 75 d from screening model calculations (Jury et al. 1987a,b; Jury & Ghodrati 1989);

moderately persistent in soils with $t_{1/2}$ = 20–100 d (Willis & McDowell 1982);

degradation rate constant k = (1.51 ± 0.086) × 10^{-2} d^{-1} with $t_{1/2}$ = 45.9 d in control soil and k = (1.76 ± 0.177) × 10^{-2} d^{-1} with $t_{1/2}$ = 39.4 d in pretreated soil in the field; k = (0.943 ± 0.047) × 10^{-2} d^{-1} with $t_{1/2}$ = 73.5 d in control soil and k = (0.864 ± 0.048) × 10^{-2} d^{-1} with $t_{1/2}$ = 80.2 d in pretreated soil once only in the laboratory (Walker & Welch 1991);

reported $t_{1/2}$ = 15–75 d, 46–174 d and 56 d; 29 d at 5°C and $t_{1/2}$ = 209 d at 30°C (Bottoni & Funari 1992);

selected field $t_{1/2}$ = 60 d (Wauchope et al. 1991, 1992; quoted, Dowd et al. 1993; Richards & Baker 1993; quoted, Halfon et al. 1996; Hornsby et al. 1996);

soil $t_{1/2}$ = 75 d (Pait et al. 1992);

degradation by microorganism in biometer systems: $t_{1/2}$ = 58 d in silty sand standard laboratory conditions, $t_{1/2}$ = 87 d for corrected standard conditions and $t_{1/2}$ = 91 d in simulated outdoor conditions; $t_{1/2}$ = 51 d in silty loam standard laboratory conditions, $t_{1/2}$ = 77 d corrected standard conditions, $t_{1/2}$ = 63 d in simulated outdoor conditions at constant soil moisture and 20°C. Degradation by microorganism in outdoor experiments in small lysimeter systems: $t_{1/2}$ = 32 d outdoor fallow, $t_{1/2}$ = 35 d outdoor barley in silty sand, and $t_{1/2}$ = 49 d outdoor fallow, $t_{1/2}$ = 53 d outdoor barley in silty loam (Rüdel et al. 1993)

$t_{1/2}$ = 49–50 d in 0–40 cm soil cores taken from: cultivated field; from meadow $t_{1/2}$ = 32–39 d and from gravel track $t_{1/2}$ = 62–51 d (Hassink et al. 1994);

degradation $t_{1/2}$ = 70–110 d (Tomlin 1994).

Biota: biochemical $t_{1/2}$ = 75 d from screening model calculations (Jury et al. 1987a,b; Jury & Ghodrati 1989).

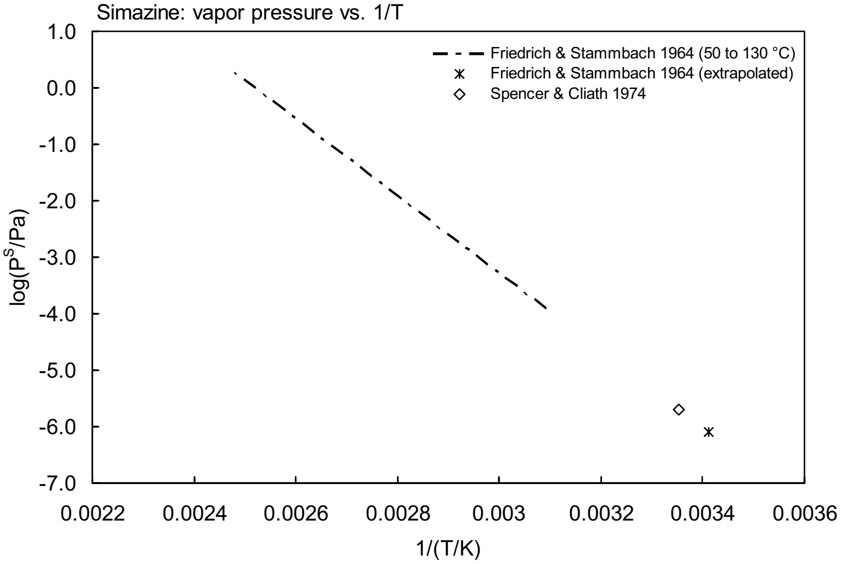
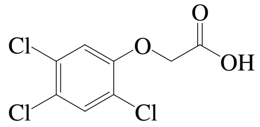


FIGURE 17.1.1.72.1 Logarithm of vapor pressure versus reciprocal temperature for simazine.

17.1.1.73 2,4,5-T



Common Name: 2,4,5-T

Synonym: Amine 2,4,5-T for rice, BCF-bushkiller, Brush rhap, Brush-Khap, Brushtox, Dacamine, Ded-Weed, Dinoxol, Envert-T, Estercide T-2 & T-245, Esterone 245, Fence rider, Forron, Fortex, Fruitone A, Gesatop, Inverton 245, Line rider, Phortox, Reddon, Reddox, Spontox, Super D Weedone, Tippon, Tormona, Transamine, Tributon, Trinoxol, Trioxone, Veon, Weddar, Weedone

Chemical Name: 2,4,5-trichlorophenoxyacetic acid

Uses: herbicide to control undesirable brush and woody plants; also used as plant hormone, defoliant.

CAS Registry No: 93-76-5

Molecular Formula: $C_8H_5Cl_3O_3$

Molecular Weight: 255.483

Melting Point (°C):

153	(Lide 2003)

Boiling Point (°C):

> 200	(dec., Howard 1991)

Density (g/cm^3 at 20°C):

1.80	(Ashton & Crafts 1981; Hartley & Kidd 1987; Montgomery 1993)
1.80	(25°C, Que Hee et al. 1981)
1.80	(Spencer 1982; Budavari 1989; Milne 1995)

Molar Volume (cm^3/mol):

226.1	(calculated-Le Bas method at normal boiling point)

Dissociation Constant pK_a:

2.88	(potentiometric titration, Nelson & Faust 1969)
2.85	(Cessna & Grover 1978; Somasundaram et al. 1991; Augustijn-Beckers et al. 1994)
2.70	(Haag & Yao 1992)
2.80–2.88	(Montgomery 1993)

Enthalpy of Vaporization, ΔH_V (kJ/mol):

107.8	(Rordorf 1989)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

34.936	(DSC method, Plato & Glasgow 1969)
34.2	(Rordorf 1989)

Entropy of Fusion, ΔS_{fus} (J/mol K):

Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F: 0.0555 (mp at 153°C)

Water Solubility (g/m^3 or mg/L at 25°C or as indicated):

268	(shake flask-UV, Leopold et al. 1960)
238	(20°C, Loos 1975)
238	(Martin & Worthing 1977)
238–280	(Weber et al. 1980)
238	(30°C, Ashton & Crafts 1981; Budavari 1989)
278	(Spencer 1982; Verschueren 1983)
278	(20°C, Hartley & Kidd 1987)
280	(selected, Gerstl & Helling 1987)
150	(Worthing & Walker 1987, Worthing & Hance 1991)
220	(20°C, Montgomery 1993)
278	(20–25°C, selected, Augustijn-Beckers et al. 1994)
238	(20°C, Milne 1995)

Vapor Pressure (Pa at 25°C or as indicated and reported temperature dependence equations):

0.0063 (effusion method, Hamaker & Kerlinger 1971)
$< 1.0 \times 10^{-6}$ (20°C, Hartley & Kidd 1983)
0.005 (20°C, selected, Suntio et al. 1988; Riederer 1990)
$< 1.0 \times 10^{-5}$ (20°C, Hartley & Kidd 1983; 1987)
2.30×10^{-6}, 1.90×10^{-4}, 8.50×10^{-3}, 0.230, 4.0 (25, 50, 70, 100, 125°C, gas saturation-GC, Rordorf 1989)
$\log (P_S/\text{Pa}) = 19.238 - 7418.9/(T/\text{K})$; measured range 80.4–145°C (solid, gas saturation-GC, Rordorf 1989)
$\log (P_L/\text{Pa}) = 15.058 - 5632.4/(T/\text{K})$; measured range 80.4–145°C (liquid, gas saturation-GC, Rordorf 1989)
7.00×10^{-7} (Worthing & Hance 1991)
0.0040 (20°C, Montgomery 1993)
0.0 (20–25°C at pH 7, selected, Augustijn-Beckers et al. 1994)

Henry's Law Constant (Pa·m^3/mol at 25°C or as indicated):

8.79×10^{-4} (Hine & Mookerjee 1975)
0.0058 (20°C, calculated-P/C, Suntio et al. 1988)
0.0049 (20°C, calculated-P/C, Montgomery 1993)

Octanol/Water Partition Coefficient, log K_{OW}:

3.13 (electrometric titration, Freese et al. 1979)
0.60 (pH dependent quoted from Dow Chemical data, Kenaga & Goring 1980)
0.85 (Rao & Davidson 1980)
2.99 (RP-HPLC-k′ correlation, Braumann et al. 1983)
3.13 (Hansch & Leo 1985)
3.40 (OECD 81 method, Kerler & Schönherr 1988)
3.36 (selected, Travis & Arms 1988)
3.31 (shake flask-HPLC/UV, Jafvert et al. 1990)
0.60–3.40 (Montgomery 1993)
3.13 (countercurrent LC, Ilchmann et al. 1993)
3.13 (selected, Sangster 1993)
3.13 (recommended, Hansch et al. 1995)
3.31 (LOGPSTAR or CLOGP data, Sabljic et al. 1995)

Bioconcentration Factor, log BCF:

–4.55 (milk biotransfer factor log B_m, correlated-K_{OW}, Bjerke et al. 1972)
1.18 (measured, Isensee 1976)
–4.82 (beef biotransfer factor log B_b, correlated-K_{OW}, Kenaga 1980)
1.63 (fish under flowing water conditions, Kenaga & Goring 1980)
1.45 (calculated-S, Kenaga 1980)
0.301 (calculated-K_{OC}, Kenaga 1980)
1.36–1.40 (fish under static ecosystem tests, Kenaga & Goring 1980; Garten & Tralbalka 1983)
1.41 (mosquito fish 32 d under unspecified conditions, Ang et al. 1989)

Sorption Partition Coefficient, log K_{OC}:

1.72 (soil, Hamaker & Thompson 1972; Kenaga 1980; Kenaga & Goring 1980; Sabljic 1987)
2.34 (soil, calculated-S as per Kenaga & Goring 1980, Kenaga 1980)
1.93, 2.27, 2,31, 2.31, 2.45, 2.31 (sand soil, whole soil, fine soil, coarse clay soil, medium silt soil, coarse silt soil, Nkedi-Kizza et al. 1983)
2.38 (calculated-MCI χ, Gerstl & Helling 1987)
1.90 (soil, screening model calculations, Jury 1987b)
1.72 (soil, Sabljic 1987)
1.77; 2.63; 1.94 (Alfisol soil, Podzol soil; sediment, von Oepen et al. 1991)
1.72, 2.27 (Montgomery 1993)
1.90 (20–25°C at pH 7, selected, Augustijn-Beckers et al. 1994)

1.72 (estimated-chemical structure, Lohninger 1994)
1.99 (soil, calculated-QSAR MCI $^1\chi$, Sabljic et al. 1995)
1.99 (1.63–2.35) (soils: organic carbon OC ≥ 0.5%, average, Delle Site 2001)

Environmental Fate Rate Constants, k, or Half-Lives, $t_{½}$:

Volatilization:

Photolysis: $t_{½}$ = 48 h for 17–80% of 1 μg/mL to degrade in buffered aqueous solution at pH 7.8 under sunlight (Crosby & Wong 1973; quoted, Cessna & Muir 1991);

$t_{½}$ = 15 d for < 2.6 μg/mL to degrade in distilled water under sunlight (Skurlatov et al. 1983; quoted, Cessna & Muir 1991);

$t_{½}$ = 8.7 d for < 2.6 μg/mL to degrade in aqueous fulvic acid solution (17 mg/L) and $t_{½}$ = 3.5 d for < 2.6 μg/mL to degrade in aqueous fulvic acid solution (55 mg/L) under sunlight (Skurlatov et al. 1983; quoted, Cessna & Muir 1991).

Oxidation:

photooxidation $t_{½}$ = 12.2–122 h in air, based on an estimated rate constant for the reaction with hydroxyl radical in the atmosphere (Atkinson 1987; quoted, Howard et al. 1991)

k(aq.) = (8.9 ± 1.3) $M^{-1}\ s^{-1}$ for direct reaction with ozone in water at pH 1.7–5.0 and 26°C, with $t_{½}$ = 1.0 h at pH 7 (Yao & Haag 1991)

$k_{OH\cdot}$(calc) = $4.0 \times 10^9\ M^{-1}\ s^{-1}$ for reaction with hydroxy radical in aqueous solutions (Haag & Yao 1992).

Hydrolysis: will not hydrolyze to any reasonable extent; however, it may undergo other abiotic transformation processes (Kollig 1993).

Biodegradation:

$t_{½}$(aerobic) = 27 d for 50 μg/mL in sediment-water microcosm by long lag phase degradation (Alexander 1974; quoted, Muir 1991)

$t_{½}$(aq. aerobic) = 240–480 h, based on unacclimated soil grab sample data (Smith 1978, 1979; quoted, Howard et al. 1991)

k = 0.001 d^{-1} by river die-away test in aquatic systems (Lee & Ryan 1979; quoted, Scow 1982)

k = 0.035 d^{-1} by soil incubation die-away studies (Rao & Davidson 1980; quoted, Scow 1982)

k = 0.01–0.03 d^{-1} at 9–21°C by river die-away test in slurry sediment of aquatic systems (Lee & Ryan 1979; quoted, Scow 1982)

$t_{½}$ = 33 d from screening model calculations (Jury et al. 1987b)

$t_{½}$(aq. anaerobic) = 672–4320 h, based on anaerobic digester sludge data (Battersby & Wilson 1989; quoted, Howard et al. 1991).

Biotransformation:

Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants:

Half-Lives in the Environment:

Air: $t_{½}$ = 12.2–122 h, based on an estimated rate constant for the vapor-phase reaction with hydroxyl radical in the atmosphere (Atkinson 1987; quoted, Howard et al. 1991).

Surface water: estimated first-order $t_{½}$ = 693 d from biodegradation rate constant k = 0.001 d^{-1} by river die-away test in aquatic systems (Lee & Ryan 1979; quoted, Scow 1982);

$t_{½}$ = 240–480 h, based on estimated unacclimated aqueous aerobic biodegradation half-life (Howard et al. 1991);

extremely resistant degradation in natural water with $t_{½}$ = 580 d for static sediment-sea water to $t_{½}$ = 1400 d for static estuarine river water (Muir 1991);

measured rate constant k = (8.9 ± 1.3) $M^{-1}\ s^{-1}$ for direct reaction with ozone in water at pH 1.7–5.0 and 21 ± 1°C, with $t_{½}$ = 3.9 h at pH 7 (Yao & Haag 1991).

Ground water: $t_{½}$ = 480–4320 h, based on estimated unacclimated aqueous aerobic and anaerobic biodegradation half-life (Howard et al. 1991).

Sediment: estimated first-order $t_{½}$ = 23–69.3 d from biodegradation rate constant k = 0.01–0.03 d^{-1} at 9–21°C by river die-away test in slurry sediment of aquatic systems (Lee & Ryan 1979; quoted, Scow 1982);

$t_{½}$ = 27 d for sediment-water microcosm under aerobic conditions (quoted, Muir 1991).

Soil: degradation $t_{½}$ = 24 d and 14 d in Quachita Highlands' forest and grassland soil, respectively, $t_{½}$ = 21 d in Gross Timbers Forest soil, average $t_{½}$ = 17 d in 3 soils (Altom & Stritzke 1973);

$t_{1/2}$ = 240–480 h, based on unacclimated soil grab sample data (Smith 1978, 1979; quoted, Howard et al. 1991);

estimated first-order $t_{1/2}$ = 19.8 d from rate constant k = 0.035 d^{-1} by soil incubation die-away studies (Rao & Davidson 1980; quoted, Scow 1982);

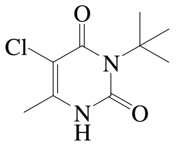
$t_{1/2}$ = 33 d from screening model calculations (Jury et al. 1987b);

aerobic degradation $t_{1/2}$ > 25 d at 29°C, to $t_{1/2}$ = 58 d at 21°C in soil suspension from pre-incubated soil (Muir 1991);

selected field $t_{1/2}$ = 30 d (Augustijn-Beckers et al. 1994).

Biota: biochemical $t_{1/2}$ = 33 d from screening model calculations (Jury et al. 1987b).

17.1.1.74 Terbacil



Common Name: Terbacil
Synonym: Sinbar, Turbacil
Chemical Name: 3-*tert*-butyl-5-chloro-6-methyluracil
CAS Registry No: 5902-51-2
Uses: control of most annual grasses and broadleaf weeds, and some perennial weeds in established apples, asparagus, blueberries, citrus, lucerne, mint, peaches, pecans, strawberries, and sugar cane, etc.
Molecular Formula: $C_9H_{13}ClN_2O_2$
Molecular Weight: 216.664
Melting Point (°C):

176	(Lide 2003)

Boiling Point (°C):
sublime(below mp, Hartley & Kidd 1987; Tomlin 1994)
Density (g/cm^3 at 20°C):

1.34	(25°C, Hartley & Kidd 1987; Montgomery 1993; Tomlin 1994)

Molar Volume (cm^3/mol):

217.7	(calculated-Le Bas method at normal boiling point)

Dissociation Constant pK_a:

9.0	(Wauchope et al. 1992)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
Entropy of Fusion, ΔS_{fus} (J/mol K):
Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F: 0.0330 (mp at 176°C)

0.027	(20°C, Suntio et al. 1988)

Water Solubility (g/m^3 or mg/L at 25°C or as indicated):

710	(Ashton & Crafts 1973; 1981; Spencer 1982)
710	(Martin & Worthing 1977; Hartley & Kidd 1987; Montgomery 1993; Tomlin 1994)
600	(20°C, selected, Suntio et al. 1988)
710	(20–25°C, selected, Wauchope et al. 1992; Hornsby et al. 1996)

Vapor Pressure (Pa at 25°C or as indicated):

6.40×10^{-5}	(29.5°C, Ashton & Crafts 1973; 1981)
6.00×10^{-5}	(30°C, Hartley & Kidd 1987)
5.00×10^{-5}	(20°C, selected, Suntio et al. 1988)
6.00×10^{-5}	(20°C, Montgomery 1993)
6.25×10^{-5}	(29.5°C, Tomlin 1994)
1.91×10^{-3}	(20–25°C, supercooled liquid value, quoted, Majewski & Capel 1995)
4.13×10^{-5}	(20–25°C, selected, Wauchope et al. 1992; Hornsby et al. 1996)

Henry's Law Constant (Pa·m^3/mol at 25°C or as indicated):

1.80×10^{-5}	(20°C, calculated-P/C, Suntio et al. 1988)
1.82×10^{-5}	(20–25°C, calculated, Montgomery 1993)
1.53×10^{-5}	(calculated-P/C, this work)

Octanol/Water Partition Coefficient, log K_{OW}:

1.89	(Karickhoff et al. 1979)
1.89	(Rao & Davidson 1980)

1.89, 1.90	(quoted, Montgomery 1993)
1.89	(recommended, Sangster 1993)
1.91	(Tomlin 1994)
1.89	(recommended, Hansch et al. 1995)

Bioconcentration Factor, log BCF:

1.18	(calculated-S, Kenaga 1980)
1.74	(Montgomery 1993)

Sorption Partition Coefficient, log K_{OC}:

1.71, 2.08	(soil: exptl., calculated, Kenaga 1980; Kenaga & Goring 1980)
1.62, 1.98	(soil, quoted, Madhun et al. 1986)
1.89, 1.76; 1.82, 1.04	(estimated-K_{OW}; solubilities, Madhun et al. 1986)
1.62	(soil, screening model calculations, Jury et al. 1987b)
1.74	(soil, Wauchope et al. 1992; Hornsby et al. 1996)
1.32–2.20	(soil, quoted, Montgomery 1993)
1.66	(soil, calculated-QSAR MCI $^1\chi$, Sabljic et al. 1995)
1.58 (1.38–1.78)	(soils: organic carbon OC $\geq$ 0.5%, average, Delle Site 2001)

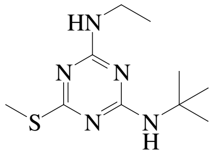
Environmental Fate Rate Constants, k, or Half-Lives, $t_{1/2}$:

Biodegradation: $t_{1/2}$ = 50 d (Jury et al. 1987b).

Half-Lives in the Environment:

Air:
Surface water:
Ground water:
Sediment:
Soil: moderately persistent in soil with $t_{1/2}$ = 20–100 d (Willis & McDowell 1982);
$t_{1/2}$ ~ 5–7 months (Hartley & Kidd 1987);
$t_{1/2}$ = 50 d from screening model calculations (Jury et al. 1987b);
field $t_{1/2}$ = 50–175 d and the selected $t_{1/2}$ = 120 d (Wauchope et al. 1992; Hornsby et al. 1996).
Biota: biochemical $t_{1/2}$ = 50 d (Jury et al. 1987b).

17.1.1.75 Terbutryn



Common Name: Terbutryn
Synonym: Clarosan, GS 14260, Igran, Prebane, Shortstop, Terbutrex, Terbutrin, Terbutryn
Chemical Name: *N*-(1,1-dimethylethyl)-*N*′-ethyl-6-(methylthio)-1,3,5-triazine-2,4-diamine; 2-(*tert*-butylamino)-4-(ethylamino)-6-(methylthio)-*s*-triazine
Uses: selective herbicide to control annual broadleaf and grass weeds in wheat.
CAS Registry No: 886-50-0
Molecular Formula: $C_{10}H_{19}N_5S$
Molecular Weight: 241.357
Melting Point (°C):

104	(Herbicide Handbook 1989, Lide 2003)

Boiling Point (°C):

154–160	(at 0.06 mmHg, Hartley & Kidd 1987; Worthing & Hance 1991; Montgomery 1993; Milne 1995)

Density (g/cm^3 at 20°C):

1.115	(Hartley & Kidd 1987; Worthing & Hance 1991; Montgomery 1993; Milne 1995)

Molar Volume (cm^3/mol):

273.8	(calculated-Le Bas method at normal boiling point)

Dissociation Constant:

4.30	(pK_a, Worthing & Hance 1991)
9.70	(pK_b, Wauchope et al. 1992; Hornsby et al. 1996)
4.07	(pK_a, Montgomery 1993)

Enthalpy of Vaporization, ΔH_V (kJ/mol):

101.4	(Rordorf 1989)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

22.4	(Rordorf 1989)

Entropy of Fusion, ΔS_{fus} (J/mol K):

59	(Rordorf 1989)

Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F: 0.168 (mp at 104°C)

Water Solubility (g/m^3 or mg/L at 25°C or as indicated):

25	(20°C, Weber 1972; Ashton & Crafts 1973, 1981)
58	(20°C, Quellette & King 1977)
25	(Martin & Worthing 1977; Worthing & Walker 1987, Worthing & Hance 1991; Herbicide Handbook 1978)
25	(shake flask-HPLC, Ellgehausen et al. 1981)
25	(20°C, Hartley & Kidd 1987; Herbicide Handbook 1989; Montgomery 1993)
22	(20–25°C, selected, Wauchope et al. 1992; Hornsby et al. 1996)

Vapor Pressure (Pa at 25°C or as indicated and reported temperature dependence equations):

0.00013	(20°C, Weber 1972; Worthing & Walker 1987; Worthing & Hance 1991)
0.00013	(20°C, Ashton & Crafts 1973; 1981)
0.00013	(20°C, Hartley & Kidd 1987; Herbicide Handbook 1989)

2.20×10^{-4}, 9.10×10^{-3}, 0.22, 3.40, 38.0 (25, 50, 70, 100, 125°C, gas saturation-GC, Rordorf 1989)
$\log (P_S/Pa) = 17.151 - 6201.4/(T/K)$; measured range 45–100°C (solid, gas saturation-GC, Rordorf 1989)
$\log (P_L/Pa) = 14.654 - 5297.1/(T/K)$; measured range 109–139°C (liquid, gas saturation-GC, Rordorf 1989)

0.00128 (20°C, Montgomery 1993)
0.00028 (20–25°C, selected, Wauchope et al. 1992; Hornsby et al. 1996)

Henry's Law Constant (Pa·m^3/mol at 25°C or as indicated):
0.0013 (20°C, calculated-P/C, Suntio et al. 1988)
0.0012 (20°C, calculated-P/C, Muir 1991)
0.0120 (20°C, calculated-P/C, Montgomery 1993)
0.0014 (calculated-P/C, this work)

Octanol/Water Partition Coefficient, log K_{OW}:
3.74 (shake flask-GC, Elkell & Walum 1979)
3.72, 3.74 (shake flask, Ellgehausen et al. 1981)
2.56 (RP-HPLC-k′ correlation, Braumann et al. 1983)
3.34 (Worthing & Walker 1987)
3.43 (RP-HPLC-RT correlation, Finizio et al. 1991)
3.49 (Worthing & Hance 1991; Milne 1995)
3.43–3.73 (Montgomery 1993)
3.34 (RP-HPLC-RT correlation, Sicbaldi & Finizio 1993)
3.74 (recommended, Sangster 1993)
3.38, 3.36 (shake flask-UV, calculated-RP-HPLC-k′ correlation, Liu & Qian 1995)
3.74 (recommended, Hansch et al. 1995)
3.44 (Pomona-database, Müller & Kördel 1996)
3.34 (RP-HPLC-RT correlation, Finizio et al. 1997)

Bioconcentration Factor, log BCF:
1.17 (*Daphnia magna*, wet wt. basis, Ellgehausen et al. 1980)
2.00, 2.00 (calculated-S, calculated-K_{OC}, Kenaga 1980)
1.95 (catfish *Ictalurus melas*, wet wt basis, Wang et al. 1996)

Sorption Partition Coefficient, log K_{OC}:
2.85 (soil, Colbert et al. 1975; Gaillardon et al. 1977;, Kenaga 1980; Kenaga & Goring 1980)
2.87 (soil, calculated-S as per Kenaga & Goring 1980, Kenaga 1980)
2.85–2.87 (soil, quoted values, Bottoni & Funari 1992)
3.30 (soil, 20–25°C, selected, Wauchope et al. 1992; Hornsby et al. 1996)
2.68 (soil, HPLC-screening method, mean value from different stationary and mobile phases, Kördel et al. 1993, 1995b)
3.21–4.07 (Montgomery 1993)
3.30 (estimated-chemical structure, Lohninger 1994)
2.84 (calculated-K_{OW}, Liu & Qian 1995)
2.85 (soil, calculated-MCI $^1\chi$, Sabljic et al. 1995)
2.68; 2.80 (HPLC-screening method; calculated-PCKOC fragment method, Müller & Kördel 1996)
4.62, 2.57, 2.90, 1.56, 3.55 soil, first generation Eurosoils ES-1, ES-2, ES-3, ES-4, ES-5, shake flask/batch equilibrium-HPLC/UV, Gawlik et al. 1998)
3.554, 2.878, 2.778, 2.505, 3.054 (soil, second generation Eurosoils ES-1, ES-2, ES-3, ES-4, ES-5, shake flask/batch equilibrium-HPLC/UV and HPLC-k′ correlation, Gawlik et al. 2000)
2.85; 2.82, 2.74 (soil, quoted obs.; estimated-class-specific model, estimated-general model using molecular descriptors, Gramatica et al. 2000)
3.79 (3.28–4.30) (soil: organic carbon OC $\geq$ 0.5%, average, Delle Site 2001)
2.59, 2.86 (Kishon river sediments, sorption isotherm, Chefetz et al. 2004)

Environmental Fate Rate Constants, k, or Half-Lives, $t_{1/2}$:
Volatilization:
Photolysis: 4 ppb contaminated water in the presence of TiO_2 and H_2O_2 completely photodegraded after 15 h by solar irradiation (Muszkat et al. 1992).
Oxidation:

Hydrolysis:

Biodegradation: aerobic $t_{½}$ = 80–240 d for 1 µg/mL to biodegrade in sediment-water and anaerobic $t_{½}$ > 650 d for 1 µg/mL to biodegrade in sediment-water both at 25°C (Muir & Yarechewski 1982; quoted, Muir 1991).

biological degradation rate followed a first order kinetics, with $t_{½}$ = 8.9–18.2 d by raw water microflora from Rivere Nile, $t_{½}$ = 4.0–6.9 d by raw water microflora + sewage (El-Dib & Abou-Waly 1998)

Biotransformation:

Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants:

k_1 = 1.70 h^{-1} (*Chironomus tentans* larvae in pond sediment-water system, 96-h exposure, calculated by using first-order kinetic and concn factors, Muir et al. 1983)

k_1 = 1.9–1.5 h^{-1} (*Chironomus tentans* larvae in river sediment-water system, 96-h exposure, calculated by using first-order kinetic and concn factors, Muir et al. 1983)

k_1 = 3.6–2.7 h^{-1} (*Chironomus tentans* larvae in sediment (sand)-water system, 96-h exposure, calculated by using first-order kinetic and concn factors, Muir et al. 1983)

k_1 = 3.6–4.4 h^{-1} (*Chironomus tentans* larvae in sediment (sand)-water system, 96-h exposure, calculated by using initial uptake data of 0–12 h, Muir et al. 1983)

k_2 = 0.053 h^{-1} (*Chironomus tentans* larvae in pond sediment-water system, calculated by initial uptake data of 0–12 h, Muir et al. 1983)

k_2 = 0.043 h^{-1} (*Chironomus tentans* larvae in river water system, calculated by concentration decay curve, Muir et al. 1983)

k_2 = 0.040 h^{-1} (*Chironomus tentans* larvae in river sediment-water system, calculated by concentration decay curve, Muir et al. 1983)

k_2 = 0.040 h^{-1} (*Chironomus tentans* larvae in sediment (sand)-water system, calculated by concentration decay curve, Muir et al. 1983)

k_1 = 3.11 h^{-1}, k_2 = 0.0346 h^{-1} (catfish *Ictalurus melas*, Wang et al. 1996)

Half-Lives in the Environment:

Air:

Surface water: $t_{½}$ = 8.9–18.2 d by raw water microflora from River Nile, $t_{½}$ = 4.0–6.9 d by raw water microflora + sewage (El-Dib & Abou-Waly 1998)

Ground water: reported half-lives or persistence, $t_{½}$ = 14–28 d (Bottoni & Funari 1992)

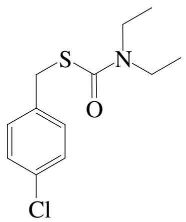
Sediment: aerobic $t_{½}$ = 80–240 d for 1 µg mL^{-1} to biodegrade in sediment-water and anaerobic $t_{½}$ > 650 d for 1 µg mL^{-1} to biodegrade in sediment-water both at 25°C (Muir & Yarechewski 1982; quoted, Muir 1991).

Soil: reported $t_{½}$ = 14–28 d (Worthing & Hance 1991; Bottoni & Funari 1992);

$t_{½}$ ~ 42 d (estimated, Wauchope et al. 1992; Hornsby et al. 1996).

Biota: elimination $t_{½}$ = 13.1 h in pond sediment-water, $t_{½}$ = 16.1 h in river water, $t_{½}$ = 17.3 h in river sediment-water, $t_{½}$ = 17.3 in sand-water systems (*Chironomus tentans* larvae, Muir et al. 1983)

17.1.1.76 Thiobencarb



Common Name: Thiobencarb
Synonym: benthiocarb, Bolero, Saturn, Saturno, Siacarb
Chemical Name: *S*-(4-chlorophenyl)methyl diethylcarbamothioate
Pesticide Class: herbicide; Group: carbamate
Uses: herbicide
CAS Registry No: 28249-77-6
Molecular Formula: $C_{12}H_{16}ClNOS$
Molecular Weight: 257.779
Melting Point (°C):
1.7 (Lide 2003)
Boiling Point (°C):
126–129/0.008 mmHg (Ashton & Crafts 1981)
126–128/0.008 mmHg (Spencer 1982; Hartley & Kidd 1987; Herbicide Handbook 1989)
Density (g/cm^3 at 20°C):
1.148–1.180 (Spencer 1982; Hartley & Kidd 1987; Herbicide Handbook 1989)
Molar Volume (cm^3/mol):
Dissociation Constant pK$_a$:
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
Entropy of Fusion, ΔS_{fus} (J/mol K):
Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F: 1.0

Water Solubility (g/m^3 or mg/L at 25°C or as indicated):
30 (Ashton & Crafts 1981)
30 (reported as 30 g/L, Spencer 1982)
30 (20°C, Hartley & Kidd 1987; Herbicide Handbook 1989)
28 (20–25°C, recommended, Wauchope et al. 1992; Hornsby et al. 1996)
17.0 (Majewski & Capel 1995)

Vapor Pressure (Pa at 25°C or as indicated):
1.96×10^{-4} (20°C, Ashton & Crafts 1981)
4.21×10^{-3} (20°C, GC-RT correlation, Kim 1985)
2.0×10^{-4} (20°C, Hartley & Kidd 1987)
1.97×10^{-4} (Herbicide Handbook 1989)
2.93×10^{-3} (20–25°C, selected, Wauchope et al. 1992; Hornsby et al. 1996)
1.78×10^{-3} (Majewski & Capel 1995)

Henry's Law Constant (Pa·m^3/mol at 25°C):
0.027 (calculated-P/C, Majewski & Capel 1995)
0.0274 (quoted lit., Armbrust 2000)

Octanol/Water Partition Coefficient, log K_{OW}:
3.42 (20°C, shake flask-GC, Kanazawa 1981)
3.40 (shake flask-GC, Schimmel et al. 1983)
3.98 (HPLC-RT correlation, Kawamoto & Urano 1989)
3.42 (Gerstl 1990)

3.40 (recommended, Sangster 1993)
3.93 (HPLC-RT correlation, Scibaldi & Finizio 1993)
3.40 (LOGPSTAR or CLOGP data, Sabljic et al. 1995)
3.78 (RP-HPLC-RT correlation, Yu et al. 1997)
4.37 (RP-HPLC-RT correlation, Nakamura et al. 2001)

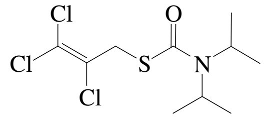
Bioconcentration Factor, log BCF or log K_B:
2.97 (Pait et al. 1992)
1.76, 1.77 (37.2, 18.6 μg/L concn in water; carp, 3–5 d exposure, Wang et al. 1992)
1.38, 1.0 (20.0, 2.0 μg/L concn in water; tilapia, 3–5 d exposure, Wang et al. 1992)
1.49, 1.13 (20.0, 2.0 μg/L concn in water; loach, 3–5 d exposure, Wang et al. 1992)
0.92, 1.08 (15.0, 7.5 μg/L concn in water; Grass carp, 3–5 d exposure, Wang et al. 1992)
1.20, 1.26 (10.0, 5.0 μg/L concn in water; eel, 3–5 d exposure, Wang et al. 1992)
2.57, 1.94 (5.0, 1.4 μg/L concn in water; black silver carp, 3–5 d exposure, Wang et al. 1992)
0.46, 0.86 (200, 20 μg/L concn in water; freshwater clam, 3v5 d exposure, Wang et al. 1992)
1.82; 2.23 (*Gnathopogon aerulescens; Pseudorasbora parva*, flow-through condition, quoted, Devillers et al. 1996)

Sorption Partition Coefficient, log K_{OC}:
2.83 (soil, Gerstl 1990)
2,49, 3.02, 2.83 (soil, Bottoni & Funari 1992)
2.95 (soil, Wauchope et al. 1992; Hornsby et al. 1996)
3.43 (soil, calculated-χ, Meylan et al. 1992)
3.27 (calculated-QSAR MCI $^1\chi$, Sabljic et al. 1995)
2.95 (quoted lit., Armbrust 2000)
3.32, 2.75 (soil, estimated-class-specific model, estimated-general model using molecular descriptors, Gramatica et al. 2000)

Environmental Fate Rate Constants or Half-Lives, $t_{1/2}$:
Volatilization:
Photolysis:
Oxidation:
Hydrolysis: stable aqueous hydrolysis rates at pH 5, 7, 9; measured hydroxy radical rate constant $k = 6.8 \times 10^{12}$ M^{-1}/h (Armbrust 2000)
Biodegradation: $t_{1/2}$ = 2–3 wk in soil varies under aerobic conditions to $t_{1/2}$ = 6–8 months under anaerobic conditions (Hartley & Kidd 1987; Herbicide Handbook 1989)
aerobic degradation rate constant $k = 0.057\ d^{-1}$ with $t_{1/2}$ = 12 d by aerobic activated sludge at 20°C (Kawamoto & Urano 1990)
aerobic rate constant, $k = 1.38 \times 10^{-3}\ h^{-1}$ (Armbrust 2000).
Biotransformation:
Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants:

Half-Lives in the Environment:
Air:
Surface water: lost from aqueous solution by volatility and photodegradation (Herbicide Handbook 1989)
biodegradation $t_{1/2}$ = 12 d by aerobic activated sludge at 20°C (Kawamoto & Urano 1990).
Ground water: reported half-lives or persistence, $t_{1/2}$ = 6–7, 23–120, and 26–40 d (Bottoni & Funari 1992)
Sediment:
Soil: laboratory studies with Stockton adobe and Crowley silty clay loam gave $t_{1/2}$ = 2–3 wk under aerobic conditions to $t_{1/2}$ = 6–8 months under anaerobic conditions (Hartley & Kidd 1987; Herbicide Handbook 1989);
reported half-lives or persistence of 6–7 d, 23–120 d, 26–40 d (Bottoni & Funari 1992);
soil; $t_{1/2}$ = 18 d (Pait et al. 1992);
field $t_{1/2}$ = 21 d (Wauchope et al. 1992; Hornsby et al. 1996).
Biota:

17.1.1.77 Triallate



Common Name: Triallate
Synonym: Avadex BW, Buckle, CP 23426, Dipthal, Far-Go
Chemical Name: 2,3,3-trichloro-2-propene-1-thiol diisopropylcarbamate; *S*-(2,3,3-trichloro-allyl)diisopropyl-(thio-carbamate); *S*-(2,3,3-trichloro-2-propenyl) bis(1-methylethyl)-carbamothioate
Uses: herbicide to control wild oats in lentils, barley, peas, and winter wheat.
CAS Registry No: 2303-17-5
Molecular Formula: $C_{10}H_{16}Cl_3NOS$
Molecular Weight: 304.664
Melting Point (°C):
 29 (Lide 2003)
Boiling Point (°C):
 148–149 (Khan 1980; Spencer 1982)
 117 (at 40 mPa, Herbicide Handbook 1989: Montgomery 1993; Milne 1995)
Density (g/cm^3 at 20°C):
 1.273 (25°C, Hartley & Kidd 1987; Herbicide Handbook 1989; Worthing & Hance 1991; Montgomery 1993; Tomlin 1994; Milne 1995)
Molar Volume (cm^3/mol):
 314.0 (calculated-Le Bas method at normal boiling point)
Dissociation Constant pK_a:
Enthalpy of Vaporization, ΔH_V (kJ/mol):
 85.86 (Rordorf 1989)
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
 27.7 (Rordorf 1989)
Entropy of Fusion, ΔS_{fus} (J/mol K):
Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F: 0.914 (mp at 29°C)

Water Solubility (g/m^3 or mg/L at 25°C or as indicated):
 4.0 (20°C, Weber 1972; Weber et al. 1980)
 4.0 (Ashton & Crafts 1973; Spencer 1973, 1982; Khan 1980)
 4.0 (Martin & Worthing 1977, Worthing & Walker 1983, 1987; Worthing & Hance 1991; Herbicide Handbook 1978, 1989)
 4.0 (Hartley & Graham-Bryce 1980; Hartley & Kidd 1987; Montgomery 1993; Tomlin 1994; Milne 1995)
 < 1.0 (27°C, Ashton & Crafts 1981)
 3.0 (20°C, selected, Suntio et al. 1988)
 4.0 (20–25°C, selected, Wauchope et al. 1992; Hornsby et al. 1996)

Vapor Pressure (Pa at 25°C or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):
 0.016 (20°C, Weber 1972; Worthing & Walker 1987)
 0.016 (Ashton & Crafts 1973; Spencer 1982; quoted, Suntio et al. 1988)
 0.0276* (gas saturation-GC, measured range 20–45°C, Grover et al. 1978)
 log (P/mmHg) = 11.045 – 4401/(T/K); temp range 20–45°C (Antoine eq., gas saturation-GC, Grover et al. 1978)
 0.0265 (29.5°C, Ashton & Crafts 1981)
 0.0276 (gas saturation method, Spencer & Cliath 1983)
 6.07×10^{-3}, 4.81×10^{-3} (20°C, GC-RT correlation, GC-RT correlation with mp correction, Kim 1985)
 0.016 (Hartley & Kidd 1987; Worthing & Hance 1991; Tomlin 1994)
 0.010 (20°C, selected, Suntio et al. 1988; quoted, Majewski & Capel 1995)

0.015	(Herbicide Handbook 1989)
0.017*	(gas saturation-GC, measured range 25–125°C, Rordorf 1989)

log (P_S/Pa) = 18.124 – 5932/(T/K); measured range 32.3–150°C (solid, gas saturation-GC, Rordorf 1989)

log (P_L/Pa) = 13.395 – 4485.1/(T/K); measured range 32.3–150°C (liquid, gas saturation-GC, Rordorf 1989)

0.026	(selected, Taylor & Spencer 1990)
0.0147	(20–25°C, selected, Wauchope et al. 1992; Hornsby et al. 1996)
0.016	(20°C, Montgomery 1993)

Henry's Law Constant (Pa·m^3/mol at 25°C or as indicated):

1.96	(calculated-P/C, Jury et al. 1983, 1984, 1987a, 1990; Jury & Ghodrati 1989)
1.02	(20°C, calculated-P/C, Suntio et al. 1988)
1.983	(calculated-P/C, Taylor & Glotfelty 1988)
1.226	(20°C, calculated-P/C, Muir 1991)
1.013	(20–25°C, calculated-P/C, Montgomery 1993)
0.762	(calculated-P/C, this work)

Octanol/Water Partition Coefficient, log K_{OW}:

4.29	(Montgomery 1993)
4.53	(LOGPSTAR or CLOGP data, Sabljic et al. 1995)

Bioconcentration Factor, log BCF:

2.45	(calculated-S, Kenaga 1980; quoted, Isensee 1991)
2.18	(calculated-K_{OC}, Kenaga 1980)

Sorption Partition Coefficient, log K_{OC}:

3.56	(Guenzi & Beard 1974)
3.34	(soil, Grover 1974; Beestman & Demming 1976)
3.32	(soil, calculated-S as per Kenaga & Goring 1980, Kenaga 1980)
3.56	(soil, screening model calculations, Jury et al. 1987a,b; Jury & Ghodrati 1989)
3.22	(soil, calculated-MCI χ and fragments contribution, Meylan et al. 1992)
3.38	(soil, 20–25°C, selected, Wauchope et al. 1992; Hornsby et al. 1996)
3.31	(calculated, Montgomery 1993)
3.38	(selected, Lohninger 1994)
3.35	(soil, calculated-MCI $^1\chi$, Sabljic et al. 1995)
3.60, 3.12	(soil, estimated-class-specific model, estimated-general model using molecular descriptors, Gramatica et al. 2000)
2.70, 2.64	(soils: organic carbon OC ≥ 0.1%, OC ≥ 0.5%, average, Delle Site 2001)

Environmental Fate Rate Constants, k, or Half-Lives, $t_{1/2}$:

Volatilization: $t_{1/2}$ = 26 d (Jury et al. 1983; quoted, Grover 1991); half-life of 100 d (Jury et al. 1984; quoted, Spencer & Cliath 1990);

estimated $t_{1/2}$ ~ 8 d from 1 m depth of water at 20°C (Muir 1991).

Photolysis:

Oxidation: calculated lifetime of 5 h for the vapor-phase reaction with OH radicals in the troposphere (Atkinson et al. 1992; Kwok et al. 1992).

Hydrolysis: $t_{1/2}$ > 24 wk for 1 μg/mL to hydrolyze in aqueous buffer at pH 4, 7, and 9 in the dark at 25°C (Smith 1969; quoted, Muir 1991).

Biodegradation: estimated $t_{1/2}$ = 680 d at pH 6.8 and $t_{1/2}$ = 1170 d at pH 7.0, both at 25°C from biodegradation rate constants in aquatic systems (Smith 1969; quoted, Scow 1982);

$t_{1/2}$ = 100 d for a 100 d leaching and screening test in 0–10 cm depth of soil (Jury et al. 1983, 1984, 1987a,b; 1990; Jury & Ghodrati 1989; Grover 1991).

Biotransformation:

Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants:

Half-Lives in the Environment:

Air: calculated life-time of 5 h for the vapor-phase reaction with OH radicals in the troposphere (Atkinson et al. 1992; Kwok et al. 1992).

Surface water: $t_{1/2}$ = 680 d at pH 6.8 and $t_{1/2}$ = 1170 d at pH 7.0, both at 25°C for biodegradation in aquatic systems (Smith 1969; quoted, Scow 1982).

Ground water:

Sediment:

Soil: biodegradation $t_{1/2}$ = 100 d from screening model calculations (Jury et al. 1984, 1987a,b; 1990; Jury & Ghodrati 1989; quoted, Montgomery 1993);

selected field $t_{1/2}$ = 82 d (Wauchope et al. 1992; Hornsby et al. 1996).

Biota: biochemical $t_{1/2}$ = 100 d from screening model calculations (Jury et al. 1987a,b; Jury & Ghodrati 1989).

TABLE 17.1.1.77.1
Reported vapor pressures of triallate at various temperatures and the coefficients for the vapor pressure equations

$\log P = A - B/(T/K)$ (1) $\ln P = A - B/(T/K)$ (1a)

$\log P = A - B/(C + t/°C)$ (2) $\ln P = A - B/(C + t/°C)$ (2a)

$\log P = A - B/(C + T/K)$ (3)

$\log P = A - B/(T/K) - C \cdot \log (T/K)$ (4)

Grover et al. 1978		Rordorf 1989	
gas saturation method-GC		gas saturation-GC	
t/°C	P/Pa	t/°C	P/Pa
20	0.0133	25	0.017
23	0.0202	50	0.59
25	0.0276	75	12.0
30	0.0446	100	170
35	0.0704	125	1700
40	0.131		for solid
45	0.267	eq. 1	P_S/Pa
		A	18.124
eq. 1	P/mmHg	B	5932
A	11.045		for liquid
B	4401	eq. 1	P_L/Pa
		A	13.395
mp/°C	33–33.5°C	B	4485.1

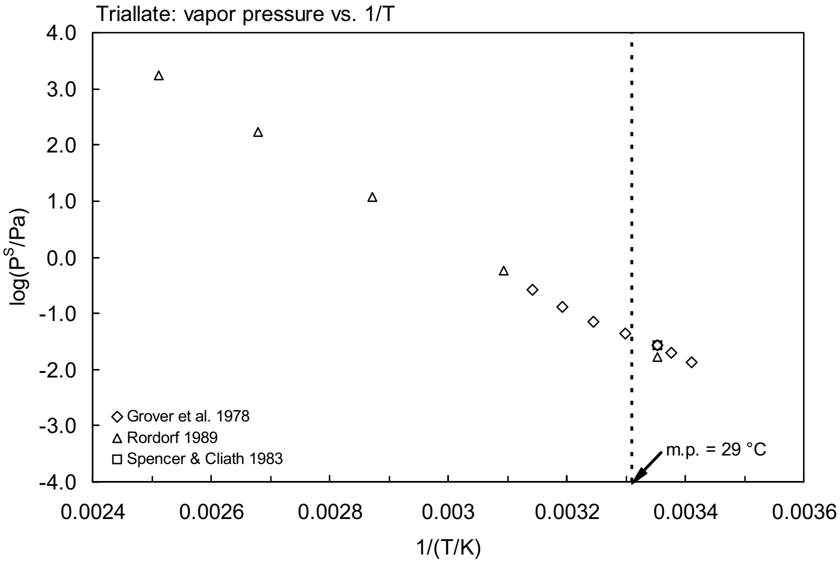
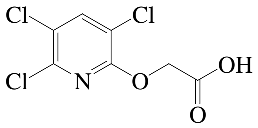


FIGURE 17.1.1.77.1 Logarithm of vapor pressure versus reciprocal temperature for triallate.

17.1.1.78 Triclopyr



Common Name: Triclopyr
Synonym: Garlon, Truflon, Crossbow
Chemical Name: 3,5,6-trichloro-2-pyridinyloxyacetic acid
CAS Registry No: 56335-06-3
Uses: herbicide
Molecular Formula: $C_7H_4Cl_3NO_3$
Molecular Weight: 256.471
Melting Point (°C):
  148–150 (Spencer 1982; Hartley & Kidd 1987; Worthing & Walker 1987)
  150.5 (Tomlin 1994)
Boiling Point (°C):
  290 (dec., Hartley & Kidd 1987; Tomlin 1994)
Density (g/cm^3 at 20°C):
Dissociation Constant pK_a:
  2.68 (Spencer 1982; Worthing & Walker 1987)
  2.93 (Woodburn et al. 1993)
  3.97 (Tomlin 1994)
Enthalpy of Vaporization, ΔH_V (kJ/mol):
  102.5 (Rordorf 1989)
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
  31.8 (Rordorf 1989)
Entropy of Fusion, ΔS_{fus} (J/mol K):
Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F:

Water Solubility (g/m^3 or mg/L at 25°C or as indicated):
  430 (Kenaga 1980a,b)
  440 (Spencer 1982; Hartley & Kidd 1987; Worthing & Walker 1987)
  408 (20°C, Tomlin 1994)
  7690, 8100, 8220 (20°C, at pH 5, 7, and 9, Tomlin 1994)
  7618 (20–25°C, quoted as 2.97E + 01 mol/m^3, Majewski & Capel 1995)

Vapor Pressure (Pa at 25°C or as indicated and reported temperature dependence equations):
  1.6×10^{-4} (Spencer 1982)
  1.68×10^{-4} (Worthing & Walker 1987; Hartley & Kidd 1987; Tomlin 1994)
  1.90×10^{-5}, 1.0×10^{-3}, 0.031, 0.59, 7.80 (25, 50, 70, 100, 125°C, gas saturation-GC, Rordorf 1989)
  $\log (P_S/Pa) = 17.65 - 6672.3/(T/K)$; measured range 85.4–145°C (gas saturation-GC, Rordorf 1989)
  $\log (P_L/Pa) = 14.445 - 5354.8/(T/K)$; measured range 150–186°C (gas saturation-GC, Rordorf 1989)
  2.0×10^{-4} (vapor pressure balance, Tomlin 1994)
  2.91×10^{-3} (20–25°C, Majewski & Capel 1995)

Henry's Law Constant ($Pa \cdot m^3/mol$ at 25°C or as indicated):
  9.79×10^{-5} (20–25°C, calculated-P/C, Majewski & Capel 1995)

Octanol/Water Partition Coefficient, log K_{OW}:
  –0.52 (Kenaga 1980a)
  0.42, –0.45, –0.96 (pH 5, 7, and 9, Tomlin 1994)
  1.30 (Isensee 1991)
  2.53 (LOGPSTAR or CLOGP data, Sabljic et al. 1995)

Octanol/Air Partition Coefficient, log K_{OA}:

Bioconcentration Factor, log BCF or log K_B:

1.49, –0.22	(fish: flowing water tests, static ecosystem tests, Kenaga 1980a)
1.30, 0	(fish: calculated-solubility, K_{OW}, Kenaga 1980b)

Sorption Partition Coefficient, log K_{OC}:

1.43	(soil, Kenaga 1980a)
1.43, 2.204	(soil: quoted, calculated, Kenaga 1980b)
1.43, 2.20	(soil, Bottoni & Funari 1992)
1.43	(quoted or calculated-MCI $^1\chi$, Sabljic et al. 1995)

Environmental Fate Rate Constants, k, or Half-Lives, $t_{½}$:

Volatilization:

Photolysis: photolysis $t_{½} < 0.4$ d in sterile, pH 5-buffered water at 40°N latitude in midday, midsummer (McCall & Gavit 1986);

photodecomposition $t_{½} < 12$ h (Worthing 1987; Tomlin 1994);

photodecomposition $t_{½} < 24$ h (Hartley & Kidd 1987);

aqueous photolysis pseudo-first order $t_{½}$(average) = 0.5 and 1.3 d in pH 7-buffered water and natural river water, respectively, at 25°C under artificial lights and midsummer sunlight, 40°N latitude (Woodburn et al. 1993);

aqueous photolysis rate constant, $k = 8.3 \times 10^{-2}\ h^{-1}$ (Armbrust 2000).

Oxidation:

Hydrolysis: hydrolysis $t_{½} > 3$ months in darkened, sterile, buffered water at pH of 5–9 and 25°C (Woodburn et al. 1993);

stable aqueous hydrolysis rates at pH 5, 7, 9; measured hydroxy radical rate constant $k = 4.3 \times 10^{12}\ M^{-1}\cdot h^{-1}$ (Armbrust 2000).

Biodegradation: in soil, fairly rapid degradation by microbial activity, with an average $t_{½} = 46$ d depending on soil and climatic conditions (Spencer 1982; Tomlin 1994);

aerobic rate constant, $k = 9.03 \times 10^{-4}\ h^{-1}$ (Armbrust 2000).

Biotransformation:

Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants:

Half-Lives in the Environment:

Air:

Surface water: stable to hydrolysis, but subject to photolysis with $t_{½} < 12$ h (Spencer 1982; Worthing 1987; Tomlin 1994);

photolysis $t_{½} < 0.4$ d in sterile, pH 5 buffered water at 40°N latitude (McCall & Gavit 1986);

$t_{½} \sim 3$ to 4 d in natural water during summer conditions (Solomon et al. 1988);

pseudo-first order photolysis $t_{½}$(ave.) = 0.5 and 1.3 d in pH-buffered water and natural river water, respectively; the photodegradation pseudo-first-order half-lives in sterile, pH 7 water, midsummer sunlight at 40°N latitude and 25°C calculated as k = 0.36 (0.33–0.39) and 0.60 (0.50–0.70) d under artificial and natural sunlight, respectively; $t_{½} = 0.71$ (0.70–0.73) and 1.86 (1.77–1.96) d in river water under artificial and natural sunlight conditions, respectively, in midsummer sunlight and approximately 40°N latitude and 25°C (Woodburn et al. 1993);

photodecomposition $t_{½} < 24$ h (Hartley & Kidd 1987).

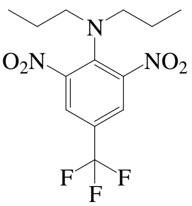
Ground water: reported half-lives or persistence, $t_{½} = 40$ and 46 d (Bottoni & Funari 1992).

Sediment:

Soil: fairly rapid degradation by microbial activity, with an average $t_{½} = 46$ d depending on soil and climatic conditions (Spencer 1982; Tomlin 1994);

Biota:

17.1.1.79 Trifluralin



Common Name: Trifluralin

Synonym: Agreflan, Crisalin, Digermin, Elancolan, L-36352, Nitran, Nitrofor, Olitref, Treflan, Trifluoramine, Trifurex, Trikepin, Trim

Chemical Name: 2,6-dinitro-*N,N*-dipropyl-4-trifluoromethylaniline; 2,6-dinitro-*N,N*-dipropyl-4-(trifluoromethyl)-benzenamine

Uses: pre-emergence herbicide to control many grass and broadleaf weeds.

CAS Registry No: 1582-09-8

Molecular Formula: $C_{13}H_{16}F_3N_3O_4$

Molecular Weight: 335.279

Melting Point (°C):
49 (Lide 2003)

Boiling Point (°C):
362 (estimated, Grain 1982)
139–140 (at 4.2 mmHg, Hartley & Kidd 1987; Montgomery 1993; Milne 1995)
96–97 (at 0.18 mmHg, Herbicide Handbook 1989)

Density (g/cm^3 at 20°C):
1.294 (25°C, Montgomery 1993)
1.36 (22°C, Tomlin 1994)

Molar Volume (cm^3/mol):
295.9 (calculated-Le Bas method at normal boiling point)

Dissociation Constant pK_a:

Enthalpy of Vaporization, ΔH_V (kJ/mol):
8754 (Rordorf 1989)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
23.85 (DSC method, Plato & Glasgow 1969)
23.5 (Rordorf 1989)

Entropy of Fusion, ΔS_{fus} (J/mol K):

Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F: 0.581 (mp at 49°C)

Water Solubility (g/m^3 or mg/L at 25°C or as indicated):
24 (27°C, Woodford & Evans 1963; Günther et al. 1968; Spencer 1973)
40 (29.5°C, Melnikov 1971)
0.35 (20°C, Weber 1972; Worthing & Walker 1987)
0.1–0.5 (Probst et al. 1975)
0.60 (Herbicide Handbook 1978; Kenaga 1980; Kenaga & Goring 1980)
0.05 (Wauchope 1978; Weber et al. 1980)
< 1.0 (20°C, Khan 1980)
8.11 (20–25°C, Kanazawa 1981)
0.30 (Beste & Humburg 1983; Jury et al.1984; Taylor & Glotfelty 1988; Herbicide Handbook 1989)
0.32 (generator column-HPLC-RI, Swann et al. 1983)
0.70 (HPLC-RT correlation, Swann et al. 1983)
4.0 (27°C, Verschueren 1983; Montgomery 1993)
0.75 (shake flask-GC or LSC, Gerstl & Mingelgrin 1984)
< 1.0 (27°C, Hartley & Kidd 1987; Worthing & Hance 1991; Milne 1995)
0.30 (20–25°C, selected, Wauchope et al. 1992; Hornsby et al. 1996)
0.184, 0.221, 0.189 (at pH 5, 7, 9, Tomlin 1994)

Vapor Pressure (Pa at 25°C or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):

0.0265 (29.5°C, Probst et al. 1967; Khan 1980)
0.0292 (29°C, effusion method, Hamaker & Kerlinger 1971)
0.0138 (20°C, Weber 1972; Worthing & Walker 1987)
0.0323 (30°C, from Spencer & Cliath 1973 unpublished data, Spencer et al. 1973)
0.0065* (20°C, gas saturation-GC, measured range 20–40°C, Spencer & Cliath 1974, Spencer 1976)
log (P/mmHg) = 17.318 – 6344/(T/K); temp range 20–40°C (Antoine eq., Spencer 1976)
0.0262 (30°C, effusion method-pressure gauge, DePablo 1976)
0.0137 (Worthing & Walker 1979, Worthing & Hance 1991; Hartley & Kidd 1987)
0.0029 (20–25°C, Weber et al. 1980)
0.0173 (Herbicide Handbook 1983)
0.015 (20°C, Jury et al. 1983)
0.0147 (Herbicide Handbook 1989)
0.010* (gas saturation-GC, measured range 25–125°C, Rordorf 1989)
log (P_S/Pa) = 17.46 – 5800.6/(T/K); measured range 48.8–124°C (solid, gas saturation-GC, Rordorf 1989)
log (P_L/Pa) = 13.65 – 4573.1/(T/K); measured range 48.8–124°C (liquid, gas saturation-GC, Rordorf 1989)
0.015 (20°C, selected, Taylor & Spencer 1990)
0.0147 (20–25°C, selected, Wauchope et al. 1992; Hornsby et al. 1996)
0.0147 (20°C, Montgomery 1993)
0.0095 (Tomlin 1994)
0.0363 (liquid P_L, GC-RT correlation; Donovan 1996)

Henry's Law Constant (Pa·m^3/mol at 25°C or as indicated and reported temperature dependence equations):

16.61 (calculated-P/C, Jury et al. 1983, 1984, 1987a,b; Jury & Ghodrati 1989)
4.02 (20°C, calculated-P/C, Suntio et al. 1988)
16.36 (calculated-P/C, Taylor & Glotfelty 1988)
5.206 (fog chamber-GC/ECD, Fendinger et al. 1989)
5.95 (wetted-wall column-GC/ECD, Fendinger et al. 1989)
16.0 (calculated-P/C, Nash 1989)
13.27 (20°C, calculated-P/C, Muir 1991)
4.903 (23°C, calculated-P/C, Montgomery 1993)
15.2, 6.67, 4.02 (quoted literature values, Grover et al. 1997)
10.31, 15.06 (20°C, distilled water, salt water 33.3% NaCl, wetted wall column-GC, Rice et al. 1997b)
log K_{AW} = –1546/(T/K) + 2.87; temp range 8.3–43.5°C, (distilled water, wetted-wall column-GC, Rice et al. 1997b)
log K_{AW} = –1232/(T/K) + 1.94; temp range 8.3–43.5°C, (salt water solution, 33.3% NaCl, wetted-wall column-GC, Rice et al. 1997b)
11.16, 11.04; 12.50 (20°C, microlayer, subsurface natural water of salinity 17% and TOC 0.4–1.0 ppm, from Pt. Lookout, Chesapeake Bay; estimated value adjusted to salinity, Rice et al. 1997b)
10.97, 10.72; 12.38 (20°C, microlayer, subsurface natural water of salinity 16% and TOC 0.5–0.6 ppm, from Solomons, Chesapeake Bay; estimated adjusted to salinity, Rice et al. 1997b)
10.40, 10.06; 11.82 (20°C, microlayer, subsurface natural water of salinity 12%, TOC 0.6 ppm, from Sandy Point, Chesapeake Bay; estimated value adjusted to salinity, Rice et al. 1997b)
12.43, 12.70; 14.84 (20°C, microlayer, subsurface water of salinity 32%, TOC 2.2–46 ppm, ocean water from Bering/Chukchi Sea; estimated value adjusted to salinity, Rice et al. 1997b)
9.49, 13.14, 19.67 (8.3, 20, 43.5°C, subsurface water from Bering Sea, TOC 2.14 ppm, wetted-wall column-GC, Rice et al. 1997b)
8.504, 12.80; 19.61 (8.3, 20, 43.5°C, surface microlayer water from Bering Sea, TOC 3.14 ppm, wetted-wall column-GC, Rice et al. 1997b)
8.87, 12.26, 19.69 (8.3, 20, 43.5°C, subsurface water from Chukchi Sea, TOC 3.3 ppm, wetted-wall column-GC, Rice et al. 1997b)
7.95, 12.04; 19.40 (8.3, 20, 43.5°C, surface microlayer water from Chukchi Sea, TOC 45.5 ppm, wetted-wall column-GC, Rice et al. 1997b)

6.99, 9.94, 15.85 (8.3, 20, 43.5°C, melted surface ice from the Arctic Ocean, TOC 48.8 ppm, wetted-wall column-GC, Rice et al. 1997b)
$\log K_{AW} = -786/(T/K) + 0.307$; temp range: 8.3–43.5°C, (ocean water from the Chukchi Sea, wetted-wall column-GC, Rice et al. 1997b)
$\log K_{AW} = -1232/(T/K) + 1.900$; temp range: 8.3–43.5°C, (subsurface microlayer of ocean water from the Chukchi Sea, wetted-wall column-GC, Rice et al. 1997b)
4.026 (calculated-P/C, this work)
9.63 (20°C, selected from literature experimentally measured data, Staudinger & Roberts 2001)
$\log K_{AW} = 2.870 - 1546/(T/K)$, (van't Hoff eq. derived from literature data, Staudinger & Roberts 2001)

Octanol/Water Partition Coefficient, log K_{OW}:

5.34	(Kenaga & Goring 1980)
3.06	(Rao & Davidson 1980)
5.34	(shake flask-UV, Briggs 1981)
5.28	(shake flask, Brown & Flagg 1981)
3.97	(shake flask-GC, Kanazawa 1981)
4.94	(HPLC-k′ correlation, McDuffie 1981)
4.86	(shake flask, Dubelman & Bremer 1983)
4.19	(shake flask-GC or LSC, Gerstl & Mingelgrin 1984)
5.07	(Herbicide Handbook 1989; Worthing & Hance 1991; Milne 1995)
5.07, 5.28, 5.34	(Montgomery 1993)
4.88	(RP-HPLC-RT correlation, Saito et al. 1993)
4.82	(RP-HPLC-RT correlation, Sicbaldi & Finizio 1993)
5.34	(recommended, Sangster 1993; Hansch et al. 1995)
5.27	(pH 7.7–8.9, Tomlin 1994)
5.13	(Pomona-database, Müller & Kördel 1996)
4.82	(RP-HPLC-RT correlation, Finizio et al. 1997)
4.98	(RP-HPLC-RT correlation using short ODP column, Donovan & Pescatore 2002)

Bioconcentration Factor, log BCF:

3.97, 3.66	(measured, Metcalf & Sanborn 1975)
3.51. 3.03	(fathead minnow, kinetic test, chronic exposure, Spacie & Hamelink 1979)
3.11	(mosquito fish, correlated-S, Spacie & Hamelink 1979)
3.01	(rainbow trout, correlated-K_{OW}, Spacie & Hamelink 1979)
3.26–3.76	(Spacie & Hamelink 1979)
3.66, 3.04	(quoted exptl., calculated-K_{OC}, Kenaga 1980)
2.92	(calculated-S, Kenaga 1980)
2.95	(calculated-K_{OW}, Briggs 1981)
3.50	(*Pseudorasbora parva*, Kanazawa 1981)
3.26–3.76	(selected, Schnoor & McAvoy 1981; Schnoor 1992)
2.67, 5.02	(dry leaf, wet leaf, Bacci et al. 1990)

Sorption Partition Coefficient, log K_{OC}:

4.14	(soil, Harvey 1974; Kenaga 1980; Kenaga & Goring 1980)
3.76	(soil, calculated-S as per Kenaga & Goring 1980, Kenaga 1980)
3.64	(av. 3 soils, McCall et al. 1980)
4.49	(Georgia's Hickory Hill pond sediment, Brown & Flagg 1981)
2.70	(selected, sediment/water, Schnoor & McAvoy 1981; Schnoor 1992)
3.78	(soil, Thomas 1982)
3.87	(soil average, Jury et al. 1983)
3.63	(soil slurry method, Swann et al. 1983)
3.98	(RP-HPLC-RT correlation, Swann et al. 1983)
3.86	(screening model calculations, Jury et al. 1987a,b; Jury & Ghodrati 1989)
5.13	(RP-HPLC-k′ correlation, cyanopropyl column, Hodson & Williams 1988)
3.59	(Nash 1988)

2.94 (average of 2 soils, Kanazawa 1989)
3.64–4.15, 3.76–4.14 (soil, quoted values, Bottoni & Funari 1992)
4.71, 4.44, 4.59 (No. 1 and 2 soil, No. 3 soil and No. 4 soil; Francioso et al. 1992)
3.90 (soil, 20–25°C, selected, Wauchope et al. 1992)
4.37 (selected, Lohninger 1994)
3.94 (soil, HPLC-screening method, mean value from different stationary and mobile phases, Kördel et al. 1993, 1995a,b)
3.93 (soil, calculated-MCI $^1\chi$, Sabljic et al. 1995)
3.94; 3.99 (HPLC-screening method; calculated-PCKOC fragment method, Müller & Kördel 1996)
3.86 (soil, estimated-general model using molecular descriptors, Gramatica et al. 2000)
3.53, 3.45, 3.96 (soils: organic carbon OC ≥ 0.1%, OC ≥ 0.5%, 0.1 ≤ OC < 0.5%, average, Delle Site 2001)
4.42 (average values for sediments with OC ≥ 0.5%, Delle Site 2001)

Sorption Partition Coefficient, log K_{OM}:
3.87 (Grover et al. 1978)
3.63 (experimental, Grover et al. 1979)
4.14 (av. soils/sediments, Kenaga & Goring 1980)
3.90 (sorption isotherm-GC, Briggs 1981)
1.36, 2.08, 2.98 (log K_P: with first-order rate 0.52, 0.2, 8.3×10^{-3} h^{-1}, Karickhoff & Morris 1985)
4.14, 3.75 (selected, estimated, Magee 1991)
2.94–4.49 (Montgomery 1993)
4.37 (selected, Lohninger 1994)
3.90 (soil, 20–25°C, selected, Hornsby et al. 1996)

Adsorption Coefficient K_d (L kg^{-1}):
8.1 (homoionic K^+-montmorillonite clay minerals, Haderlein et al. 1996)

Environmental Fate Rate Constants, k, or Half-Lives, $t_{½}$:
Volatilization: initial rate constant $k = 2.6 \times 10^{-2}$ h^{-1} and predicted rate constant $k = 6.6 \times 10^{-2}$ h^{-1} from soil with $t_{½}$ = 10.5 h (Thomas 1982);
$t_{½}$ = 18 d (Jury et al. 1983; quoted, Grover 1991);
measured rate constant k = 2–6 d^{-1} (Glotfelty et al. 1984; quoted, Glotfelty 1989);
estimated rate constant k = 0.7 d^{-1} (Glotfelty et al. 1989);
estimated $t_{½}$ ~ 1.6 d from 1 m depth of water at 20°C (Muir 1991).
Photolysis: $t_{½}$ < 1 h under acidic conditions in aqueous methanolic solution (Crosby & Leitis 1973)
k = 2.0 d^{-1} with $t_{½}$ = 22 min for direct sunlight photolysis near surface water at 40°N in the summer (Zepp & Cline 1977; Zepp 1980; Zepp et al. 1984)
$t_{½}$(calc) = 0.94 h for disappearance via direct sunlight photolysis in aqueous media (Zepp & Baughman 1978; quoted, Harris 1982)
k = 0.03 d^{-1} with $t_{½}$ = 22 d for direct sunlight near surface (Schnoor & McAvoy 1981)
k = 0.028–0.012 min^{-1} corresponding to $t_{½}$ = 25–60 min for July, midday sunlight in an outdoor chamber (Mongar & Miller 1988)
$t_{½}$ = 0.5 h estimated from photolysis reaction rate by direct sunlight of midday in mid-summer at 40°N near surface water (Zepp 1991)
$t_{½}$ ~ minutes to several months depending on the substrate under sunlight in all media (summary of literature data, Grover et al. 1997)
Oxidation:
Hydrolysis: $t_{½}$(calc) > 1yr buffered at pH 4, 7, 9 and incubated at 50°C (Grover et al. 1997)
Abiotic Transformations: Degradation by abiotic reductive transformations:
$k = 1.79 \times 10^{-3}$ min^{-1} at pH 6.5, 1.08×10^{-2} min^{-1} at pH 6.72–6.75, 1.64×10^{-2} min^{-1} at pH 6.84, 4.90×10^{-2} min^{-1} at pH 6.94, 7.09×10^{-2} min^{-1} at pH 6.97, 0.141 min^{-1} at pH 7.14, 0.390 min^{-1} at pH 7.46, 0.566 min^{-1} at pH 7.53, and 0.727 min^{-1} at pH 7.73 covering half-lives of 1–400 min., in reaction mixture of 0.5 mM Fe(II) and 100 mg/L goethite solutions (Klupinski & Chin 2003)
k = 1.88 M^{-1} s^{-1} in H_2S with (mecapto)juglone (hydroquinone moiety, an abiotic reductant found in natural systems) solution at pH 6.65 (Wang & Arnold 2003)

Aqueous solutions with surface-bound Fe(II) species and their first-order rate constants as:

$k = 1.13 \times 10^{-3}$ h^{-1} at pH 6.5, $k = 1.11 \times 10^{-2}$ h^{-1} at pH 7.0, $k = 0.0251$ h^{-1} at pH 7.4, and $k = 3.40$ h^{-1} at pH 7.8 for aqueous ferrous ion system;

$k = 0.361$ h^{-1} at pH 6.5, $k = 0.750$ h^{-1} at pH 6.7, $k = 2.57$ h^{-1} at pH 7.0, and $k = 6.66$ h^{-1} at pH 7.3 for Fe(II)/goethite system; and

$k = 4.23 \times 10^{-3}$ h^{-1} at pH 6.5, $k = 5.38 \times 10^{-3}$ h^{-1} at pH 7.0, $k = 1.10 \times 10^{-2}$ h^{-1} at pH 7.4 and $k = 2.36 \times 10^{-2}$ h^{-1} at pH 7.8 for Fe(II)/clay system, all with total dissolved Fe(II) = 1 mM (Wang & Arnold 2003)

Biodegradation:

$t_{½}$ = 4–5 d for 4 µg/mL to biodegrade in flooded soils at 24.5°C and $t_{½}$ > 21 d at 3.3°C (Probst et al. 1967; quoted, Means et al. 1983; Muir 1991);

$t_{½}$ > 20 d for 0.33 µg/mL to biodegrade in soil suspension at 25°C (Willis et al. 1974; quoted, Muir 1991);

$t_{½}$ = 20 d for 0.5 µg/mL to biodegrade in flooded soil with 0.5–1.0 cm of water on top of the soil at 20–42°C (Savage 1978; quoted, Muir 1991);

Degradation $t_{½}$ < 1 month in three soils, Goldsborol loamy sand, Cecil loamy sand Drummer clay loam treated with 1 ppm trifluralin) for 4 month under aerobic conditions, no degradation in sterile controls. (shake flask-TLC, Camper et al. 1980)

$t_{½}$ < 1 month for 1.0 µg/mL to biodegrade in flooded soils at 25°C (derived from Camper et al. 1980; Muir 1991)

$k = 0.008$ d^{-1} by soil incubation die-away test and $k = 0.025$ d^{-1} by flooded soil incubation die-away test (Rao & Davidson 1980; quoted, Scow 1982);

$t_{½}$ = 132 d for a 100 d leaching and screening test in 0–10 cm depth of soil (Rao & Davidson 1980; quoted, Jury et al. 1983, 1984, 1987a,b; Jury & Ghodrati 1989; Grover 1991);

$t_{½}$ = 46 wk for 2.0 µg/mL to biodegrade in flooded soils at 25°C (Brewer et al. 1982; quoted, Muir 1991);

$t_{½}$ = 20 h for 0.36 µg/mL to biodegrade in sediment-water microcosm at 20°C (Spain & Van Veld 1983; quoted, Muir 1991);

$k = -0.00504$ to -0.00730 h^{-1} in nonsterile sediment, $k = -0.00160$ to -0.00651 h^{-1} in sterile sediment by shake-tests at Range Point; $k = -0.00827$ to -0.01140 h^{-1} in nonsterile water, and $k = -0.00499$ to -0.00712 h^{-1} in sterile water by shake-tests at Range Point (Walker et al. 1988)

$k = -0.00621$, -0.0121 h^{-1} in nonsterile sediment, $k = -0.00476$, -0.00409 h^{-1} in sterile sediment by shake-tests at Davis Bayou and $k = -0.00439$, -0.00349 h^{-1} in nonsterile water, and $k = -0.00299$, -0.00598 h^{-1} in sterile water by shake-tests at Davis Bayou (Walker et al. 1988).

Biotransformation:

Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants:

Half-Lives in the Environment:

Air: mean $t_{½}$ = 42 min under August conditions in California range from 21–63 min (Woodrow et al. 1978)

$t_{½}$ = 25–60 min for July, midday sunlight in an outdoor chamber (Mongar & Miller 1988)

$t_{½}$ = 182–193 min under fall sunlight conditions in October (Woodrow et al. 1983)

Surface water: calculated $t_{½}$ = 21 min from midday direct sunlight photolysis rate constant of 2.0 h^{-1} (Zepp 1978; Zepp & Cline 1977; quoted, Zepp et al. 1984);

calculated $t_{½}$ = 0.94 h for disappearance via direct sunlight photolysis in aqueous media (Zepp & Baughman 1978; quoted, Harris 1982);

$t_{½}$ < 20 d for 2.5–5 cm water over flooded soils, $t_{½}$ ~ 20 h in water above sediment in estuarine sediment-water microcosm (Muir 1991);

$t_{½}$ < 9 h in buffered aqueous solution of pH 7 under Xenon lamp (quoted, Grover et al. 1997)

$t_{½}$ = 1–400 min in reaction mixture of 0.5 mM and 100 mg/L goethite solution for pHs from 6.5 to 7.73 (Klupinski & Chin 2003).

Ground water: reported $t_{½}$ = 4–67, 57–126, 70, 83, and 105–132 d (Bottoni & Funari 1992)

Sediment: degradation $t_{½}$ = 9 d in estuarine sediment (18‰) system (Means et al. 1983).

$t_{½}$ = 18.5 d in flooded sediment (quoted, Grover et al. 1997)

Soil: $t_{½}$ = 4–5 d for 4 µg/mL to biodegrade in flooded soils at 24.5°C and $t_{½}$ > 21 d at 3.3°C (Probst et al. 1967; quoted, Means et al. 1983; Muir 1991);

estimated persistence of 6 months in soil (Kearney et al. 1969; Edwards 1973; quoted, Morrill et al. 1982; Jury et al. 1987a);

degradation $t_{½}$ = 93 d in soil (Parr & Smith 1973; quoted, Means et al. 1983);

$t_{1/2} > 20$ d for 0.33 μg mL^{-1} to biodegrade in soil suspension at 25°C (Willis et al. 1974; quoted, Muir 1991);
degradation $t_{1/2} = 1$ d (Kearney et al. 1976; quoted, Means et al. 1983); and $t_{1/2} = 54$ d in soil (Zimdahl & Gwynn 1977; quoted, Means et al. 1983);
$t_{1/2} = 20$ d for 0.5 μg/mL to biodegrade in flooded soil with 0.5–1.0 cm of water on top of the soil at 20–42°C (Savage 1978; quoted, Muir 1991);
persistence of more than 6 months (Wauchope 1978);
$t_{1/2} < 21$ d in flooded soil at 20–25°C (Golab et al. 1979)
biodegradation $t_{1/2} < 1$ month in 3 flooded soils at 25°C (Camper et al. 1980);
estimated first-order $t_{1/2} \sim 86.6$ d in soil from biodegradation rate constant $k = 0.008\ d^{-1}$ by soil incubation die-away test and $t_{1/2} = 27.7$ d in anaerobic systems from rate constant $k = 0.025\ d^{-1}$ by flooded soil incubation die-away test (Rao & Davidson 1980; quoted, Scow 1982);
$t_{1/2} = 2$ d on Bosket silt loam, $t_{1/2} = 2$ d on Sharkey clay for the first 3 to 5 days when sprayed onto soil surface, rate of loss much slower for the remainder of the 7- or 12-d sampling period with $t_{1/2} = 70$ d on Bosket silt loam, $t_{1/2} = 50$ d on Sharkey clay (Savage & Jordon 1980)
$t_{1/2} = 30$ d flooded soil in aquatic ecosystem (Yockim et al. 1980)
field $t_{1/2} = 0.1–0.3$ d in moist fallow soil (Glotfelty 1981; quoted, Nash 1983);
Field studies: $t_{1/2} = 9.5$ wk - 1978 first study; $t_{1/2} = 11.8$ wk -1978 second study; $t_{1/2} = 12.2$ wk –1979, in a Crowley silt loam at Stuttgart, Arkansas (Brewer et al. 1982)
Laboratory studies: $t_{1/2} = 19.6$ wk at 4°C, $t_{1/2} = 7.1$ wk at 25°C for soil of field capacity moisture (27% w/w for Crowley silt), $t_{1/2} = 16.2$ wk at 4°C, $t_{1/2} = 3.9$ wk at 25°C for flooded soils, Crowley silt loam; and $t_{1/2} = 27.0$ wk at 4°C, $t_{1/2} = 8.1$ wk at 25°C for soil of field capacity moisture (34% w/w for Sharkey silty clay), $t_{1/2} = 18.6$ wk at 4°C and $t_{1/2} = 5.4$ wk at 25°C for flooded soils, Sharkey silty clay (Brewer et al. 1982)
microagroecosystem $t_{1/2} = 3–4$ d in moist fallow soil (Nash 1983);
$t_{1/2} = 46$ wk for 2.0 μg/mL to biodegrade in flooded soils at 25°C (derived from Brewer et al. 1982, Muir 1991);
very persistent in soils with $t_{1/2} > 100$ d (Willis & McDowell 1982);
$t_{1/2} = 20$ h for 0.36 μg/mL to biodegrade in sediment-water microcosm at 20°C (Spain & Van Veld 1983; quoted, Muir 1991);
measured dissipation rate $k = 0.69\ d^{-1}$ (Nash 1983; quoted, Nash 1988);
estimated dissipation rate $k = 1.6$ and $0.24\ d^{-1}$ (Nash 1988);
first-order adsorption rate constants: $k = 0.52,\ 0.2,\ 8.3 \times 10^{-3}\ h^{-1}$ (Karickhoff & Morris 1985; quoted, Brusseau & Rao 1989);
$t_{1/2} \sim 22$ d in submerged soils in a model ecosystem (Muir 1991);
reported $t_{1/2} = 4–67$ d, 57–126 d, 70 d, 83 d, 105–132 d (Bottoni & Funari 1992);
selected field $t_{1/2} = 60$ d (Wauchope et al. 1992; Hornsby et al. 1996; quoted, Halfon et al. 1996)
Estimated $t_{1/2} \sim 25$ to > 201 d under a variety of agronomic conditions in agriculture soils depending on depth of incorporation, soil moisture, soil temperature, sil air, and soil organic matter content (summary of literature data, Grover et al. 1997)

Biota: $t_{1/2} = 22–31$ d in river saugers, $t_{1/2} = 17–57$ d in river shorthead redhorse, $t_{1/2} = 23$ d in river golden redhorse, $t_{1/2} = 3$ d in lab. fathead minnow (Spacie & Hamelink 1979);
biochemical $t_{1/2} = 132$ d (Jury et al. 1987a,b; Jury & Ghodrati 1989).

TABLE 17.1.1.79.1
Reported vapor pressures of trifluralin at various temperatures and the coefficients for the vapor pressure equations

$\log P = A - B/(T/K)$	(1)	$\ln P = A - B/(T/K)$	(1a)
$\log P = A - B/(C + t/°C)$	(2)	$\ln P = A - B/(C + t/°C)$	(2a)
$\log P = A - B/(C + T/K)$	(3)		
$\log P = A - B/(T/K) - C\cdot\log(T/K)$	(4)		

Spencer & Cliath 1974		Rordorf 1989	
gas saturation method		gas saturation-GC	
t/°C	P/Pa	t/°C	P/Pa
20	0.0065	25	0.010
30	0.0323	50	0.32
40	0.155	75	6.30
		100	82.0
		125	780
			for solid
		eq. 1	P_S/Pa
		A	17.46
		B	5800.6
			for liquid
		eq. 1	P_L/Pa
		A	13.65
		B	4573.1

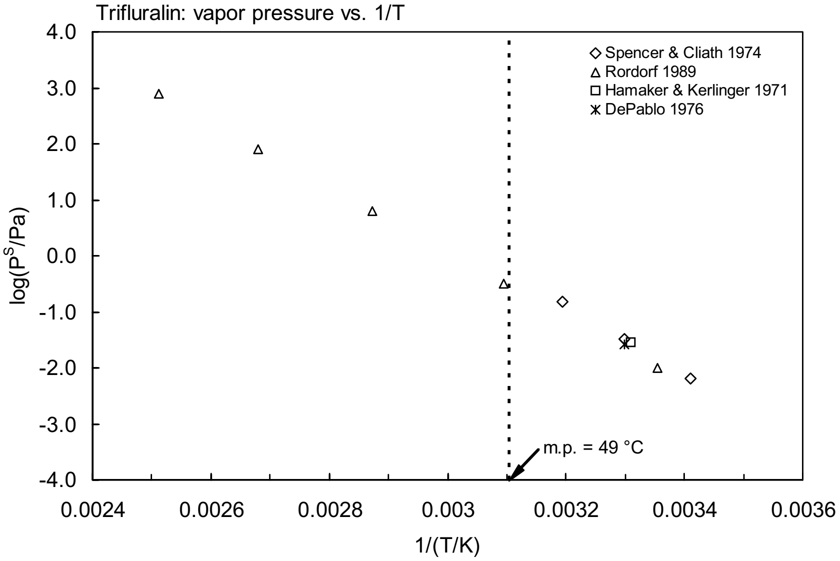
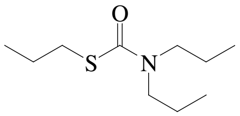


FIGURE 17.1.1.79.1 Logarithm of vapor pressure versus reciprocal temperature for trifluralin.

17.1.1.80 Vernolate



Common Name: Vernolate
Synonym: PPTC, R1607, Vanalate, Vernam, Vernnolaolate
Chemical Name: *S*-propyldipropylthiocarbamate; *S*-propyldipropylcarbamothioate
Uses: herbicide incorporated with soil for pre-planting or pre-emergence control of broadleaf and grass weeds in groundnuts, soybeans, maize, tobacco, and sweet potatoes.
CAS Registry No: 1929-77-7
Molecular Formula: $C_{10}H_{21}NOS$
Molecular Weight: 203.345
Melting Point (C): liquid
Boiling Point (°C):

150	(at 30 mmHg, Herbicide Handbook 1989; Worthing & Hance 1991; Tomlin 1994; Milne 1995)
149–150	(at 30 mmHg, Budavari 1989)

Density (g/cm^3 at 20°C):

0.954	(Ashton & Crafts 1981; Herbicide Handbook 1989; Worthing & Hance 1991)
0.952	(Hartley & Kidd 1987; Tomlin 1994; Milne 1995)

Molar Volume (cm^3/mol):

269.2	(calculated-Le Bas method at normal boiling point)

Dissociation Constant pK_a:
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
Entropy of Fusion, ΔS_{fus} (J/mol K):
Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F: 1.0

Water Solubility (g/m^3 or mg/L at 25°C or as indicated):

107	(Martin & Worthing 1977)
90	(20°C, Khan 1980; Spencer 1982; Ashton & Crafts 1981; Herbicide Handbook 1989)
107	(21°C, Verschueren 1983)
90	(20°C, Hartley & Kidd 1987; Worthing & Walker 1987, Worthing & Hance 1991)
107	(Budavari 1989; Milne 1995)
95	(Wauchope 1989)
108	(20–25°C, selected, Wauchope et al. 1992; Hornsby et al. 1996)

Vapor Pressure (Pa at 25°C or as indicated):

0.84	(20°C, Hartley & Graham-Bryce 1980)
1.386	(Khan 1980; Spencer 1982; Herbicide Handbook 1989)
1.333	(Ashton & Crafts 1981)
0.244	(20°C, GC-RT correlation, Kim 1985)
1.39	(Hartley & Kidd 1987)
0.9	(20°C, selected, Suntio et al. 1988)
1.386	(Budavari 1989)
1.39	(Worthing & Hance 1991; Tomlin 1994)
1.293	(20–25°C, selected, Wauchope et al. 1992; Hornsby et al. 1996)

Henry's Law Constant (Pa·m^3/mol at 25°C or as indicated):

2.05	(20°C, calculated-P/C, Suntio et al. 1988)
2.034	(calculated-P/C, this work)

Octanol/Water Partition Coefficient, log K_{OW}:

3.84	(20°C, Worthing & Hance 1991; Tomlin 1994)

3.84	(20°C, Milne 1995)
3.84	(recommended, Hansch et al. 1995)
3.86	(RP-HPLC-RT correlation, Finizio et al. 1997)

Bioconcentration Factor, log BCF:

1.64	(calculated-S, Kenaga 1980)
1.70	(calculated, Pait et al. 1992)

Sorption Partition Coefficient, log K_{OC}:

2.52	(calculated-S, Kenaga 1980)
2.41	(soil, 20–25°C, selected, Wauchope et al. 1992; Hornsby et al. 1996)
2.03, 1.93	(quoted exptl.; calculated-MCI and fragment contribution method, Meylan & Howard 1992)
2.41	(estimated-chemical structure, Lohninger 1994)
2.33	(soil, calculated-MCI $^1\chi$, Sabljic et al. 1995)
2.33; 2.40, 2.11	(soil, quoted exptl.; estimated-class-specific model, estimated-general model using molecular descriptors, Gramatica et al. 2000)

Environmental Fate Rate Constants, k, or Half-Lives, $t_{½}$:

Biodegradation: microbial degradation $t_{½}$ = 8–16 d at 27°C, $t_{½}$ > 64 d at 4°C in soil (Tomlin 1994).

Half-Lives in the Environment:

Soil: $t_{½}$ ~ 1.5 wk in moist loam soil at 21–27°C (Herbicide Handbook 1989);
selected field $t_{½}$ = 12 d (Wauchope et al. 1992; Hornsby et al. 1996);
soil $t_{½}$ = 11 d (Pait et al. 1992);
microbial degradation $t_{½}$ = 8–16 d at 27°C, $t_{½}$ > 64 d at 4°C (Tomlin 1994).

Biota:

17.2 SUMMARY TABLES

TABLE 17.2.1
Common names, chemicals names and physical properties of herbicides

Compound	Synonym	Chemical name	Molecular formula	Molecular weight, MW g/mol	m.p. °C	Fugacity ratio, F at 25°C*	pK_a	pK_b
Alachlor [15972-60-8]	Lasso, Metachlor	α-chloro-2,6-diethyl-*N*-methoxy-methylacetanilide	$C_{14}H_{20}ClNO_2$	269.768	40	0.713	0.62	
Ametryn [834-12-8]	Evik, Gesapax	2-methylthio-4-(ethylamino)-6-(isopropylamino)-*s*-triazine	$C_9H_{17}N_5S$	227.330	88	0.241	4.00 4.10	10.07
Amitrole [61-82-5]	Amerol, Aminotriazole	3-amino-1*H*-1,2,4-triazole	$C_2H_4N_4$	84.080	159	0.0484		9.83
Atrazine	Gesaprim	2-chloro-4-(ethylamino)-6-(isopropylamino)-*s*-triazine	$C_8H_{14}ClN_5$	215.684	173	0.0353	1.68 1.70	12.32
Barban [101-27-9]	Carbyne	4-chlorobut-2-ynyl-3-chlorocarbanilate	$C_{11}H_9Cl_2NO_2$	258.101	75	0.323		
Benefin [1861-40-1]	Balan, Bonalan Benfluralin	*N*-butyl-*N*-ethyl-α,α,α-trifluoro-2,6-di-nitro-*p*-toluidine	$C_{13}H_{16}N_3O_4F_3$	335.279	66	0.396		
Bifenox [42576-02-3]	Modown	methyl-5-(2,4-dichlorophenoxy)-2-nitrobenzoate	$C_{14}H_9Cl_2NO_5$	342.131	85	0.258		
Bromacil [314-40-9]	Borea, Hyvar X	5-bromo-3-*sec*-butyl-6-methyl-uracil	$C_9H_{13}BrN_2O_2$	261.115	158	0.0496	9.10 < 7.0	
Bromacil lithium salt			$C_9H_{12}N_2O_3Li$	267.0			9.27	
Bromoxynil [1689-84-5]	Brominal, Buctril	3,5-dibromo-4-hydroxybenzonitrile	$C_7H_3Br_2NO$	276.913	190	0.0241	4.06 4.20	
Bromoxynil butyrate ester [3861–41–4]			$C_{13}H_9BrNO_3$	307.119			4.10	
Bromoxynil octanoate [1689–99–2]		2,6-dibromo-4-cyanophenyl octanoate	$C_{15}H_{17}Br_2NO_2$	403.109	45–46	0.629	4.08	
sec-Bumeton [26259-45-0]	Etazine, Sumitol	*N*-ethyl-6-methoxy-*N'*-(1-methyl-propyl)-1,3,5-triazine-2,4-diamine	$C_{10}H_{19}N_5O$	225.291	87	0.246	4.40	
Butachlor [23184-66-9]	Machete	*N*-butoxymethyl-2-chloro-2',6'-diethylacetanilide	$C_{17}H_{26}ClNO_2$	311.847	< –5	1		
Butralin [33629-47-9]	Amex, Tamex	*N*-*sec*-butyl-4-*tert*-butyl-2',6'- dinitroaniline	$C_{14}H_{21}N_3O_4$	295.335	60	0.454		
Butylate [2008-41-5]	Sutan	*S*-ethyl bis(2-methylpropyl) carbamothioate	$C_{11}H_{23}NOS$	217.372	liquid	1		
Chloramben [133-90-4]	Amiben, Amoben	3-amino-2,5-dichlorobenzoic acid	$C_7H_5Cl_2NO_2$	206.027	200	0.0192	3.40	

(Continued)

TABLE 17.2.1 (*Continued*)

Compound	Synonym	Chemical name	Molecular formula	Molecular weight, MW g/mol	m.p. °C	Fugacity ratio, F at 25°C*	pK_a	pK_b
Chloramben salts [133-90-4]	Amiben	ammonium or sodium salt of chloramben	$C_7H_5Cl_2NO_2$	206.027				
Chlorazine [580–48–3]		6-chloro-*N,N,N'N'*-tetraethyl-1,3,5-triazine-2,4-diamine	$C_{11}H_{20}ClN_5$	257.764	27	0.956		
Chlorbromuron [13360-45-7]	Maloran	3-(4-bromo-3-chlorophenyl)-1-methoxy-1-methylurea	$C_9H_{10}BrClN_2O_2$	293.544	96	0.201		
Chlorfenac [85-34-7]	Fenac	(2,3,6-trichlorophenyl)acetic acid	$C_8H_5Cl_3O_2$	239.484	161	0.046		
Chlorpropham [101-21-3]	Furloe	isopropyl 3-chlorocarbanilate	$C_{10}H_{12}ClNO_2$	213.661	41	0.697		
Chlorsufuron [64902-72-3]	Glean, Telar	1-(2-chlorophenylsulfonyl)-3-(4-methoxy-6-methyl-1,3,5-trizaon-2-yl)urea	$C_{12}H_{12}ClN_5O_4S$	357.773	176	0.0330	3.60	
Chlortoluron [15545-48-9]	Dicuran	3-(3-chloro-*p*-tolyl)-1,1-dimethylurea	$C_{10}H_{13}ClN_2O$	212.675	147	0.0635		
Cyanazine [21725-46-2]	Bladex, Fortrol	2-(4-chloro-6-ethylamino-1,3,5-triazin-2-ylamino)-2-methylpropionotrile	$C_9H_{13}ClN_6$	240.692	168	0.0395	1 0.63	12.9
2,4-D [94-75-7]	Agratect, Farmco, Weed Tox	2-(2,4-dichlorophenoxy)acetic acid	$C_8H_6Cl_2O_3$	221.038	140.5	0.0736	2.64 3.31	
2,4-D dimethylamine salt [2008–39–1]		$C_{10}H_{13}Cl_2NO_3$	266.121	85–87	0.252			
2,4-D esters			$C_8H_6Cl_2O_3$ (a)	221.038			2.80	
Dalapon [75-99-0]	Dowpon, Radapon	2,2-dichloropropionic acid	$C_3H_4Cl_2O_2$	142.969	liquid	1	1.74 1.84	
Dalapon sodium salt [120-20-8]		sodium 2,2-dichloropropionate	$C_3H_3Cl_2Na$	164.95	166.5 dec			
2,4-DB [94-82-6]	Embutox	4-(2,4-dichlorophenoxy)butyric	$C_{10}H_{10}Cl_2O_3$	249.090	118	0.122	4.80	
2,4-DB butoxyethyl ester			$C_{16}H_{22}O_4Cl_2$	349.249			4.80	
Diallate [2303-16-4]	Avadex	*S*-(2,3-dichloroallyl)diiso-propylthiocarbamate	$C_{10}H_{17}Cl_2NOS$	270.219				
Dicamba [1918-00-9]	Banvel, Dianat, Mediben	3,6-Dichloro-*o*-anisic acid	$C_8H_6Cl_2O_3$	221.038	115	0.131	1.91 1.95	
Dichlobenil [1194-65-6]	Casoron	2,6-dichlorobenzonitrile	$C_7H_3Cl_2N$	172.012	144.5	0.0672		
Dichlorophen (F.A.B) [97-23-4]	Super Mosstox	4,4'-dichloro-2,2'-methylenediphenol	$C_{13}H_{10}Cl_2O_2$	269.123	177.5	0.0320		
Dichloroprop [120-36-5]	2,4-DP	(*RS*)-2-(2,4-dichorophenoxy)-propionic acid	$C_9H_8Cl_2O_3$	235.064	117.5	0.124	3.0	

Dichlorprop-P [15165-67-0]	Cornox RK	(*R*)-2-(2,4-dichorophenoxy)propionic acid	$C_9H_8Cl_2O_3$	235.064	122	0.112	3.0 2.86	
Dichlorprop ester	Weedone	butoxyethyl ester of	$C_9H_8Cl_2O_3$	335.3			2.85	
Diclofop [40843-25-2]		(*R*-2-(2,4-dichloro-2-(4-aryloxyphenoxy) propionic acid	$C_{15}H_{12}Cl_2O_4$	327.159				
Diclofop-methyl [51338-27-3]	Hoelon	2-(4-(2,4-dichlorophenoxy)phenoxyl)-propanoic acid methyl ester	$C_{16}H_{14}Cl_2O_4$	341.186	40	0.713	3.10	
Dinitramine [29091-05-2]	Cobexo	*N,N*-diethyl-2,6-dinitro-4-trifluoro-methyl-*m*-phenyenediamine	$C_{11}H_{13}N_4O_4F_3$	322.241	98	0.192		
Dinoseb [88-85-7]	Antox, Aretit, BNP 30, DNBP	2-*sec*-butyl-4,6-dinitrophenol	$C_{10}H_{12}N_2O_5$	240.212	40	0.713	4.62	
Dinoseb salts [88–85–7]	Premerge, Dinitro	2-*sec*-butyl-4,6-dinitrophenyl ammonium, amine, acetate salts					4.50	
Diphenamid [957-51-7]	Dymid, Enide	*N,N*-dimethyldiphenylacetamide	$C_{16}H_{17}NO$	239.312	135	0.0833		
Diquat [2764-72-9]	Reglone, Pathclear Cleansweep, Weedol	1,1'-ethylene-2,2'-dipyridine	$C_{12}H_{14}N_2$	186.236				
Diquat dibromide salt [85-00-7]			$C_{12}H_{12}Br_2N_2$	344.1			10	
Diuron [330-54-1]	DMU, Karmex DCMU	3-(3,4-dichlorophenyl)-1,1-dimethylurea	$C_9H_{10}Cl_2N_2O$	233.093	158	0.0496		
EPTC [759-94-4]	Eptam, Eradicane	*S*-ethyl dipropylthiocarbamate	$C_9H_{19}NOS$	189.318	liquid	1		
Ethalfluralin [55283–68–6]	Benzenamine, Somilan, Sonalan, Sonalen	*N*-ethyl-*N*-(2-methyl-2-propenyl)-2,6-dinitro-(trifluoromethyl)-benzenamine	$C_{13}H_{14}F_3N_3O_4$	333.263	57	0.485		
Fenoprop (G.R.) [93-72-1]	Silvex, 2,4,5-TP	(±)-2-(2,4,5-trichlorophenoxy)-propionic acid	$C_9H_7Cl_3O_3$	269.509	181.6	0.0291		
Fenuron [101-42-8]	Dybar, Urab	1,1-dimethyl-3-phenylurea	$C_9H_{12}N_2O$	164.203	132	0.0892		
Fenuron-TCA [4482-55-7]		1,1-dimethyl-3-phenyluronium trichloroacetate	$C_{11}H_{13}Cl_3N_2O_3$	327.592	65–68	0.392		
Fluchloralin [33245-39-5]	Basalin Basalin, BAS-392H	*N*-(2-chloroethyl) α,α,α-trifluoro-2,6-dinitro-*N*-propyl-*p*-toluidine	$C_{12}H_{13}ClF_3N_3O_4$	355.697	42	0.681		
Fluometuron [2164-17-2]	Cotoran, Cottonex, Meturon	*N,N*-dimethyl-*N*'-[3-trifluoromethyl)-phenylurea	$C_{10}H_{11}F_3N_2O$	232.201	164	0.0433		
Fluorodifen [15457-05-3]	Soyex	4-nitrophenyl α,α,α-trifluoro-2-nitro-*p*-tolyl ether	$C_{13}H_7F_3N_2O_5$	328.200	94	0.210		
Fluridone [59756-60-4]	Fluridon, Pride, Sonar	1-methyl-3-phenyl-5-[3-(trifluoromethyl) phenyl]-4-(1*H*)-pyridinone	$C_{19}H_{14}F_3NO$	329.315	155	0.0530		12.3

(*Continued*)

TABLE 17.2.1 (*Continued*)

Compound	Synonym	Chemical name	Molecular formula	Molecular weight, MW g/mol	m.p. °C	Fugacity ratio, F at 25°C*	pK_a	pK_b
Glyphosate [1071-83-6]	Roundup, Polado	*N*-(phosphoromethyl)glycine	$C_3H_8NO_5P$	169.074	230 dec	0.0097	5.70	
Glyphosate-mono(*iso*-propylammonium) [38641–94–0]			$C_6H_{17}N_2O_5P$	228.2	200	0.0190		
Ioxynil [1689-83-4]	Actril, Totril	4-hydroxy-3,5-di-iodobenzonitrile	$C_7H_3I_2NO$	370.914	201 dec	0.0190	3.96	
Ioxynil-octanoate [3681–47–0]		4-cyano-2,6-iodophenyl octanoate	$C_{15}H_{17}I_2NO_2$	497.1	59–60	0.459		
Ioxynil-sodium salt [2961–62–8]			$C_7H_2I_2NNaO$	392.9	360	0.00052		
Isopropalin [33820-53-0]	Paralan	4-isopropyl-2,6-dinitro-*N*-dipropylaniline	$C_{15}H_{23}N_3O_4$	309.362	liquid	1		
Isoproturon [34123-59-6]	Alon, Arelon, Graminon	3-*p*-cumenyl-1,1-dimethylurea	$C_{12}H_{18}N_2O$	206.284	155–156	0.0520		
Linuron [330-55-2]	Afalon, Lorox	3-(3,4-dichlorophenyl)-1-methoxy-1-methylurea	$C_9H_{10}Cl_2N_2O_2$	249.093	93	0.215		
MCPA (G.R., H) [94-74-6]	Metaxon, Agroxone, Agritox	4-chlor-*o*-tolyloxyacetic acid	$C_9H_9ClO_3$	200.618	120	0.117	3.05 3.13	
MCPA dimethylamine salt [94–74–6]			$C_{11}H_{16}ClNO_3$	243.7			3.12	
MCPA ester	Weedone, Weedar		$C_9H_9ClO_3$	200.6				
MCPA sodium salt			$C_9H_8ClNaO_3$	222.6				
MCPA-thioethyl [25319–90–8]		*S*-ethyl 4-chloro-*o*-tolyoxythioacetate	$C_{11}H_{13}ClO_2S$	244.7	41–42	0.689		
MCPB [94-81-5]	Tropotox	4-(4-chloro-2-methylphenoxy)butyric acid	$C_{11}H_{13}ClO_3$	228.672	100	0.184	4.84 4.80	
MCPB sodium salt [6062–26–6]			$C_{11}H_{12}ClNaO_2$	250.7				
Mecoprop [7085-19-0]	Iso-Cornox, MCPP	(±)-2-(4-chloro-*o*-tolyloxy)-propionic acid	$C_{10}H_{11}ClO_3$	214.645	94-95	0.208	3.78 3.75	
Mecoprop-P [16484–77–8]		(*R*)-2-(4-chloro-*o*-tolyoxy)propionic acid	$C_{10}H_{11}ClO_3$	214.645	95	0.206	3.78	
Metobromuron [3060-89-7]	Patoran	3-(4-bromophenyl)-1-methoxy-1-methyl urea	$C_9H_{11}BrN_2O_2$	259.099	95	0.206		

Metolachlor [51218-45-2]	Codal, Dual, Primagram	2-chloro-6'-ethyl-*N*-(2-methoxy-1-methylethyl)acet-*o*-toluidide	$C_{15}H_{22}ClNO_2$	283.795	liquid	1		
Metoxuron [19937-59-8]	Dosanex	3-(3-chloro-4-methoxyphenyl)-1,1-dimethylurea	$C_{10}H_{13}ClN_2O_2$	228.675	126-127	0.101		
Metribuzin [21087–64–9]	Metribuzine, Lexone, Preview, Sencor	4-amino-6-(*t*-butyl)-3-(methylthio)-1,2,4-triazin-5-(4*H*)-one	$C_8H_{14}N_4OS$	214.288	126	0.102		
Molinate [2212-67-1]	Ordram	*S*-ethyl azepane-1-carbothioate	$C_9H_{17}NOS$	187.302	liquid	1		
Monolinuron [1746-81-2]	Aresin	3-(4-chlorophenyl)-1-methoxy-1-methylurea	$C_9H_{11}ClN_2O_2$	214.648	77	0.309		
Monuron [150-68-5]	Telvar, Urox	1,1-dimethyl-3-(*p*-chloro-phenyl)-urea	$C_9H_{11}ClN_2O$	198.648	170.5	0.0374		
Napropamide [15299–99–7]	Devrinol	2-(α-naphthloxy)-*N,N*-diethylpropionamide	C17H21NO2	271.355	75	0.323	2.93	
Neburon [555-37-3]	Kloben	1-butyl-3-(3,4-dichlorophenyl)-1-methyl urea	$C_{12}H_{16}Cl_2N_2O$	275.174	102-103	0.174		
Nitralin [4726-14-1]	Planavin	4-(methylsulfonyl)-2,6-dinitro-*N,N*-dipropylaniline	$C_{13}H_{19}N_3O_6S$	345.371	150	0.0594		
Nitrofen [1836–75–5]	nitrophen, Tok, Tokkron	2,4-dichloro-1-(4-nitrophenoxy)benzene	$C_{12}H7Cl_2NO_3$	284.095	70	0.362		
Norfluorazon [27314–13–2]			$C_{12}H_9ClF_3N_3O$	303.666	184	0.0275		
Oryzalin [19044-88-3]	Rycelan, Rycelon, Surflan	4-(dipropylamino)-3,5-dinitro-benzenesulfonamide	$C_{12}H_{18}N_4O_6S$	346.359	141	0.0728	9.40 8.60	
Paraquat [4685-14-7]	Cyclone, Gramoxone	1,1'-dimethyl-4,4'-pyridinium	$C_{12}H_{14}N_2$	186.252	dec.			
Paraquat dichloride salt [1910–42–5]			$C_{12}H_{14}Cl_2N_2$	257.2				< 4
Pebulate [1114-71-2]	Tillam	*s*-propyl butylethylcarbamothioate	$C_{10}H_{21}NOS$	203.345	liquid	1		
Pendimethalin [40487–42–1]	penoxalin	*N*-(1-ethylpropyl-3,4-dimethyl-2,6-dinitrobenzenamine	$C_{13}H_{19}N_30_4$	281.308	56	0.496		
Pentachlorophenol [87–86–5]	PCP	pentachlorophenol	C_6Cl_5OH	266.336	174	0.0350	4.74	
Pentachlorophenol sodium salt (Pentacon)								
Pentanochlor [2307-68-8]	Solan	3'-chloro-2-methylvaler-*p*-toluidide	$C_{13}H_{18}ClNO$	239.741	85-86	0.255		
Picloram [1918-02-1]	Tordon	4-amino-3,5,6-trichloro-picolinic acid	$C_6H_3Cl_3N_2O_2$	241.459	218.5	0.0126	1.90 3.60	

(*Continued*)

TABLE 17.2.1 (*Continued*)

Compound	Synonym	Chemical name	Molecular formula	Molecular weight, MW g/mol	m.p. °C	Fugacity ratio, F at 25°C*	pK_a	pK_b
Picloram-potassium salt [2425–60–0]			$C_6H_2Cl_3KN_2O_2$	279.6				
Profluralin [26399-36-0]	Pregard	*N*-(cyclopropylmethyl)-2,6-dinitro-*N*-propyl-4-(trifluoromethyl)-benzenamine	$C_{14}H_{16}F_3N_3O_4$	347.290	34	0.816		
Prometon [1610-18-0]	Primatol, Gesagram	2,4-bis(isopropylamino)-6-methoxy-*s*-triazine	$C_{10}H_{19}N_5O$	225.291	91.5	0.223	4.28 4.30	9.73
Prometryn [7287-19-6]	Caparol, Gesagard	*N*,*N*-1,3,5-triazine-2,4-diamine-bis(isopropylamino)-6-(methylthio)	$C_{10}H_{19}N_5S$	241.357	119	0.120	4.05 4.10	9.95
Pronamide [23950-58-5]	Kerb, Promamide	3,5-dichloro-*N*-(1,1-dimethyl-propynyl)-benzamide	$C_{12}H_{11}Cl_2NO$	256.127	155	0.0530		
Propachlor [1918-16-7]	Ramrod	2-chloro-*N*-(1-methylethyl)-*N*-phenylacetamide	$C_{11}H_{14}ClNO$	211.688	77	0.309		
Propanil [709-98-8]	Propanex, Riselect, Stampede 3E	*N*-(3,4-dichlorophenyl)-propionamide	$C_9H_9Cl_2NO$	218.079	92	0.220		
Propazine [139-40-2]	Gesamil, Milogard	2-chloro-4,6-bis(isopropylamino)-*s*-triazine	$C_9H_{16}ClN_5$	229.710	213	0.0143	1.85 1.80	12.15
Propham [122-42-9]	IPC	isopropyl carbanilate	$C_{10}H_{13}NO_2$	179.216	90	0.230		
Pyrazon [1698-60-8]	Chloridazon	5-amino-4-chloro-2-phenyl-3(2*H*)-pyridazinone	$C_{10}H_8ClON_3$	221.643	205	0.0171		
Simazine [122-34-9]	Gesatop, Weedex, Aquazine	2-chloro-4,6-di(ethylamino)-*s*-triazine	$C_7H_{12}ClN_5$	201.657	226	0.0107	1.65 1.60	12.35
Simetryne [1014-70-6]	Gy-bon	*N*,*N*'-diethyl-6-methylthio-1,3,5-triazine -2,4-diyldiamine	$C_8H_{15}N_2S$	171.283	82-83	0.273		11
2,4,5-T [93-76-5]	Gesatop	2,4,5-trichlorophenoxyacetic acid	$C_8H_5Cl_3O_3$	255.483	153	0.0555	2.80 2.88	
2,3,6-TBA [50-31-7]	Trysben, Cambilene	2,3,6-trichlorobenzoic acid	$C_7H_3Cl_3O_2$	225.457	124.5	0.106		
Terbacil [5902-51-2]	Sinbar	3-*tert*-butyl-5-chloro-6-methyluracil	$C_9H_{13}ClN_2O_2$	216.664	176	0.0330	9.0	
Terbumeton [33693-04-8]	Caragard	*N*-*tert*-butyl-*N*'-ethyl-6-methoxy-1,3,5-triazine	$C_{10}H_{19}N_5O$	225.290	123-124	0.108		9.41
Terbuthylazine [5915-41-3]	Gardoprim	*N*-*tert*-butyl-6-chloro-*N*'-ethyl-1,3,5-triazine-2,4-diamine	$C_9H_{16}ClN_5$	229.710	178	0.0320		12
Terbutryn [886-50-0]	Igran, Clarosan, Prebane	*N*-*tert*-butyl-*N*'-ethyl-6-methyl-thio-1,3,5-triazine-2,4-diamine	$C_{10}H_{19}N_5S$	241.357	104	0.168	4.30 4.07	9.7

Thiobencarb [28249-77-6]	Benthiocarb, Bolero, Saturno	*S*-4-chlorobenzyl-diethyl-thiocarbamate	$C_{12}H_{16}ClNOS$	257.779	1.7	1	
Triallate [2303-17-5]	Avadex BW, Far-Go	*S*-(2,3,3-trichloro-2-propenyl)-bis(1-methylethyl)carbamothioate	$C_{10}H_{16}Cl_3NOS$	304.664	29	0.914	
Triclopyr [55335–06–3]	Garlon, Truflon, Crossbow	3,5,6-trichloro-2-pyridinyloxyacetic acid	$C_7H_4Cl_3NO_3$	256.471	148–150	0.0607	2.68
Trifluralin [1582-09-8]	Treflan, Triflurex, Elancolan	2,6-dinitro-*N,N*-dipropyl-4-trifluoromethylaniline	$C_{13}H_{16}F_3N_3O_4$	335.279	49	0.581	
Vernolate [1929-77-7]	Surpass, Vernam	*S*-propyldipropylthiocarbamate	$C_{10}H_{21}NOS$	203.345	liquid	1	

Note: F.A.B. – fungicide algicide bactericide; G.R. – growth regulator
pK_a – acid dissociation constant; pK_b - basicity constant
(a) ester is quickly converted to parent acid.
* Assuming ΔS_{fus} = 56 J/mol K.

TABLE 17.2.2
Summary of selected physical-chemical properties of herbicides at 25°C

	Selected properties						Henry's law constant	
	Vapor pressure		Solubility					
Compound	P^S/Pa	P_L/Pa	S/(g/m³)	C^S/(mol/m³)	C_L/(mol/m³)	log K_{OW}	H/(Pa·m³/mol) calcd P/C	log K_{OC} reported
Alachlor	0.0020	2.88×10^{-3}	240	0.890	1.281	2.8	0.0022	2.23
Ametryn	0.0001	3.92×10^{-4}	185	0.814	3.191	2.58	1.23×10^{-4}	2.59
Amitrole	5.50×10^{-7}*	1.14×10^{-5}	280000	3330	68850	0.52	1.65×10^{-10}	2.04
Atrazine	4.00×10^{-5}	1.19×10^{-3}	30	0.139	4.140	2.75	2.88×10^{-4}	2.00
Barban	5.00×10^{-5}*	1.60×10^{-4}	11	0.043	0.1362	2.68	1.17×10^{-3}	2.66
Benefin	0.0088	0.0226	0.1	0.003	0.0077	5.29	29.4	3.95
Bifenox	3.20×10^{-4}	1.25×10^{-3}	0.35	0.0010	0.0040	4.48	0.313	
Bromacil	4.00×10^{-5}	8.46×10^{-4}	815	3.121	66.018	2.11	1.28×10^{-5}	1.86
Bromacil lithium salt	4.13×10^{-5}							1.51
Bromoxynil	6.40×10^{-4}	0.0307	130	0.469	22.54	< 2.0	1.36×10^{-3}	
Bromoxynil octanoate	6.40×10^{-4}	1.03×10^{-3}				5.4		4.25
sec-Bumeton	0.00097	3.98×10^{-3}	620	2.756	11.31		3.52×10^{-4}	2.30
Butachlor	6.0×10^{-4}	6.00×10^{-4}	23	0.074	0.074	4.50	8.14×10^{-3}	2.8
Butralin	0.0017	3.86×10^{-3}	1	0.0034	7.69×10^{-3}	4.54	0.502	3.75
Butylate	1.73	1.73	45	0.182	0.182	4.15	8.36	2.60
Chloramben	0.93	51.19	700	3.398	187.05	1.11	0.274	1.32
Chloramben salts	0		900000					1.18
Chlorbromuron	5.33×10^{-5}	2.69×10^{-4}	50	0.170	0.858		3.13×10^{-4}	2.7
Chlorfenac	1	19.75	200	0.835	16.50		1.20	
Chlorpropham	0.001	0.001	89*	0.417	0.600	3.51	2.40×10^{-3}	2.85, 2.8
Chlorsufuron	6.13×10^{-4}*	0.019	7000	19.56	609.4	–1.0	3.13×10^{-5}	1.6
Chlortoluron	1.70×10^{-5}	2.80×10^{-4}	70	0.329	5.418	2.38	5.17×10^{-5}	2.81
Cyanazine	2.13×10^{-7}	5.41×10^{-6}	171	0.710	18.03	2.22	3.00×10^{-7}	2.3
2,4-D	8.0×10^{-5}*	1.11×10^{-3}	400	1.810	25.12	2.81	4.42×10^{-5}	1.68-2.73
2,4-D (a)	0.001	0.0139	890	4.026	55.92	2.81	2.48×10^{-4}	
2,4-D DMA salt	0		796000	2991	12000			1.3
2,4-D esters			100					2.00
Dalapon	1.0×10^{-5}*	1.0×10^{-5}	502000	3510	3510	0.78	2.85×10^{-9}	0.48, 2.13
Dalapon sodium salt			900000	5455			0	
2,4-DB	0		46	0.185	1.539	3.53		2.64
2,4-DB butoxyethyl ester	0.00001		8					2.7
2,4-DB DMA salt	0		709000					1.30

Diallate	0.02	0.0224	50*	0.185	0.207	5.23	0.108	2.70
Dicamba	0.0045*	0.0349	4500	20.36	158.1	2.21	2.21×10^{-4}	0.342, –0.4
Dicamba salt			400000	1646				0.301
Dichlobenil	0.07*	1.076	18	0.105	1.609	2.74	0.669	2.91
Dichlorophen (F.A.B)	1.30×10^{-8}	4.24×10^{-7}	30	0.111	3.635		1.17×10^{-7}	
Dichloroprop	0.0004	3.25×10^{-3}	350	1.489	12.099	3.43	2.69×10^{-4}	3.0
Dichlorprop-P	6.20×10^{-5}	5.65×10^{-4}	590	2.510	22.855	1.95	2.47×10^{-5}	2.23
Dichlorprop(2,4-DP)ester	1.0×10^{-5}		50	0.149				3.00
Diclofop-methyl	4.67×10^{-4}*	6.57×10^{-4}	0.8	2.34×10^{-3}	3.30×10^{-3}	4.58	0.199	4.2
Dinitramine	0.00048	2.59×10^{-3}	1	0.0031	0.017	4.30	0.155	3.6
Dinoseb	0.01*	0.0141	50	0.208	0.293	3.56	0.048	2.85
Diphenamid	4.0×10^{-6}*	4.95×10^{-5}	260	1.087	13.46	1.92	3.68×10^{-6}	2.31
Diquat	1.30×10^{-5}	0.0170	700000	3800	4.96×10^{6}	–3.05*	3.42×10^{-9}	
Diquat dibromide	0		718000	2087				
Diuron	9.2×10^{-5}*	1.9×10^{-3}	40	0.172	3.630	2.78	6.83×10^{-4}	2.6
EPTC	2*	2.0	370	1.954	1.954	3.2	1.023	2.3
Fenopro (H., G.R.)	1.33×10^{-5}*	4.54×10^{-4}	140	0.519	17.73		2.56×10^{-5}	2.48
Fenuron	0.0267	0.305	3800	23.14	264.7	0.98	1.15×10^{-3}	1.43
Fenuron-TCA			4800	14.65	38.13			
Fluchloralin	0.004	6.03×10^{-3}	1	0.00281	0.0042	4.60*	1.343	3.50
Fluometuron	6.70×10^{-5}	1.61×10^{-3}	90	0.388	9.292	2.42	1.73×10^{-4}	2.24
Fluridone	1.3×10^{-5}	2.5×10^{-4}	12	0.036	0.7039	2.98	0.357	2.544-3.04
Fluorodifen	9.5×10^{-6}	4.47×10^{-6}	2	0.0061	0.0293	3.65		3.13
Glyphosate	4.0×10^{-5}*	2.15×10^{-3}	12000	70.96	3818.4	–1.6	5.64×10^{-7}	3.43-3.69
Ioxynil	0.001	0.066	50	0.135	8.904		7.42×10^{-3}	
Ioxynil-octanoate	0.0037	8.21×10^{-3}						
Isopropalin	0.0019	0.0019	0.11	3.56×10^{-4}	3.56×10^{-4}	4.71	5.34	4.0
Isoproturon	3.30×10^{-6}	6.52×10^{-5}	55	0.267	5.266	2.25	1.24×10^{-5}	1.86
Linuron	0.023*	6.74×10^{-2}	75	0.301	1.449	3.0	7.54×10^{-2}	2.91
MCPA (H., G.R.)	0.0002	1.70×10^{-3}	1605	8.001	68.05	2.69*	2.50×10^{-5}	2.03-2.07
MCPA dimethylamine salt							1.30	
MCPA ester	0.0002		5.0					3.00
MCPA-thioethyl	0.021	0.0309	2.3	0.0094	0.0138		2.234	
MCPB	5.77×10^{-5}*	3.18×10^{-4}	41	0.179	0.989	3.43	3.22×10^{-4}	
MCPB sodium salt	0		200000	798				1.30
Mecoprop	3.1×10^{-4}	1.53×10^{-3}	620	2.89	14.23	3.94	7.43×10^{-5}	
Mecoprop-P	4.0×10^{-4}	1.97×10^{-3}	860	4.007	19.73		9.98×10^{-5}	
Metobromuron	4.0×10^{-4}	2.02×10^{-3}	330	1.274	6.416	2.41	3.14×10^{-4}	

(Continued)

TABLE 17.2.2 (*Continued*)

	Selected properties							
	Vapor pressure		Solubility					
Compound	P^S/Pa	P_L/Pa	S/(g/m^3)	C^S/(mol/m^3)	C_L/(mol/m^3)	log K_{OW}	Henry's law constant H/(Pa·m^3/mol) calcd P/C	log K_{OC} reported
Metolachlor	0.0042*	4.20×10^{-3}	430	1.80	1.80	3.13	2.33×10^{-3}	2.26
Metoxuron	0.0043	0.0439	678	2.965	30.26	1.6	1.45×10^{-3}	
Molinate	0.75	0.750	970	5.179	5.179	3.21	0.145	1.92
Monolinuron	0.02	0.0732	735	3.425	12.54	2.30	5.84×10^{-3}	2.3
Monuron	6.66×10^{-5}	2.12×10^{-3}	230	1.007	32.08	1.94	6.62×10^{-5}	2.00
Neburon			4.8	0.017	0.1031	3.8		3.36
Nitralin	0.2	3.526	0.5	0.0014	0.0255		138.2	
Oryzalin	1.30×10^{-6}	1.87×10^{-5}	2.4	0.0069	0.0995	3.73	1.88×10^{-4}	2.78
Paraquat	< 0.0001		~700000					
Paraquat dichloride salt	0		620000					6.0
Pebulate	1.2*	1.20	92*	0.452	0.452	3.84	2.653	2.63
Pentanochlor			8	0.033	0.134			
Picloram	6.0×10^{-5}*	4.98×10^{-3}	430	1.781	147.7	0.3	3.37×10^{-5}	1.23
Picloram-potassium salt			1430.6				1.20	
Profluralin	0.009	0.0116	0.10	2.88×10^{-4}	3.7×10^{-4}	6.34	31.35	4.0
Prometon	0.0003	1.38×10^{-3}	750	3.329	15.31	2.99	9.01×10^{-5}	2.54
Prometryn	0.0001	8.70×10^{-4}	48	0.199	1.730	3.51	5.03×10^{-4}	2.60
Pronamide	0.011	0.208	15	0.059	1.105	3.26	0.188	2.90
Propachlor	0.03	0.0958	600	2.834	9.055	2.18	0.011	1.90
Propanil	0.005*	0.0230	200	0.917	4.218	3.07	5.45×10^{-3}	2.17
Propazine	3.90×10^{-6}	2.89×10^{-4}	8.6	0.037	2.766	2.90	1.04×10^{-3}	2.19
Propham	sublime		250	1.395	5.804	2.60		1.71
Propyzamide	5.80×10^{-5}	1.15×10^{-3}	15	0.059	1.157	3.28	9.90×10^{-4}	2.90
Pyrazon (chloridazon)	7*	441.8	360	1.625	102.5	1.14	4.309	2.08
Simazine	8.50×10^{-6}	8.27×10^{-4}	5	0.025	2.412	2.18	3.43×10^{-4}	2.11
Simetryne	9.47×10^{-5}	3.55×10^{-4}	450	2.110	7.904		4.49×10^{-5}	2.30
2,4,5-T	0.005*	0.0922	220	0.861	15.89	3.13	5.81×10^{-3}	1.72
2,3,6-TBA			7700	34.15	340.6	4.34		
Terbacil	5.0×10^{-5}	1.56×10^{-3}	710	3.277	102.1	1.89	1.53×10^{-5}	1.74
Terbumeton	2.70×10^{-4}	2.57×10^{-3}	130	0.577	5.500	3.04	4.68×10^{-4}	
Terbuthylazine	1.50×10^{-4}	4.89×10^{-3}	8.5	0.037	1.206	3.04	4.05×10^{-3}	2.21-2.44
Terbutryn	0.00013*	8.04×10^{-4}	22	0.091	0.564	3.74	1.43×10^{-3}	2.85
Thiobencarb	2.2	2.20	19.1	0.074	0.0741	3.42	29.69	

Triallate	0.015	0.0164	4	0.013	0.0144	4.29	1.14	3.38
Trifluralin	0.026*	0.0259	0.5*	1.49×10^{B3}	2.57×10^{B3}	5.34	10.08	4.14
Vernolate	0.90	0.90	90	0.443	0.443	3.84	2.034	2.414

Note: F.A.B. – fungicide algicide bactericide; G.R. – growth regulator, H - herbicide

2,4-D(a) physical-chemical properties modified from values used in Vol. IV.

* The reported values for this quantity vary considerably, whereas this selected value represents the best judgment of the authors. The reader is cautioned that it may be subject to large error.

TABLE 17.2.3
Suggested half-life classes of herbicides in various environmental compartments 25°C

Compound	Air class	Water class	Soil class	Sediment class
Atrazine	1	8	6	6
2,4-D	2	3	5	6
Dalapon	5	6	6	6
2,4-DB	3	4	4	5
Diallate	2	6	6	7
Dicamba	3	5	5	6
Diuron	2	5	6	7
EPTC	2	4	4	6
Glyphosate	4	6	6	7
Isopropalin	2	5	6	7
Linuron	2	5	6	7
Mecoprop	2	4	4	6
Metolachlor	4	6	6	7
Simazine	3	5	6	7
2,4,5-T	3	5	5	6
Triallate	4	6	4	5
Trifluralin	4	6	6	7

Class	Mean half-life (hours)	Range (hours)
1	5	< 10
2	17 (~ 1 day)	10–30
3	55 (~ 2 days)	30–100
4	170 (~ 1 week)	100–300
5	550 (~ 3 weeks)	300–1,000
6	1700 (~ 2 months)	1,000–3,000
7	5500 (~ 8 months)	3,000–10,000
8	17000 (~ 2 years)	10,000–30,000
9	55000 (~ 6 years)	> 30,000

17.3 REFERENCES

Abernethy, J.R., Davidson, J.M. (1971) Effect of calcium chloride on prometryne and fluometuron adsorption in soil. *Weed Sci.* 19, 517–521.

Abu-Qare, A.Q., Duncan, H.J. (2002) Photodegradation of the herbicide EPTC and the safener dichlormid, alone and in combination. Chemospere 1183–1189.

Agrochemicals Handbook (1989) *The Agrochemicals Handbook*, The Royal Society of Chemistry, Nottingham, England.

Alexander, M. (1973) Nonbiodegradable and other recalcitrant molecules. *Biotech. Bioeng*. 15, 611–647.

Alexander, M. (1974) Microbial formation of environmental pollutants. *Appl. Environ. Microbiol.* 15, 611–647.

Alexander, M., Aleem, M.I.H. (1961) Effect of chemical structure on microbial decomposition of aromatic herbicides. *J. Agric. Food Chem*. 9, 44–47.

Altom, J.D., Stritzke, J.F. (1973) Degradation of dicamba, picloram, and few phenoxy herbicides in soils. *Weed Sci.* 21, 556–560.

Anderson, J.P.E., Domsch, K.H. (1976) Microbial degradation of thiocarbamate herbicide diallate in soils and by pure cultures of soil microorganisms. *Arch. Environ. Contam. Toxicol.* 4, 1–7.

Ang, C., Meleady, K., Wallace L. (1989) Pesticide residues in drinking water in the north coast region of New South Wales, Australia. *Bull. Environ. Contam. Toxicol.* 42, 595–602.

Aquasol Database (1994) *Aquasol Database.* 5th Edition, Yalkowsky, S.H., Dannenfelzer, R.M., Editors, University of Arizona, Arizona.

Armbrust, K.L. (2000) Pesticide hydroxyl radical rate constants: measurements and estimates of their importance in aquatic environments. *Environ. Toxicol. Chem*. 19, 2175–2180.

Armstrong, D.E., Chesters, G., Harris, R.R. (1967) Atrazine hydrolysis in soil. *Soil Sci. Am. Proc.* 31, 61–66.

Ashton, F.M., Crafts, A.S. (1973) *Mode of Action of Herbicides*. John Wiley & Sons, New York.

Ashton, F.M., Crafts, A.S. (1981) *Mode of Action of Herbicides*. John Wiley & Sons, New York.

Atkinson, R. (1985) Kinetics and mechanisms of gas-phase reactions of hydroxyl radicals with organic compounds under atmospheric conditions. *Chem. Rev.* 85, 69–201.

Atkinson, R. (1987) Structure-activity relationship for estimation of rate constants for the gas-phase reactions of OH radicals with organic compounds. *Int'l. J. Chem. Kinetics* 19, 799–828.

Atkinson, R., Carter, W.P.L. (1984) Kinetics and mechanisms of the gas-phase reactions of ozone with organic compounds under atmospheric conditions. *Chem. Rev.* 84, 437–470.

Atkinson, R., Kwok, E.S.C., Arey, J. (1992) Photochemical processes affecting the fate of pesticides in the atmosphere. *Brighton Crop Prot. Conf.-Pests Dis.* (2), 469–476.

Attaway, H.H., Camper, N.D., Paynter, M.J.B. (1982a) Anaerobic microbial degradation of diuron by pond sediment. *Pest. Biochem. Physiol.* 17, 96.

Attaway, H.H., Paynter, M.J.B., Camper, N.D. (1982b) Degradation of selected phenylurea herbicides by anaerobic pond sediment. *J. Environ. Sci. Health* B17, 683–689.

Augustijn-Beckers, P.W.M., Hornsby, A.G., Wauchope, R.D. (1994) The SCS/ARS/CES pesticides database for environmental decision-making. II. Additional compounds. *Rev. Environ. Contam. Toxicol*. 137, 1–82.

Bacci, E., Calamari, D., Gaggi, C., Vighi, M. (1990) Bioconcentration of organic chemical vapors in plant leaves: Experimental measurements and correlation. *Environ. Sci. Technol.* 24, 885–889.

Bahnick, D.A., Doucette, W.J. (1988) Use of molecular connectivity indices to estimate soil sorption coefficients for organic chemicals. *Chemosphere* 17, 1703–1715.

Bailey, G.W., White, J.L. (1965) Herbicides - A compilation of their physical, chemical and biological properties. *Res. Rev.* 10, 1–97.

Baker, E.A., Hayes, A.L., Butler, R.C. (1992) Physicochemical properties of agrochemicals: their effects on foliar penetration. *Pestic. Sci*. 34, 167–182.

Ballantine, L.G., Newby, L.C., Simoneaux, B.J. (1978) Fate of atrazine in a marine environment. 4th International Congress of Pesticide Chemistry. Abstract No. V-528. IUPAC, Zurich, Switzerland.

Banks, P.A., Ketchersid, M.L., Merkle, M.G. (1979) The persistence of fluridone in various soils under field conditions and controlled conditions. *Weed Sci*. 27, 631.

Barak, E., Dinoor, A., Jacoby, B. (1983) Adsorption of systemic fungicides and a herbicide by some components of plant tissues, in relation to some physicochemical properties of the pesticides. *Pestic. Sci*. 14, 213–219.

Barnsley, G.E., Rosher, P.H. (1961) The relationship between the herbicidal effect of 2,6-dichlorobenzonitrile and its persistence in soil. *Weed Res*. 1, 147–158.

Battersby, N.S. (1990) A review of biodegradation kinetics in the aquatic environments. *Chemosphere* 21(10/11), 1243–1284.

Battersby, N S., Wilson, V. (1989) Survey of the anaerobic biodegradation potential of organic chemicals in digesting sludge. *Appl. Environ. Microbiol.* 55, 433–439.

Baur, J.R., Bovey, R. (1974) Ultraviolet and volatility loss of herbicides. *Arch. Environ. Contam. Toxicol.* 2, 275–288.

Beestman, G.B., Demming, J.M. (1974) Dissipation of acetamide herbicides from soils. *Agron. J.* 66, 308–544.

Beestman, G.B., Demming, J.M. (1976) Triallate mobility in soils. *Weed Sci.* 24, 541–544.

Behrendt, H., Bruggemann, R. (1993) Modelling the fate of organic chemicals in the soil plant environment: model study of root uptake of pesticides. *Chemosphere* 27, 2325–2332.

Belluck, D., Felsot, A. (1981) Bioconcentration of pesticides by egg masses of the caddisfly, *Triaenodes tardus* milne. *Bull. Environ. Contam. Toxicol*. 26, 299–306.

Benoit-Guyod, J.L., Crosby, D.G., Bowers, J.B. (1986) Degradation of MCPA by ozone and light. *Water Res.* 20, 67–72.

Beste, C.E., Humburg, N.E. (1983) *Herbicide Handbook of the Weed Science Society of America.* 5th Edition, Weed Science Society, Champaign, Illinois.

Beynon, K.I., Stoydin, G., Wright, A.N. (1972) The breakdown of the triazine herbicide cyanazine in soils and maize. *Pest. Sci*. 3, 293–305; 379–401.

Beynon, K.I., Stoydin, G., Wright, A.N. (1972) Comparison of the breakdown of the triazine herbicides cyanazine, atrazine and simazine in soils and in maize. *Pest. Biochem. Physiol.* 2, 153–161.

Beynon, K.I., Wright, A.N. (1972) The fates of herbicides chlorthiamid and dichlobenil in relation to residues in crops, soils and animals. *Res. Rev.* 43, 23–53.

Biagi, G.L., Guerra, M.C., Barbaro, A.M., Recanatini, M., Borea, P.A., Sapone, A. (1991) Lipophilicity for *s*-triazine herbicides. In: *QSAR in Environmental Toxicology IV.* Hermens, J.L., Opperhuizen, A., Editors, pp. 33–40, Elsevier, Amsterdam, The Netherlands.

Bintein, S., Devillers, J. (1994) QSAR for organic chemical sorption in soils and sediments. *Chemosphere* 28(6), 1171–1188.

Bjerke, E.L., Herman, J.L., Miller, P.W., Wetters, J.H. (1972) Residue study of phenoxy herbicides in milk and cream. *J. Agric. Food Chem*. 20, 963–967.

Bottoni, P., Funari, E. (1992) Criteria for evaluating the impact of pesticides on groundwater quality. *Sci. Total Environ*. 123/124, 581–590.

Bouchard, D C., Wood, A.L. (1988) Pesticides sorption on geologic material of varying organic carbon content. *Toxicol. Ind. Health* 4, 341–349.

Bowman, B.T. (1990) Mobility and persistence of alachlor, atrazine and metolachlor in plain field sand, and atrazine and isazofos in honeywood silt loam, using lysimeters. *Environ. Toxicol. Chem.* 9, 453–461.

Bowman, B.T., Sans, W.W. (1979) The aqueous solubility of twenty-seven insecticides and related compounds. *J. Environ. Sci. Health* B14(6), 625–634.

Bowman, B.T., Sans, W.W. (1983a) Further water solubility determination of insecticidal compounds. *J. Environ. Sci. Health* B18(2), 221–227.

Bowman, B.T., Sans, W.W. (1983b) Determination of octanol-water partitioning coefficients (K_{OW}) of 61 organophosphorous and carbamate insecticides and their relationship to respective water solubility (S) values. *J. Environ. Sci. Health* B18(6), 667–683.

Braumann, T., Grimme, L.H. (1981) Determination of hydrophobic parameters for pyridazinone herbicides by liquid-liquid partition and reversed-phase high-performance liquid chromatography. *J. Chromatogr.* 206(1), 7–15.

Braumann, T., Weber, G., Grimme, H. (1983) Quantitative structure-activity relationship for herbicides. Reversed-phase liquid chromatographic retention parameter log k_w *versus* liquid-liquid partition coefficient as a model of the hydrophobicity of phenylureas *s*-triazines and phenoxycarbonic acid derivatives. *J. Chromatogr.* 261, 329–343.

Brewer, F., Lavy, T.L., Talbert, R.E. (1982) Effects of flooding on dinitroaniline persistence in soybean (*Glycine max*)-rice (*Oryza sativa*) rotation. *Weed Sci.* 30, 531–539.

Briggs, G.G. (1969) Molecular structure of herbicides and their sorption by soils. *Nature* 223, 1288.

Briggs, G.G. (1981) Theoretical and experimental relationships between soil adsorption, octanol-water partition coefficients, water solubilities, bioconcentration factors, and the parachor. *J. Agric. Food Chem.* 29, 1050–1059.

Brooke, D., Nielsen, I., De Bruijn, J., Hermens, J. (1990) An interlaboratory evaluation of the stir-flask method for the determination of octanol water partition coefficients. (LOG POW). *Chemosphere* 21, 119–133.

Broto, P., Moreau, G., Vandycke, C. (1984) Molecular structure: Perception, autocorrelation descriptor and SAR studies. System of atomic contribution for the calculation of the *n*-octanol/water partition coefficients. *Eur. J. Med. Chem. Chim. Term*. 19, 71–78.

Brown, D.F., McDonough, L.M., McCool, D.K., Papendick, R.I. (1984) High performance liquid chromatographic determination of bromoxynil octanoate and metribuzin in runoff water from wheat fields. *J. Agric. Food Chem.* 32, 195–200.

Brown, D.S., Flagg, E.W. (1981) Empirical prediction of organic pollutant sorption in natural sediments. *J. Environ. Qual.* 10, 382–386.

Brusseau, M.L., Rao, P.S.C. (1989) The influence of sorbate-organic matter interactions of sorption nonequilibrium. *Chemosphere* 18, 1691–1706.

Brust, H.F. (1966) A summary of chemical and physical properties of Dursban. *Down to Earth* 22(3), 21–22.

Budavari, S., Editor (1989) *The Merck Index. An Encyclopedia of Chemicals, Drugs and Biologicals.* 11th Edition, Merck and Co., Rahway, New Jersey.

Burkhard, N., Eberle, D.O., Guth, J.A. (1975) Model systems for studying the environmental behaviour of pesticides. *Environ. Quality & Safety* Supplement VIII, 204–213.

Burkhard, N., Guth, J.A. (1976) Photodegradation of atrazine, altraton and ametryne in aqueous solution with acetone as a photosensitizer. *Pest. Sci.* 7, 65–71.

Burkhard, N., Guth, J.A. (1981) Rate of volatilization of pesticides from soil surfaces; comparison of calculated results with those determined in a laboratory model system. *Pest. Sci.* 12, 37–44.

Burkhard, N., Guth, J.A. (1981) Chemical hydrolysis of 2-chloro-4,6-bis(alkylamino)-1,3,5-triazine herbicides and their breakdown in soil under the influence of adsorption. *Pest. Sci.* 12(1), 45–52.

Buxton, G.V., Greenstock, C.L., Helman, W.P., Ross, A.B. (1988) Critical review of rate constants for reactions of hydrated electrons, hydrogen atoms and hydroxyl radicals (-OH/-O^-) in aqueous solution. *J. Phys. Chem. Ref. Data* 17, 513–886.

Bysshe, S.E. (1982) Chapter 5, Bioconcentration factor in aquatic organisms. In: *Handbook on Chemical Property Estimation Methods, Environmental Behavior of Organic Compounds.* Lyman, W.J., Reehl, W.F., Rosenblatt, D.H., Editors, McGraw-Hill, Inc., New York.

Call, D.J., Brooke, L.T., Kent, R.J., Poirier, S.H., Knuth, M.L., Shubat, P.J., Slick, E J. (1984) Toxicity, uptake, and elimination of the herbicides alachlor and dinoseb in freshwater fish. *J. Environ. Qual.* 13, 493–498.

Call, D.J., Brooke, L.T., Kent, R.J., Knuth, M.L., Poirier, S.H., Huot, J.M., Lima, A.R. (1987) Bromacil and diuron herbicides: Toxicity, uptake, and elimination in freshwater fish. *Arch. Environ. Contam. Toxicol.* 16, 607–613.

Camper, N.D., Stralka, K., Skipper, H.D. (1980) Aerobic and anaerobic degradation of profluralin and trifluralin. *J. Environ. Sci. Health* B15, 457–473.

Capel, P.D., Larson, S.J. (1995) A chemodynamic approach for estimating losses of target organic chemicals from water during sample holding time. *Chemosphere* 30, 1097–1107.

Carlson, W.C., Lignowski, E.M., Hopen, H.J. (1975) Mode of action of pronamide. *Weed Sci.* 23, 155–161.

Carringer, R.D., Weber, J.B., Monaco, T.J. (1975) Adsorption-desorption of selected pesticides by organic matter and montmorillonite. *J. Agric Food Chem.* 23, 568–572.

Carsel, R.F. (1989) Hydrologic processes affecting the movement of organic chemicals in soils. In: *Reactions and Movement of Organic Chemicals in Soils*. SSSA Special Publication No. 22, Sawhney, B.L., Brown, K., Eds., pp. 439–445, Soil Science Society of America and Society of Agronomy, Madison, Wisconsin.

Caux. P.-Y., Kent, R.A., Taché, M., Grande, C., Fan, G.T., MacDonald, D.D. (1993) Environmental fate and effects of dicamba: A Canadian perspective. *Rev. Environ. Contam. Toxicol.* 133, 1–58.

Celis, R., Barriuso, E., Houot, S. (1998) Effect of liquid sewage sludge addition on atrazine sorption and desorption by soil. *Chemosphere* 37, 1091–1107.

Cessna, A.J., Grover, R. (1978) Spectrophotometric determination of dissociation constants of selected acidic herbicides. *J. Agric. Food Chem.* 26, 289–293.

Cessna, A.J., Muir, D.C.G. (1991) Photochemical transformations. In: *Environmental Chemistry of Herbicides.* Vol. II, Grover, R., Cessna, A.J., Editors, Chapter 6, pp. 199–264, CRC Press, Boca Raton, Florida.

Chaumat, E., Chamel, A., (1991) Sorption and permeation to phenylurea herbicides of isolated cuticles of fruit and leaves. Effect of cuticular characteristics and climatic parameters. *Chemosphere* 22, 85–97.

Chau, A.S.Y., Thomson, K. (1978) Investigation of the integrity of seven herbicidal acids in water samples. *J. Assoc. Off. Anal. Chem.* 61, 481–485.

Chefetz, B., Bilkis, Y.I., Polubesova, T. (2004) Sorption-desorption behavior of triazine and phenylurea herbicides in Kishon river sediments. *Water Res.* 38, 4383–4394.

Chen, Y-L., Chen, J-S. (1979) Degradation and dissipation of herbicide butachlor in paddy fields. *J. Pest. Sci.* 4, 431.

Chen, Y.-L., Lo, C.-C., Wong, Y.-S. (1982) Photodecomposition of herbicide butachlor in aqueous solution. *J. Pest. Sci.* 7, 41.

Cheung, M.W., Biggar, J.W. (1974) Solubility and molecular structure of 4-amine-3,5,6-trichloropicolinic acid in relation to pH and temperature. *J. Agric. Food Chem.* 22, 202–206.

Chung, K.H., Ro, K.S., Roy, D. (1996) Fate and enhancement of atrazine biotransformation in anaerobic wetland sediment. *Water Res.* 30, 341–346.

Colbert, F.O., Volk, V.V., Appleby, A.P. (1975) Sorption of atrazine, terbutryn and GS-14254 on natural and lime-amended soils. *Weed Sci.* 23, 390–394.

Comfort, S.D., Inskeep, W.P., Macut, R.E. (1992) Degradation and transport of dicamba in a clay soil. *J. Environ. Qual.* 21, 653–658.

Corbin, F.T., Upchurch, R.P. (1967) Influence of pH on detoxification of herbicides in soils. *Weeds* 15, 370–377.

Corwin, D.L., Farmer, W.J. (1984) Non-single-valued adsorption-desorption of bromacil and diquat by freshwater sediments. *Environ. Sci. Technol.* 18, 507–514.

Crosby, D.G., Leitis, E. (1973) The photodecomposition of trifluralin in water. *Bull. Environ. Contam. Toxicol.* 10, 237.

Crosby, D.G., Tang, C.-S. (1969) Photodecomposition of 3-(*p*-chlorophenyl)-1,1-dimethylurea (monuron). *J. Agric. Food. Chem.* 17, 1041–1043.

Crosby, D.G., Wong, A.S. (1973) Photodecomposition of 2,4,5-trichlorophenoxyacetic acid (2,4,5-T) in water. *J. Agric. Food. Chem.* 21, 1052.

Cunningham, J.J., Kemp, W.M., Stevenson, J.C., Boynton, W.R., Means, J.C. (1981) Stress effects of agricultural herbicides on submerged macrophytes in estuarine microcosms. pp. 147–182. In: Submerged aquatic vegetation in Chesapeake Bay. Annual Report to USEPA, UMCEES, Horn Point Environmental Laboratories, Cambridge, Maryland.

Dao, T.H., Lavy, T.L., Sorensen, R.C. (1979) Atrazine degradation and residue distribution in soil. *Soil Sci. Soc. Am. J.* 43, 1129–1134.

Dao, T.H., Lavy, T.L., Dragun, J. (1983) Rationale of the solvent selection for soil extraction of pesticide residues. *Res. Rev.* 87, 91–104.

Davidson, J.M., McDougal, J.R. (1973) Experimental and predicted movement of three herbicides in a water-saturated soil. *J. Environ. Qual.* 2, 428–433.

Davidson, J.M. et al. (1980) Adsorption, Movement and Biological Degradation of Large Concentration of Selected Pesticides in Soils. U.S. EPA-600/2-80-124.

Day, B.E., Jordon, L.S., Russell, R.C. (1963) Persistence of dalapon residues in California soils. *Soil Sci.* 95, 326–330.

Day, K.E. (1991) Pesticide transformation products in surface waters. Effects on aquatic biota. pp. 217–241. In: *Pesticide Transformation Products. Fate and Significance in the Environment.* ACS Sym. series 457, Somasundaram, L., Coats, J.R., Editors, Chapter 16, American Chemical Society, Washington DC.

Dean, J.D., Editor (1985) *Lange's Handbook of Chemistry.* 13th Edition, McGraw-Hill, New York.

Delle Site, A. (1997) The vapor pressure of environmentally significant organic chemicals: A review of methods and data at ambient temperature. *J. Phys. Chem. Ref. Data* 26, 157–193.

Delle Site, A. (2001) Factors affecting sorption of organic compounds in natural sorbent/water systems and sorption coefficients for selected pollutants. A review. *J. Phys. Chem. Ref. Data* 30, 187–439.

DePablo, R.S. (1976) Determination of saturated vapor pressure in range 10^{-1}–10^{-4} torr by effusion method. *J. Chem. Eng. Data* 21, 141–143.

Deuel, L.E., Turner, F.T., Brown, K.W., Price, J.D. (1978) Persistence and factors affecting dissipation of molinate under flooded rice culture. *J. Environ. Quality* 7, 373.

Devillers, J., Bintein, S., Domine, D. (1996) Comparison of BCF models based on log P. *Chemosphere* 33(6), 1047–1065.

Di Guardo, A., Calamari, D., Zanin, G., Consalter, A., Mackay, D. (1994) A fugacity model of pesticide runoff to surface water: development and validation. *Chemosphere* 28, 511–531.

Dixon, D., Rissman, E. (1985) Physical-Chemical Properties and Categorization of RCRA Wastes According to Volatility. U.S. EPA Report No. 450/3-85-007. NTIS PB 85-404527, Springfield, Virginia.

Dobbs, A.J., Cull, M.R. (1982) Volatilization of chemicals-relative loss rates and the estimation of vapor pressures. *Environ. Pollut.* (series B) 3, 289–298.

Dobbs, A.J., Hart, G.F., Parsons, A.H. (1984) The determination of vapour pressures from relative volatilization rates. *Chemosphere* 13, 687–692.

Donati, L., Keizer, J., Bottoni, P., Scenati, R., Funar, E. (1994) Koc estimation of diethylatrazine, diisopropylatrazine, hexazionone, and terbuthylazine by reversed phase chromatography and sorption isotherms. *Toxicol. Environ. Chem.* 44(1–2), 1–10.

Donovan, S.F. (1996) New method for estimating vapor pressure by the use of gas chromatography. *J. Chromatogr. A*, 749, 123–129.

Donovan, S.F., Pescatore, M.C. (2002) Method for measuring the logarithm of the octanol-water partition coefficient by using short octadecyl-poly(vinyl alcohol) high-performance liquid chromatography columns. *J. Chromatog*. A, 952, 47–61.

Dörfler, U., Alder-Köhler, R., Schneider, P., Scheunert, I., Korte, F. (1991) A laboratory model system for determining the volatility of pesticides from soil and plant surfaces. *Chemosphere* 23(4), 485–496.

Dousset, C., Mouvet, C., Schiavon, M. (1994) Sorption of terbuthylazine and atrazine in relation to the physicochemical properties of three soils. *Chemosphere* 28, 467–476.

Dowd, J.F., Bush, P.B., Neary, D.G., Taylor, J.W., Berisford, Y.C. (1993) Modeling pesticide movement in forested watersheds: Use of PRZM for evaluating pesticide options in loblolly pine stand management. *Environ. Toxicol. Chem.* 12, 429–439.

Doyle, R.C., Kaufman, D.D., Burt, G.W. (1978) Effect of dairy manure and sewage sludge on ^{14}C-pesticide degradation in soil. *J. Agric. Food Chem.* 26, 987–989.

Draper, W.M., Crosby, D.G. (1984) Solar photooxidation of pesticides in dilute hydrogen peroxide. *J. Agric. Food Chem.* 32, 231.

Duah-Yentumi, S., Kuwatsuka, S. (1980) Effect of organic matter and chemical fertilizers on the degradation of benthiocarb and MCPA herbicides in the soil. *Soil Sci. Plant Nutr.* 26, 541.

Dubelman, S., Bremer, M.J. (1983) Determination of the octanol/water partition coefficient of MAPC products. Report No. MSL-3219, Monsanto Company Agricultural Research Division, St. Louis.

Eadsforth, C.V., Moser, P. (1983) Assessments of reversed phase chromatographic methods for determining partition coefficients. *Chemosphere* 12, 1459–1475.

Edwards, C.A. (1973) *Persistent Pesticides in the Environment*. 2nd Edition, CRC Press, Cleveland, Ohio.

Edwards, C.A. (1977) Nature and origins of pollution of aquatic systems by pesticides. In: *Pesticides in Aqatic Environments*. Khan, M.A.Q., Editor, Plenum Press, New York.

Eichelberger, J.W., Lichtenberg, J.J. (1971) Persistence of pesticides in river water. *Environ. Sci. Technol.* 5, 541–544.

Eisler, R. (1985) *Atrazine Hazards to Fish, Wildlife, and Invertebrates: A Synoptic Review.* U.S. Fish and Wildlife Service Biological Rep. 53pp.

El-Dib, M.A., Aly, O.M. (1976) Persistence of some phenylamide pesticides in the aquatic environment. I. Hydrolysis. *Water Res.* 10, 1047.

El-Dib, M.A., Abou-Waly, H.F. (1998) Biodegradation of some triazines and phenylureas in surface waters. *Water Res.* 32, 1881–1887.

Elgar, K.E. (1983) Pesticide residues in water-An appraisal. In: *International Union of Pure and Applied Chemistry. Pesticide Chemistry: Human Welfare and the Environment*. Vol. 4, Miyamoto, J., Kearney, P.C., Editors, Pergamon Press, Oxford, England.

Ellgehausen, H., Guth, J.A., Esser, H.O. (1980) Factors determining bioaccumulation potential of pesticides in the individual compartments of aquatic food chains. *Ecotoxicol. Environ. Saf.* 4, 134–157.

Ellgehausen, H., D'Hondt, C., Fuerer, R. (1981) Reversed-phase chromatography as a general method for determining octanol/water partition coefficients. *Pest. Sci.* 12, 219.

Ellington, J.J., Stancil, F.E., Payne, W.D. (1987) Measurement of Hydrolysis Rate Constants for Evaluation of Hazardous Waste Land Disposal. Volume 1, Data on 32 chemicals. U.S. EPA-600/3-86/043, Washington, DC.

Ellington, J.J., Stancil, F.E., Payne, W.D. (1987) Measurement of Hydrolysis Rate Constants for Evaluation of Hazardous Waste Land Disposal. Volume 2, Data on 54 chemicals. U.S. EPA, EPA-600/53-87/019, Washington, DC.

Ellington, J.J., Stancil, F.E., Payne, W.D., Trusty, C.D. (1988) Measurement of Hydrolysis Rate Constants for Evaluation of Hazardous Waste Land Disposal. Volume 3, Data on 70 chemicals. U.S. EPA, EPA-600/3-88/028, NTIS PB 88-234042, Springfield, Virginia.

Ellis, P.A., Camper, N.D. (1982) Aerobic degradation of diuron by aquatic microorganisms. *J. Environ. Sci. Health* B17, 277–290.

Erkell, L., Walum, E. (1979) Differentiation of cultured neuroblastoma cells by urea derivatives. *Febs Letters* 104, 401.

Evelyne, C., André, C., Georges, T., Michel, T. (1992) Quantitative relationships between structure and penetration of phenylurea herbicides through isolated plant cuticles. *Chemosphere* 24(2), 189–200.

Farmer, W.J. (1976) *A Literature Survey of Benchmark Pesticides.* Science Communication Division of Dept. of Medical and Public Affairs, Medical Center of George Washington University, Washington DC.

Faust, B.C., Hoigné, J. (1990) Photolysis of Fe(III)-hydroxy complexes as sources of OH radicals in clouds, fog and rain. *Atmos. Environ*. 24A, 79–89.

Feigenbrugel, V., Le Calvé, S., Mirabel, P. (2004) Temperature dependence of Henry's law constants of metolachlor and diazinon. *Chemosphere* 57, 319–327.

Fendinger, N.J., Glotfelty, D.E. (1988) A laboratory method for the determination of air-water Henry's law constants for several pesticides. *Environ. Sci. Technol.* 22, 1289–1293.

Fendinger, N.J., Glotfelty, D.E., Freeman, H.P. (1989) Comparison of two experimental techniques for determining air-water Henry's law constants. *Environ. Sci. Technol.* 23(12), 1528–1531.

Finizio, A., Di Guardo, A., Arnoldi, A., Vighi, M., Fanelli, R. (1991) Different approaches for the evaluation of K_{OW} for *s*-triazine herbicides. *Chemosphere* 23, 801–812.

Finizio, A., Vighi, M., Sandroni, D. (1997) Determination of *n*-octanol/water partition coefficient (K_{OW}) of pesticide. Critical review and comparison of methods. *Chemosphere* 34, 131–161.

Foy, C.L. (1976) The chlorinated aliphatic acid. In: *Herbicides: Chemistry, Degradation and Mode of Action.* Marcel Dekker, New York.

Francioso, O., Bak, E., Rossi, N., Sequi, P. (1992) Sorption of atrazine and trifluralin in relation to the physico-chemical characteristics of selected soils. *Sci. Total Environ.* 123/124, 503–512.

Frank, R., Clegg, B.S., Patni, N.K. (1991) Dissipation of cyanazine and metolachlor on a clay loam, Ontario, Canada, 1987–1990. *Arch. Environ. Contam. Toxicol.* 21, 253–262.

Freed, V.H. (1953) Herbicides mechanisms – Mode of action other than aryloxyalkyl acids. *J. Agric. Food Chem.* 1, 47–51.

Freed, V.H. (1966) Chemistry of herbicides. In: *Pesticides and Their Effects on Soils and Water.* Breth, S.A., Editor, pp. 28–39, Soil Science Society of America.

Freed, V.H. (1976) Solubility, hydrolysis, dissociation constants and other constants of benchmark pesticides. In: *A Literature Survey of Benchmark Pesticides*. pp. 1–18, Medical Center of George Washington University, Washington DC.

Freed, V.H., Burschel, P. (1957) The relationship of water solubility to dosage of herbicides. *Z. Pflanzenkrankh,* μ. *Pflanzenschutz* 64, 477.

Freed, V.H., Haque, R. (1973) Chapter 10, Adsorption, movement, and distribution of pesticides in soil. In: *Pesticide Formulations*. Van Valkenburg, Editor, pp. 441–459, Marcel Dekker, New York.

Freed, V.H., Haque, R., Vernetti, J. (1967) Thermodynamic properties of some carbamates and thiocarbamates in aqueous solutions. *J. Agric. Food Chem.* 15, 1121–1123.

Freese, E., Levin, B.C., Pearce, R., Sreevalson, T., Kaufman, J.J., Koski, W.S., Semo, N.M. (1979) Correlation between the growth inhibitory effects, partition coefficients and teratogenic effects of lipophilic acids. *Teratology* 20(3), 413–440.

Freiberg, M.B., Crosby, D.G. (1986) Loss of MCPA from simulated spray droplets. *J. Agric. Food Chem.* 34, 92–95.

Freitag, D., Balhorn, L., Geyer, H., Körte, F. (1985) Environmental hazard profile of organic chemicals. An experimental method for the assessment of the behaviour of chemicals in the ecosphere by simple laboratory tests with C-14 labelled chemicals. *Chemosphere* 14, 1589–1616.

Freitag, D., Geyer, H., Kraus, A., Viswanathan, R., Kotzias, D., Attar, A., Klein, W., Körte, F. (1982) Ecotoxicological profile analysis. VII. Screening chemicals for their environmental behavior by comparative evaluation. *Ecotoxicol. Environ. Saf.* 6, 60–81.

Freitag, D., Lay, J.P., Körte, F. (1984) Environmental hazard profile - Test results to structure and translation into the environment. In: *QSAR in Environmental Toxicology.* Kaiser, K.L.E., Editor, pp. 111–136, D. Reidel Publishing Company, Dordrecht, The Netherlands.

Friedrich, K., Stammbach, K. (1964) Gas chromatographic determination of small vapour pressures. Determination of the vapour pressures of some triazine herbicides. *J. Chromatogr.* 16, 22–28.

Fujita, T., Iwasa, J., Hansch, C. (1964) A new substituent constant derived from partition coefficients. *J. Am. Chem. Soc*. 86(23), 5175–5180.

Funderburk, Jr., H.H., Bozarth, G.A. (1967) Review of the metabolism and decomposition of diquat and paraquat. *J. Agric. Food Chem*. 15(4), 563–567.

Funderburk, Jr., H.H., Negi, N.S., Lawrence, J.M. (1960) Photochemical decomposition of diquat and paraquat. *Weeds*. 14, 240.

Furmidge, C.G., Osgerby, J.M. (1967) Persistence of herbicides in soil. *J. Sci. Food Agric.* 18, 269.

Gao, J.P., Maguhn, J., Spitzauer, P., Kettrup, A. (1997) Distribution of pesticides in the sediment of the small Teufelsweiher pond (Southern Germany). *Wat. Res*. 31, 2811–2819.

Gao, J.P., Maguhn, J., Spitzauer, P., Kettrup, A. (1998) Sorption of pesticides in the sediment of the Teufelsweiher pond (Southern Germany). I: Equilibrium assessments, effect of organic carbon content and pH. *Wat. Res*. 32, 1662–1672.

Gaillardon, P., Calvert, R., Terce, M. (1977) Adsorption and desorption of terbutryne by a calcium-montmorerillonite and humic acid alone or in combination. *Weed Res.* 17, 41–48.

Garten, Jr., C.T., Trablka, J.R. (1983) Evaluation of models for predicting terrestrial food chain behavior of xenobiotics. *Environ. Sci. Technol.* 17, 590–595.

Gautier, C. Le Calvé, C., Miabel, P. (2003) Henry's law constants measurements of alachlor and dichlorvos between 283 and 298 K. *Atmos. Environ*. 37, 2437–2453.

Gawlik,. B.M., Feicht, E.A., Karcher, W., Kettup, A., Mujntau, H. (1998) Application of the European reference soil set (EUROSOILS) to a HPLC-screening method for the estimation of soil adsorption coefficients of organic compounds. *Chemosphere* 36, 2903–2919.

Gawlik, B.M., Bo, F., Kettrup, A., Muntau, H. (1999a) Characterisation of a second generation of European reference soils for sorption studies in the framework of chemical testing - Part I: chemical composition and pedological properties. *Sci. Total Environ*. 229, 99–107.

Gawlik, B.M., Kettrup, A., Muntau, H. (1999b) Characterisation of a second generation of European reference soils for sorption studies in the framework of chemical testing - Part II: soil adsorption behaviour of organic chemicals. *Sci. Total Environ*. 229, 109–120.

Gawlik, B.M., Kettrup, A., Muntau, H. (2000) Estimation of soil adsorption coefficients of organic compounds by HPLC screening using the second generation of the European reference soil set. *Chemosphere* 41,7–1347.

Geller, A. (1980) Studies on degradation of atrazine by bacterial communities enriched from various biotypes. *Arch. Environ. Contam. Toxicol.* 9, 289.

GEMS (1986) Graphical Exposure Modeling Systems. Fate of atmospheric pollutants (FAP) database. Office of Toxic Substances, U.S. Environmental Protection Agency.

Gerstl, Z. (1990) Estimation of organic chemical sorption by soils. *J. Contam. Hydrology* 6, 367–375.

Gerstl, Z., Helling, C.S. (1987) Evaluation of molecular connectivity as a predictive method for the adsorption of pesticides by soils. *J. Environ. Sci. Health* B22, 55–69.

Gerstl, Z., Kilger, L. (1990) Fractionation of the organic matter in soils and sediments and their contribution to the sorption of pesticides. *J. Environ. Sci. Health* 825, 729–741.

Gerstl, Z, Mingelgrin, U. (1984) Sorption of organic substances by soils and sediments. *J. Environ. Sci. Health* B19(3), 297–312.

Getzen, F.W., Ward, T.M. (1971) Influence of water structure on aqueous solubility. *Ind. Eng. Chem. Prod. Res. Develop.* 10, 122–132.

Geyer, H., Kraus, A.G., Klein, W., Richter, E., Korte, F. (1980) Relationship between water solubility and bioaccumulation potential of organic chemicals in rats. *Chemosphere* 9, 277–291.

Geyer, H., Politzki, G., Freitag, D. (1984) Prediction of ecotoxicological behaviour of chemicals: Relationship between *n*-octanol/water partition coefficient and bioaccumulation of organic chemicals by alga *Chlorella*. *Chemosphere* 13, 269–284.

Geyer, H., Scheunert, I., Brüggemann, R., Steinberg, C., Korte, F., Kettrup, A. (1991) QSAR for organic chemical bioconcentration in daphnia, algae, and mussels. *Sci. Total Environ.* 109/110, 387–394.

Geyer, H., Sheenhan, P., Kotzias, D., Freitag, D., Korte, F. (1982) Prediction of ecotoxicological behaviour of chemicals: relationship between physicochemical properties and bioaccumulation of organic chemicals in the mussel *mytilus edulis. Chemosphere* 11, 1121–1134.

Geyer, H., Visvanathan, R., Freitag, D., Korte, F. (1981) Relationship between water solubility of organic chemicals and their bioaccumulation by the alga *Chlorella*. *Chemosphere* 10, 1307–1313.

Ghossemi, M., Fargo, L., Painter, P., Quinlivan, S., Scofield, R., Takata, A. (1981) Environmental fates and impacts of major forest use pesticides and toxic substances. A-149 (Citing glyphosate registration data). Washington DC.

Ghosh, P.K., Philip, L. (2004) Atrazine degradation in anaerobic environment by a mixed microbial consortium. *Wat. Res*. 38, 2276–2283.

Gingerich, L.L., Zimdahl, R.L. (1976) Soil persistence of isopropalin and oryzalin. *Weed Sci.* 24, 431–434.

Gish, T.J., Sadeghi, A., Wienhold, B.J. (1995) Volatilization of alachlor and atrazine as influenced by surface litter. *Chemosphere* 31, 2971–2982.

Glass, B.L. (1975) Photosensitization and luminescence of picloram. *J. Agric. Food Chem*. 23, 1109.

Glotfelty, D.E. (1981) Atmospheric dispersion of pesticides from treated fields. Ph.D. Thesis of University of Maryland, College Park, Maryland.

Glotfelty, D.E., Taylor, A.W., Turner, B.C., Zoller, W.H. (1984) Volatilization of surface-applied pesticides from fallow soils. *J. Agric. Food Chem.* 32, 638–643.

Glotfelty, D E., Leech, M.M., Jersey, J., Taylor, A.W. (1989) Volatilization and wind erosion of soil surface applied atrazine, simazine, alachlor, and toxaphene. *J. Agric. Food Chem.* 37, 546–551.

Golab, T., Althaus, W.A., Wooten, H.L. (1979) Fate of ^{14}C trifluralin in soil. *J. Agric. Food Chem*. 27, 163–179.

Goodman, M.A. (1997) Vapor pressure of agrochemicals by the Knudsen effusion method using a quartz crystal microbalance. *J. Chem. Eng. Data* 42, 1227–1231.

Görge, G., Nagel, R. (1990) Kinetics and mechanism of ^{14}C-lindane and ^{14}C-atrazine in early life stages of zebra fish (*Brachdanio rerio*). *Chemosphere* 21, 1125–1137.

Goswami, K.P., Green, R.E. (1971) Microbial degradation of the herbicide atrazine and its 2-hydroxy analog in submerged soils. *Environ. Sci. Technol.* 5, 426.

Grain, C.F. (1982) Chapter 14, Vapor pressure. In: *Handbook on Chemical Property Estimation Methods. Environmental Behavior of Organic Compounds.* Lyman, W.J., Reehl, W.F., Rosenblatt, D.H., Editors, McGraw-Hill, New York.

Gramatica, P., Corradi, M., Consonni, V (2000) Modelling and prediction of soil sorption coefficients of non-ionic organic pesticides by molecular descriptors. *Chemosphere* 41, 762–777.

Grayson, B.T., Fosbracey, L.A. (1982) Determination of the vapor pressure of pesticides. *Pest. Sci.* 13, 269–278.

Grayson, B.T., Kleiser, D.A. (1990) Phloem mobility of xenobiotics. IV. Modeling of pesticide movement in plants. *Pestic. Sci.* 30, 67–79.

Grover, R. (1974) Adsorption and desorption of trifluralin, triallate and diallate by various adsorbents. *Weed Sci.* 22(4), 405–408.

Grover, R. (1991) Chapter 2, Nature transport, and fate of airborne residues. In: *Environmental Chemistry of Herbicides.* Vol. II., Grover, R., Cessna, A.J., Editors, pp. 90–117, CRC Press, Boca Raton, Florida.

Grover, R., Cessna, A.J., Editors (1991) *Environmental Chemistry of Herbicides.* Volume II, CRC Press, Boca Raton, Florida.

Grover, R., Cessna, A.J., Banting, J.D., Morse, P.M. (1979) Adsorption and bioactivity of diallate, triallate and trifluralin. *Weed Res.* 19, 363–369.

Grover, R., Spencer, W.F., Farmer, W., Shoup, T.D. (1978) Triallate vapor pressure and volatilization from glass surfaces. *Weed Sci.* 26, 505–508.

Grover, R., Wolt, J.D., Cessna, A.J., Schiefer, H.B. (1997) Environmental fate of trifluralin. *Rev. Environ. Contam. Toxicol.* 153, 1–64.

Guenzi, W.D., Beard, W.E. (1974) In: *Pesticides in Soil and Water.* Guenzi, W.D., Editor, American Soil Science Society, Madison, Wisconsin. pp. 108–122.

Gunkel, G., Streit, B. (1980) Mechanisms of bioaccumulation of a herbicide (atrazine, *s*-triazine) in a freshwater mollusc (*Ancylus fluviatilis* müll) and a fish (*Coregonus fera* jurine). *Wat. Res.* 14, 1573–1584.

Günther, F.A., Westlake, W.E., Jaglan, P.S. (1968) Reported solubilities of 738 pesticide chemicals in water. *Res. Rev.* 20, 1–148.

Gustafson, D.I. (1989) Groundwater ubiquity score: A simple method for assessing pesticide leachability. *Environ. Toxicol. Chem.* 8, 339–357.

Guzik, F.F. (1978) Photolysis of isopropyl 3-chlorocarbanilate in water. *J. Agric. Food. Chem.* 26, 53.

Gysin, H. (1962) Triazine herbicides - their chemistry, biological properties and mode of action. *Chem. Ind.* 31, 1393.

Haag, W.R., Yao, C.C.D. (1992) Rate constants for reaction of hydroxyl radicals with several drinking water contaminants. *Environ. Sci. Technol.* 26, 1005–1013.

Haderlein, S B., Weissnahr, K.W., Schwarzenbach, R.P. (1996) Specific adsorption of nitro-aromatic explosives and pesticides to clay minerals. *Environ. Sci. Technol.* 30, 612–622.

Hahn, R.R., Burnside, O.C., Lavy, T.L. (1969) Dissipation and phytotoxicity of dicamba. *Weed Sci.* 17, 3–8.

Halfon, E., Galassi, S., Brüggermann, R., Provini, A. (1996) Selection of priority properties to assess environmental hazard of pesticides. *Chemosphere* 33(8), 1543–1562.

Hall, R.C., Giam, C.S., Merkle, M.G. (1968) The photolytic degradation of picloram. *Weed Res.* 8, 292.

Hamaker, J.W. (1972) Decomposition: Quantitative aspects. In: *Organic Chemicals in the Soil Environment.* Goring, C.A.I., Hamaker, J.W., Editors, pp. 253–341, Marcel Dekker, New York.

Hamaker, J.W. (1975) The interpretation of soil leaching experiments. In: *Environmental Dynamics of Pesticides.* Haque, R., Freed, V.H., Editors, pp. 115–133, Plenum Press, New York.

Hamaker, J.W., Karlinger, H.G. (1971) Vapor pressure of pesticides. In: *Pesticidal Formulation Research: Physical and Colloidal Chemical Aspects.* Gould, R.F., Ed., pp. 39–54, Adv. Chem. Ser. 86, Am. Chem. Soc., Washington, DC.

Hamaker, J.W., Thompson, J.M. (1972) Adsorption. In: *Organic Chemicals in the Soil Environment.* Volume I. Goring, C.A.I., Hamaker, J.W., Editors, pp. 49–143, Marcel Dekker, New York.

Hance, R.J. (1969) Decomposition of herbicides in soil. *J. Sci. Food Agric.* 20(3), 144–145.

Hance, R.J. (1974) Soil organic matter and the adsorption and decomposition of the herbicides atrazine and linuron. *Soil Biol. Biochem.* 6, 39–42.

Hance, R.J. (1976) Adsorption of glyphosate by soils. *Pest. Sci.* 7, 363–366.

Hance, R.J. (1979) Effect of pH on the degradation of atrazine, dichlorprop, linuron and propyzamide in soil. *Pest. Sci.* 10, 83–86.

Hance, R.J., Haynes, R.A. (1981) The kinetics of linuron and metribuzin decomposition in soil using different laboratory systems. *Weed Res.* 21, 87–92.

Hansch, C., Anderson, S.M. (1967) The effect of intramolecular hydrophobic boding on partition coefficients. *J. Org. Chem.* 32, 2583–2586.

Hansch, C., Leo, A. (1979) *Substituent Constants for Correlation Analysis in Chemistry and Biology.* Wiley, New York, New York.

Hansch, C., Leo, A. (1985) Medchem. Project Issue No. 26, Pomona College, Claremont, California.

Hansch, C., Leo, A. (1987) Medchem. Project Issue No. 28, Pomona College, Claremont, California.

Hansch, C., Leo, A., Hoekman, D. (1995) *Exploring QSAR. Hydrophobic, Electronic, and Steric Constants.* ACS Professional Reference Book, American Chemical Society, Washington, DC.

Harris, J.C. (1982) Chapter 8, Rate of aqueous photolysis. In: *Handbook on Chemical Property Estimation Methods. Environmental Behavior of Organic Compounds.* Lyman, W.J., Reehl, W.F., Rosenblatt, D.H., Editors, McGraw-Hill, New York.

Harris, C.I., Warren, G.F. (1964) Detection of phosphorus fixation capacity in organic soil. *Weeds* 12, 120–126.

Hartley, D., Kidd, H. (1983) *The Agrochemicals Handbook.* Royal Society of Chemistry, Union Brothers Ltd., Old Working Surrey, England.

Hartley, D., Kidd, H. (1987) *The Agrochemicals Handbook.* 2nd Edition, Royal Society of Chemistry, Union Brothers Ltd., Old Working Surrey, England.

Hartley, G.S., Graham-Bryce, I.J. (1980) *Physical Principles of Pesticide Behaviour.* Academic Press, New York.

Harvey, Jr., J., Pease, H.L. (1973) Decomposition of methomyl in soil. *J. Agric. Food Chem.* 21, 784–786.

Harvey, R.G. (1974) Soil adsorption and volatility of dinitroaniline herbicides. *Weed Sci.* 22, 120–124.

Hassink, J., Klein, A., Kördel, W., Klein, W. (1994) Behaviour of herbicides in non-cultivated soils. *Chemosphere* 28, 285–295.

Hay, J.V. (1990) Chemistry of sulfonyl herbicides. *Pestic. Sci.* 29, 247–261.

Hedlund, R.T., Youngson, C.R. (1972) The rates of photodecomposition of picloram in aqueous systems. In: *Fate of Organic Pesticides in the Aquatic Environment.* Advances in Chemistry Series No. 111, Faust, S., Editor, p. 159, American Chemical Society, Washington, DC.

Heller, S.R., Scott, K., Bigwood, D.W. (1989) The need for data evaluation of physical and chemical properties of pesticides: The ARS pesticide properties database. *J. Chem. Inf. Comput. Sci.* 29, 159–162.

Helling, C.S. (1976) Dinitroaniline herbicides in soils. *J. Environ. Qual.* 5, 1–15.

Hemond, H.F., Fechner, E.J. (1994) *Chemical Fate and Transport in the Environment*. Academic Press, New York.

Herbicide Handbook (1974) *Herbicide Handbook.* 3rd Edition, Weed Science Society of America, Champaign, Illinois.

Herbicide Handbook (1978) *Herbicide Handbook.* 4th Edition, Weed Science Society of America, Champaign, Illinois.

Herbicide Handbook (1983) *Herbicide Handbook.* 5th Edition, Beste, C.E., Editor, Weed Science Society of America, Champaign, Illinois.

Herbicide Handbook (1989) *Herbicide Handbook.* 6th Edition, Weed Science Society of America, Champaign, Illinois.

Herrmann, M., Kotzias, D., Korte, F. (1985) Photochemical behaviour of chlorsulfuron in water and in adsorbed phase. *Chemosphere* 14, 3.

Hiltibran, R.C. (1972) Fate of diquat in the aquatic environment. Research Report No. 52, Water Resources Center, University of Illinois, Urbana, Illinois.

Hine, J., Mookerjee, P K. (1975) The intrinsic hydrophilic character of organic compounds. Correlations in terms of structural contributions. *J. Org. Chem.* 40, 292–298.

Hinman, M.L., Klaine, S.J. (1992) Uptake and translocation of selected organic pesticides by the rooted aquatic plant *Hydrilla verticillata* royale. *Environ. Sci. Technol*. 26, 609–613.

Hodge, H.C., Downs, W.L., Panner, B.S., Smith, D.W., Maynard, E.A. (1967) *Fed. Cosmet. Toxicol.* 5, 513–531.

Hodgman, C.R., Editor (1952) *Handbook of Chemistry and Physics.* 34th Edition, Chemical Rubber Publishing Co., Cleveland, Ohio.

Hodson, J., Williams, N.A. (1988) The estimation of the adsorption coefficient (K_{OC}) for soils by high performance liquid chromatography. *Chemosphere* 17, 67–77.

Hormann, W.D., Eberle, D.O. (1972) The aqueous solubility of 2-chloro-4-ethylamino-6-isopropylamino-1,3,5-triazine (atrazine) obtained by an improved analytical method. *Weeds Res.* 12, 199–202.

Hornsby, A.G., Wauchope, R.D., Herner, A.E. (1996) *Pesticide Properties in the Environment.* Springer-Verlag, New York.

Horowitz, M., Herzlinger, G. (1974) Soil conditions affecting the dissipation of diuron, flumeturon and propham from the soil surface. *Weed Res.* 14, 257.

Howard, P.H., Editor (1989) *Handbook of Environmental Fate and Exposure Data for Organic Chemicals. Volume I. Large Production and Primary Pollutants*. Lewis Publishers, Chelsea, Michigan.

Howard, P.H., Editor (1991) *Handbook of Environmental Fate and Exposure Data for Organic Chemicals. Volume III. Pesticides*. Lewis Publishers, Chelsea, Michigan.

Howard, P.H., Boethling, R.S., Jarvis, W.F., Meylan, W.M., Michalenko, E.M. (1991) *Handbook of Environmental Degradation Rates.* Lewis Publishers, Chelsea, Michigan.

Huber, G., Gemes, E. (1981) Decomposition of urea herbicide linuron (3-(3,4-dichlorophenyl)-1-methoxy-1-methylurea) in water of Lake Balaton. *Hungar. J. Ind. Chem*. 9, 113.

Hurle, R.J., Freed, V.H. (1972) Effect of electrolytes on the solubility of some 1,3,5-triazines and substituted ureas and their adsorption of soil. *Weeds Res.* 12, 1–10.

Ilchmann, A., Wienke, G., Meyer, T., Gmehling, J. (1993) Concurrent liquid/liquid chromatography - A reliable method for determination of partition coefficients. *Chem.-Ing.-Tech*. 65(1), 72–75.

Isensee, A.R. (1976) Variability of aquatic model ecosystem-derived data. *Inst. J. Environ. Studies* 10, 35.

Isensee, A.R. (1991) Chapter 5, Bioaccumulation and food chain accumulation. In: *Environmental Chemistry of Herbicides.* Vol. II, Grover, R., Cessna, A.J., Editors, pp. 188–198, CRC Press, Boca Raton, Florida.

Jafvert, C T., Westall, J.C., Grieder, E., Schwarzenbach, R P. (1990) Distribution of hydrophobic ionogenic organic compounds between octanol and water: organic acids. *Environ. Sci. Technol.* 24(12), 1795–1803.

Johnson, W.W., Julin, A M. (1974) A Review of the Literature on the Use of Diuron in Fisheries. Bureau of Sport Fish and Wildlife. PB 235446, U.S. Dept. of Interior, Columbia, Missouri.

Jones, T.W., Kemp, W.M., Stevenson, J.C., Means, J.C. (1982) Degradation of atrazine in estuarine water/sediments systems and soils. *J. Environ. Qual.* 11(4), 632–638.

Jury, W.A., Farmer, W.J., Spencer, W.F. (1984) Behavior assessment model for trace organics in soil: II. Chemical classification and parameter sensitivity. *J. Environ. Qual.* 13, 567–572.

Jury, W.A., Farmer, W.J., Spencer, W.F. (1984) Behavior assessment model for trace organics in soil: III. Application of screening model. *J. Environ. Qual.* 13, 573–579.

Jury, W.A., Spencer, W.F., Farmer, W.J. (1983) Use of models for assessing relative volatility, mobility, and persistence of pesticides and other trace organics in soil systems. In: *Hazard Assessment of Chemicals: Recent Developments.* Vol. 2, Saxena, J., Editor, Academic Press, New York.

Jury, W.A., Focht, D.D., Farmer, W.J. (1987b) Evaluation of pesticide groundwater pollution potential from standard indices of soil-chemical adsorption and biodegradation. *J. Environ. Qual.* 16, 422–428.

Jury, W.A., Ghodrati, M. (1989) Overview of organic chemical environmental fate and transport modeling approaches. In: *Reactions and Movement of Organic Chemicals in Soils*. SSSA Special Publication No. 22, Sawhney, B.L., Brown, K., Editors, pp. 271–304, Soil Science Soceity of America and Society of Agronomy, Madison, Wisconsin.

Jury, W.A., Russo, D., Streile, G., El Abd, H. (1990) Evaluation of volatilization by organic chemicals residing below the soil surface. *Water Resources Res.* 26(1), 13–20.

Jury, W.A., Winer, A.M., Spencer, W F., Focht, D.D. (1987a) Transport and trans-formations of organic chemicals in the soil-air-water ecosystem. *Rev. Environ. Contam. Toxicol.* 99, 120–164.

Kanazawa, J. (1981) Measurement of the bioconcentration factors of pesticides by fresh-water fish and their correlation with physicochemical properties of acute toxicities. *Pest. Sci.* 12, 417–424.

Kanazawa, J. (1989) Relationship between the soil sorption constants for pesticides and their physicochemical properties. *Environ. Toxicol. Chem.* 8, 477–484.

Karcher, W., Devillers, J. (1990) SAR and QSAR in environmental chemistry and toxicology: Scientific tool or wishful thinking? In: *Practical Applications of Quantitative-Structure Relationships (QSAR) in Environmental Chemistry and Toxicology, 1–12.* Karcher, W., Devillers, J., Editors, ECSC, EEC, EAEC, Brussels and Luxembourg.

Karickhoff, S.K. (1981) Semi-empirical estimation of sorption of hydrophobic pollutants on natural sediments and soils. *Chemosphere* 10, 833–846.

Karickhoff, S.K., Morris, K.R. (1985) Sorption dynamics of hydrophobic pollutants in sediment suspensions. *Environ. Toxicol. Chem.* 4, 469–479.

Karickhoff, S.W., Brown, D.S., Scott, T.A. (1979) Sorption of hydrophobic pollutants on natural water sediments. *Water Res.* 13, 241–248.

Kaufman, D.D. (1966) Microbial degradation of herbicide combinations: Amitrole and dalapon. *Weeds* 14, 130–134.

Kaufman, D.D. (1976) Soil degradation and persistence. In: *A Literature Survey of Benchmark Pesticides*. pp. 19–71. The George Washington University Medical Center, Dept. of Medical and Public Affairs, Science Communication Division, Washington DC.

Kaufman, D.D., Doyle, R.D. (1977) Biodegradation of organics. National Conf. Composting Municipal Residues Sludges. 75 pp.

Kawamoto, K., Urano, K. (1989a) Parameters for predicting fate of organochlorine pesticides in the environment. (I) Octanol-water and air-water partition coefficients. *Chemosphere* 18, 1987–1996.

Kawamoto, K., Urano, K. (1989b) Parameters for predicting fate of organochlorine pesticides in the environment. (II) Adsorption constant to soil. *Chemosphere* 19(8/9), 1223–1231.

Kawamoto, K., Urano, K. (1990) Parameters for predicting fate of organochlorine pesticides in the environment. (III) Biodegradation rate constants. *Chemosphere* 21(10–11), 1141–1152.

Kearney, P.C., Kaufman, D.D. (1975) *Herbicides: Chemistry, Degradation and Mode of Action.* 2nd Edition, Vol. 2, Marcel Dekker, New York.

Kearney, P.C., Nash, R.G., Isensee, A.R. (1969) Persistence of pesticides in soil. In: *Chemical Fallout: Current Research on Persistence Pesticides.* Chapter 3, pp. 54–67, Miller, M.W., Berg, C.C., Editors, Charles C. Thomas, Springfield, Illinois.

Kearney, P.C., Plimmer, J.R., Wheeler, W.B., Konston, A. (1976) Persistence and metabolism of dinitroaniline herbicides in soils. *Pestic. Biochem. Physiol.* 6, 229–238.

Kenaga, E.E. (1974) Toxilogical and residue data useful in the environmental safety evaluation of dalapon. *Res. Rev.* 53, 109–151.

Kenaga, E.E. (1975) In: *Environmental Dynamics of Pesticides.* Haque, R., Freed, V.H., Editors, Plenum Press, New York. pp. 217–273.

Kenaga, E.E. (1980) Predicted bioconcentration factors and soil sorption coefficients of pesticides and other chemicals. *Ecotoxicol. Environ. Saf.* 4, 26–38.

Kenaga E.E., Goring, C.A.I. (1980) Relationship between water solubility, soil sorption, octanol-water partitioning, and concentration of chemicals in biota. In: *Aquatic Toxicology.* ASTM STP 707, Eaton, J.G., Parrish, P.R., Hendricks, A.C., Editors, pp. 78–115, American Soc. for Testing and Materials, Philadelphia, Pennsylvania.

Kerler, F., Schönherr, J. (1988) Accumulation of lipophilic chemicals across plant cuticles: prediction from octanol/water partition coefficients. *Arch. Environ. Contam. Toxicol.* 17, 1–6.

Khan, S.U. (1978) Kinetics of hydrolysis atrazine in aqueous fulvic acid solution. *Pest. Sci.* 9, 39–45.

Khan, S.U. (1980) *Pesticides in the Soil Environment, Fundamental Aspects of Pollution Control and Environmental Series 5.* Elsevier, Amsterdam, The Netherlands.

Kim, Y.H. (1985) Evaluation of a gas chromatographic method for estimating vapor pressures with organic pollutants. Ph.D. Thesis, University of California, Davis, California.

Kim, Y.H., Woodrow, J.E., Seiber, J.N. (1984) Evaluation of a gas chromatographic method for calculating vapor pressures with organophosphorous pesticides. *J. Chromatogr.* 314, 37–53.

Kirkland, K., Frayer, J.D. (1972) Degradation of several herbicides in soil previously treated with MCPA. *Weed Res.* 12, 90–95.

Klecka, G. (1985) Biodegradation. In: *Environmental Exposure from Chemicals.* Volume I., Neely, W.B., Blau, G.E., Editors, Chapter 6, pp. 110–155, CRC Press, Boca Raton, Florida.

Klein, W., Geyer, H., Freitag, D., Rohleder, H. (1984) Sensitivity of schemes for ecotoxicological hazard ranking of chemicals. *Chemosphere* 13(1), 203–211.

Klein, W., Kördel, W., Weiβ, M., Poremski, H.J. (1988) Updating of the OECD test guideline 107 "Partition coefficient *n*-octanol/water": OECD laboratory intercomparison test on HPLC method. *Chemosphere* 17, 361–386.

Klupinski, T.P., Chin, Y.-P. (2003) Abiotic degradation of trifluralin by Fe(II): Kinetics and transformation pathways. *Environ. Sci. Technol.* 37, 1311–1318.

Kochany, J. (1992) Effects of carbonates on the aquatic photodegradation rate of bromoxynil (3,5-dibromo-4-hydroxybenzonitrile) herbicide. *Chemosphere* 24, 1119–1126.

Kollig, H.P., Editor (1993) Environmental Fate Constants for Organic Chemicals under consideration for EPA's Hazardous Waste Identification Projects. EPA/600/R-93/132. Environmental Research Laboratory, U.S. EPA, Athens, Georgia.

Kollig, H.P., Ellington, J.J., Hamrick, K.J., Jafverts, C.T., Weber, E.J., Wolfe, N.L. (1987) *Hydrolysis Rate Constants, Partition Coefficients, and Water Solubilities for 129 Chemicals*. A Summary of Fate Constants Provided for the Concentration-Based Listing Program. U.S. EPA, Environmental Research Lab., Office of Research and Development, Athens, Georgia.

Kolpin, D.W., Kalkhoff, S.J. (1993) Atrazine degradation in a small stream in Iowa. *Environ. Sci. Technol*. 27, 134–139.

Kördel, W., Stuffe, J., Kotthoff, G. (1993) HPLC-screening method for the determination of the adsorption-coefficient on soil. Comparison of different stationary phases. *Chemosphere* 27, 2341–2352.

Kördel, W., Kotthoff, G., Müller, J. (1995a) HPLC-screening method for the determination of adsorption coefficient on soil-results of a ring-test. *Chemosphere* 30, 1373–1384.

Kördel, W., Stutte, J., Kotthoff, G. (1995b) HPLC-screening method to determine the adsorption coefficient in soil-comparison of immobilized humic acid and clay mineral phases for cyanopropyl columns. *Sci. Total Environ*. 162, 119–125.

Körte, F., Freitag, D., Geyer, H., Klein, W., Kraus, A.G., Lahaniatis, E. (1978) Ecotoxicologic profile analysis: A concept for establishing ecotoxicologic priority lists for chemicals. *Chemosphere* 1, 79–102.

Kotzias, D., Klein, W., Korte, F. (1974) Beiträge zur ökologischen chemie. LXXXIX. Reaktionen von buturon und monolinuron in fester und flüssiger phase bei UV-bestrahlung. *Chemosphere* 3, 161.

Kruger, E.L., Somasundaram, L., Kanwar, R.S. (1993) Persistence and degradation of [^{14}C]atrazine and [^{14}C]deisopropylatrazine as affected by soil depth and moisture conditions. *Environ. Toxicol. Chem*. 12, 1959–1967.

Kühne, R., Ebert, R.-U., Kleint, F., Schmidt, G., Schüürmann, G. (1995) Group contribution methods to estimate water solubility of organic chemicals. *Chemosphere* 30, 2061–2077.

Kulshrestha, G., Mukerjee, S.K. (1986) The photochemical decomposition of the herbicide isoproturon. *Pest. Sci*. 17, 489.

Kulshrestha, G., Singh, S.B. (1992) Influence of soil moisture and microbial activity on pendimethalin degradation. *Bull. Environ. Contam. Toxicol*. 48, 269–274.

Kulshrestha, G., Yaduraju, N.T. (1987) Persistence of pendimethalin in soil following pre-emergence application to wheat. *Indian J. Agron*. 32, 271–274.

Kuwatsuka, S. (1972) Degradation of several herbicides in soils under different conditions. In: *Environmental Toxicology of Pesticides.* Matsumura, F., Boush, G.M., Misato, T., Editors, pp. 385, Academic Press, New York.

Kwok, E.S.C., Atkinson, R., Arey, J. (1992) Gas-phase atmospheric chemistry of selected thiocarbamates. *Environ. Sci. Technol*. 26(9), 1798–1807.

Lane, L.J., Morton, H.L., Wallace, D.E., Wilson, R.E., Martin, R.D. (1977) Nonpoint source pollutants to determine runoff source areas. *Hydrology and Water Resources in Arizona and the Southwest* 7, 89.

Lartiges, S.B., Garrigues, P.P. (1995) Degradation kinetics of organophosphorus and organonitrogen pesticides in different waters under various environmental conditions. *Environ. Sci. Technol.* 29, 1246–1254.

Lee, L.S., Bellin, C.A., Pinal, R., Rao, P.S.C. (1993) Cosolvent effects on sorption of organic acids by soils from mixed solvents. *Environ. Sci. Technol*. 27, 165–171.

Lee, R.F., Ryan, C. (1979) Microbial degradation of organochlorine compounds in estuarine waters and sediments. In: *Proceedings of the Workshop: Microbial Degradation of Pollutants in Marine Environments.* EPA 600/9-79-012, Washington DC.

Lee, Y.-C., Myrdal, P.B., Yalkowsky, S.H. (1996) Aqueous functional group activity coefficients (AQUAFAC). 4: Applications to complex organic compounds. *Chemosphere* 33(11), 2129–2144.

Leistra, M., Smelt, J.H., Verlaat, J.G., Zandvoort, R. (1974) Measured and computed concentration patterns of propyzamide in field soils. *Weed Res.* 14, 87–95.

Leo, A., Hansch, C., Elkins, D. (1971) Partition coefficients and their uses. *Chem. Rev.* 71, 525–616.

Leopold, A.C., van Schaik, P., Neal, M. (1960) Molecular structure and herbicide adsorption. *Weeds* 8, 48.

Li, G.C., Felbeck, Jr., G.T. (1972) Atrazine hydrolysis as catalyzed by humic acids. *Soil Sci.* 114, 201–208.

Lichtner, F.T. (1983) Amitrole absorption by bean (*Phaseolus vulgaris L.* cv "Red Kidney" roots. *Plant Physiol*. 71, 307–312.

Lide, D.R., Editor (2003) *Handbook of Chemistry and Physics*. 84th Edition, CRC Press, Boca Raton, Florida.

Liu, D., Strachan, W.M J., Thomson, K., Kwasniewska, K. (1981) Determination of the biodegradability of organic compounds. *Environ. Sci. Technol.* 15, 788–793.

Liu, J., Qian, C. (1995) Hydrophobic coefficients of *s*-trazine and phenylurea herbicides. *Chemosphere* 31(8), 3951–3959.

Lohninger, H. (1994) Estimation of soil partition coefficients of pesticides from their chemical structure. *Chemosphere* 29, 1611–1626.

Loos, M.A. (1975) Phenoxyalkanoic acids. In: *Herbicides, Chemistry, Degradation and Mode of Action.* Vol. I, 2nd Edition, Kearney, P.C., Kaufmann, D.D., Editors, Marcel Dekker, New York.

Lopez-Avila, V., Hirata, P., Kraska, S., Flanagan, M., Taylor, J.H., Hern, S.C., Melanon, S., Pollard, J.P. (1989) Movement of selected pesticides and herbicides through columns of sandy loam. In: *Evaluation of Pesticides in Ground Water.* Garner, W.Y., Honeycutt, R.C., Editors, American Chemical Society, Washington DC.

Lord, K.A., Briggs, G.C., Neale, M.C., Manlove, R. (1980) Uptake of pesticides from water and soil by earthworms. *Pestic. Sci.* 11, 401–408.

Lund-Høie, K., Friestad, H.O. (1986) Photodegradation of the herbicide glyphosate in water. *Bull. Environ. Contam. Toxicol.* 36, 723–729.

Lyman, W.J. (1985) Chapter 2, Estimation of physical properties. In: *Environmental Exposure from Chemicals*. Vol. 1, Neely, W.B., Blau, G E., Editors, pp. 13–48, CRC Press, Boca Raton Florida.

Lyman, W.J., Reehl, W.F., Rosenblatt, D.H., Editors (1982) *Handbook on Chemical Property Estimation Methods. Environmental Behavior of Organic Compounds.* McGraw-Hill, New York.

Lynch, T.R., Johnson, H.E., Adams, W.J. (1982) The fate of atrazine and a hexachlorophenyl isomer in naturally-derived model stream ecosystems. *Environ. Toxicol. Chem.* 1, 179–192.

Mabey, W., Mill, T. (1978) Critical review of hydrolysis of organic compounds in water under environmental conditions. *J. Phys. Chem. Ref. Data* 7, 383–415.

Mabury, S., Crosby, D.G. (1996) Pesticide reactivity toward hydroxyl and its relationship to field persistence. *J. Agric, Food Chem.* 44, 1920–1924.

Mackay, D. (1982) Correlation of bioconcentration factors. *Environ. Sci. Technol.* 16, 274–278.

Mackay, D., Stiver, W. (1991) Chapter 8, Predicatability and environmental chemistry. In: *Environmental Chemistry of Herbicides.* Vol. II, Grover, R., Cessna, A.J., Editors, pp. 281–297, CRC Press, Boca Raton, Florida.

Madhun, Y.A., Freed, V.H. (1987) Degradation of herbicides bromacil, diuron, and chlortoluron in soil. *Chemosphere* 16, 1003–1011.

Madhun, Y.A., Freed, V.H., Young, J.L., Fang, S.C. (1986) Sorption of bromacil, chlortoluron, and diuron by soils. *Soil Sci. Soc. Am. J.* 50, 1467–1471.

Magee, P.S. (1991) Complex factors in hydrocarbon/water, soil/water and fish/water partitioning. *Sci. Total Environ*. 109/110, 155–178.

Majewski, M.S., Capel, P.D. (1995) *Pesticides in the Atmosphere. Distribution, Trends, and Governing Factors.* Vol. 1 of the series *Pesticide in the Hydrologic System.* Gilliom, R.J., Editor, Ann Arbor Press Chelsea, Michigan.

Mansour, M., Feicht, E., Meallier, P. (1989) Improvement of the photostability of selected substances in aqueous medium. *Toxicol. Environ. Contam.* 20–21, 139–147.

Martin, H. (1961) *Guide to the Chemicals used in Crop Protection.* 4th Edition, Canadian Dept. of Agriculture Publication 1093, Ottawa, Ontario.

Martin, H., Worthing, C R., Editors (1977) *Pesticide Manual.* 5th Edition, British Crop Protection Council, United Kingdom.

Martin, R.A., Edgington, L.V. (1981) Comparative systemic translocation of several xenobiotics and sucrose. *Pestic. Biochem. Physiol.* 16, 87–96.

Massad, W., Criado, S., Bertolotti, S., Pajares, A., Gianotte, J., Escalada, J.P., Amat-Guerri, F., Carcia, N.A. (2004) Photodegradation of the herbicide norflurazon sensitised by riboflavin. A kinetic and mechanistic study. *Chemosphere* 57, 455–461.

Massini, P. (1961) Movement of 2,6-dichlorobenzonitrile in soils and in plants in relation to its physical properties. *Weed Res.* 1, 142–146.

McCall, P.J., Agin, G.L. (1985) Desorption kinetics of picloram as affected by residence time in the soil. *Environ. Toxicol. Chem.* 4, 37–44.

McCall, P.J., Gavit, P.D. (1986) Aqueous photolysis of triclorpyr and its butoxyethyl ester and calculated environmental photodecomposition rates. *Environ. Toxicol. Chem.* 5(10), 879–885.

McCall, P.J., Swann, R.L., Laskowski, D.A., Unger, S.M., Vrona, S.A., Dishburger, H.J. (1980) Estimation of chemical mobility in soil from liquid chromatographic retention times. *Bull. Environ. Contam. Toxicol.* 24, 190–195.

McCall, P.J., Swann, R.L., Laskowski, D.A., Vrona, S.A., Unger, S.M., Dishburger, H.J. (1981) Prediction of chemical mobility in soil from sorption coefficients. In: *Aquatic Toxicology and Hazard Assessment*. ASTM STP 737, Branson, D.R., Dickson, K.L., Editors, pp. 49–58, Am. Soc. for Testing and Materials, Philadelphia, Pennsylvania.

McCall, P.J., Vrona, S.A., Kelley, S.S. (1981) Fate of uniformly carbon-14 ring labelled 2,4,5-trichlorophenoxyacetic acid and 2,4-dichlorophenoxyacetic acid. *J. Agric. Food Chem.* 29, 100–107.

McDuffie, B. (1981) Estimation of octanol/water partition coefficients for organic pollutants using reverse-phase HPLC. *Chemosphere* 10, 73–83.

Meakins, N.C., Bubb, J.M., Lester, J.N. (1994) The behaviour of the *s*-triazine herbicides, atrazine and simazine, during primary and secondary biological waste water treatment. *Chemosphere* 28, 1611–1622.

Means, J.C., Wijayaratne, R.D. (1982) Role of natural colloids in the transport of hydrophobic pollutants. *Science* 215, 968.

Means, J.C., Wijayaratne, R.D., Boynton, W.R. (1983) Fate and transport of selected herbicides in an estuarine environment. *Can. J. Fish Aquat. Sci.* 40 (Suppl. 2), 337–345.

Melnikov, N.N. (1971) Chemistry of pesticides. *Res. Rev.* 36, 1–447.

Mersie, W., Seybold, C. (1996) Adsorption and desorption of atrazine, deethylatrazine, deisopropylatrazine, and dydroxyatrazine on Levy wetland soil. *J. Agric. Food Chem.* 44, 1925–1929.

Metcalf, R.L., Sanborn, J.R. (1975) Pesticides and environmental quality in Illinois. *Illinois Natural History Survey Bulletin* 31, 381–436.

Meylan, W., Howard, P.H. (1991) Bond contribution method for estimating Henry's law constants. *Environ. Toxicol. Chem.* 10, 1283–1293.

Meylan, W., Howard, P.H., Boethling, R.S. (1992) Molecular topology/fragment contribution method for predicting soil sorption coefficients. *Environ. Sci. Technol.* 26, 1560–1567.

Milne, G.W.A., Editor (1995) *CRC Handbook of Pesticides.* CRC Press, Boca Raton, Florida.

Mingelgrin, U., Gerstl, Z. (1983) Reevaluation of partitioning as a mechanism of nonionic chemicals adsorption in soils. *J. Environ. Qual.* 12(1), 1–11.

Mitsutake, K.-I., Iwasmura, H., Shimizu, R., Fujita, T. (1986) Quantitative structure-activity relationships of photosystem II inhibitors in chloroplasts and its link to herbicidal action. *J. Agric. Food Chem.* 34, 725–732.

Miyazaki, S., Sikka, H.C., Lynch, R.S. (1975) Metabolism of dichlobenil by microorganism in the aquatic environment. *J. Agric. Food Chem.* 23, 365.

Moilanen, K.W., Crosby, D.G. (1972) Photodecomposition of 3′,4′-dichloropropionanilide (propanil). *J. Agric. Food Chem.* 20, 950–953.

Mongar, K., Miller, G.C. (1988) Vapor phase photolysis of trifluralin in an outdoor chamber. *Chemosphere* 17, 2183–2188.

Montgomery, J.H. (1993) *Agrochemicals Desk Reference. Environmental Data.* Lewis Publishers, Chelsea, Michigan.

Morrill, L.G., Mahilum, B.C., Mohiuddin, S.H. (1982) *Organic Compounds in Soils.* Ann Arbor Science Publishers, Inc., Ann Arbor, Michigan.

Mosier, A.R., Guenzi, W.D. (1973) Picloram photolytic decomposition. *J. Agric. Food Chem.* 21, 835–837.

Moyer, J.R.R., Hance, R.J., McKone, C.E. (1972) The effect of adsorption of adsorbents on the rate of degradation of herbicides incubated with soil. *Soil. Biol. Biochem.* 4, 307–311.

Muir, D.C.G. (1991) Dissipation and transformation in water and sediment. In: *Environmental Chemistry of Herbicides*. Vol. II, Grover, R., Cessna, A.J., Editors, Chapter 1, pp. 1–88, CRC Press, Boca Raton, Florida.

Muir, D.C.G., Grift, N.P. (1982) Fate of fluoridone in sediment and water in laboratory and field experiments. *J. Agric. Food Chem.* 30, 238.

Muir, D.C.G., Grift, N.P., Blouw, A.P., Lockhart, W.L. (1980) Persistence of fluridone in small ponds. *J. Environ. Qual.* 9, 151–156.

Muir, D.C.G., Teixeira, C, Wania, F. (2004) Empirical and modeling evidence of regional atmospheric transport of current-use pesticides. *Environ. Toxicol. Chem.* 23, 2421–2432.

Muir, D.C.G., Townsend, B.E., Lockhart, W.L. (1983) Bioavailability of six organic chemicals to *Chironomus tentans* larvae in sediment and water. *Environ. Toxicol. Chem.* 2, 269–281.

Muir, D.C.G., Yarechewski, A.L. (1982) Degradation of terbutryn in sediments and water under various redox conditions. *J. Environ. Sci. Health* B17, 363.

Müller, M., Kördel, W. (1996) Comparison of screening methods for the estimation of adsorption coefficients on soil. *Chemosphere* 32, 2493–2504.

Müller, M.D., Buser, H.-R. (1995) Environmental behavior of acetamide pesticide stereoisomers. 2. Stereo- and enantioselective degradation in sewage sludge and soil. *Environ. Sci. Technol*. 29, 2031–2037.

Muszkat, L., Halmann, M., Raucher, D., Bir, L. (1992) Solar photodegradation of xenobiotic contaminants in polluted well water. *J. Photochem. Photobiol. A: Chem.* 65, 409–417.

Nakamura, M., Suzuki, T., Amano, K., Yamada, S. (2001) Relation of sorption behavior of agricultural chemicals in solid-phase extraction with their *n*-octanol/water partition coefficients evaluated by high-performance liquid chromatography (HPLC). *Anal. Chim. Acta* 428, 219–226.

Nandihalli, U.B., Duke, M.V., Duke, S.O. (1993) Prediction of RP-HPLC log P from semiempirical molecular properties of diphenyl ether and phenopylate herbicides. *J. Agric. Food Chem.* 41, 582–587.

Nash, R.G. (1980) Dissipation rate of pesticides from soils. In: *CREAMS.* Vol. 3, Niesel, W.G., Editor, pp. 560–594, U.S. Dept. of Agriculture, Washington DC.

Nash, R.G. (1983) Distribution of butylate, heptachlor, lindane, and dieldrin emulsifiable concentrated and butyrated microencapsulated formulations in microagroecosystem chambers. *J. Agric. Food Chem.* 31, 1195.

Nash, R.G. (1983) Comparative volatilization and dissipation rates of several pesticides from soil. *J. Agric. Food Chem.* 31, 210.

Nash, R.G. (1983) Determining environmental fate of pesticides with microagroecosystems. *Res. Rev.* 85, 199–215.

Nash, R.G. (1988) Chapter 5, Dissipation from soil. In: *Environmental Chemistry of Herbicides.* Vol. I, Grover, R., Editors, pp. 131–169, CRC Press, Boca Raton, Florida.

Nash, R.G. (1989) Models for estimating pesticide dissipation from soil and vapor decline in air. *Chemosphere* 18(11/12), 2375–2381.

Nash, R.G., Beall, M.L. (1980) Distribution of silvex, 2,4-D, and TCDD applied to turf in chambers and field plots. *J. Agric. Food Chem.* 28, 614.

Neary, D.G., Bush, P.B., Michael, J.L. (1993) Fate, dissipation and environmental effects of pesticides in southern forests: A review of a decade of research progress. *Environ. Toxicol. Chem.* 12, 411–428.

Neely, W.B., Blau, G.E. (1985) Chapter 1, Introduction to environmental exposure from chemicals. In: *Environmental Exposure From Chemicals.* Volume I, Neely, B.W., Blau, G.E., Editors, pp. 1–11. CRC Press, Boca Raton, Florida.

Nelson, N.H., Faust, S.D. (1969) Acidic dissociation constants of selected aquatic herbicides. *Environ. Sci. Technol.* 3, 1186–1188.

Nesbitt, H.J., Watson, J.R. (1980a) Degradation of the herbicide 2,4-D in river water-I. Description of study area and survey of rate determining factors. *Water Res.* 14, 1683–1688.

Nesbitt, H.J., Watson, J.R. (1980b) Degradation of the herbicide 2,4-D in river water-II, the role of suspended sediment. Nutrients and water temperature. *Water Res.* 14, 1689–1694.

Newsome, H.C., Woods, W.G. (1973) Photolysis of the herbicide dinitramine (N^3, N^3-diethyl-2,4-dinitro-6-trifluromethyl-*m*-phenylenediamine). *J. Agric. Food Chem.* 21, 598.

Nex, R W., Swezey, A.W. (1954) Some chemical and physical properties of weed killers. *Weeds* 3, 241–253.

Nicholls, P.H. (1988) Factors influencing entry of pesticides into soil water. *Pestic. Sci.* 22, 123–137.

Nilles, G.P., Zabik, M.J. (1974) Photochemistry of bioactive compounds. Multiphase photodegradation of basalin. *J. Agric. Food Chem.* 22, 684–688.

Nkedi-Kizza, P., Rao, P.S C., Johnson, J.W. (1983) Adsorption of diuron and 2,4,5-T on soil particle-size separates. *J. Environ. Qual.* 12, 195–197.

Nkedi-Kizza, P., Rao, P.S.C., Hornsby, A.G. (1985) Influence of organic cosolvents on sorption of hydrophobic organic chemicals by soils. *Environ. Sci. Technol.* 19, 975–979.

Nomura, N.S., Hilton, H.W. (1977) The adsorption and degradation of glyphosate in five Hawaiian sugarcane soils. *Weed Res.* 17, 113–121.

Novick, N.J., Alexander, M. (1985) Cometabolism of low concentration of propachlor, alachlor and cycloate in sewage and lake water. *Appl. Environ. Microbiol.* 49, 737.

Nyholm, N., Jacobsen, B.N., Pedersen, B.M., Poulsen, O., Damboroj, A., Schultz, B. (1992) Removal of organic micro pollutants at ppb levels in laboratory activated sludge reactors under various operating conditions: Biodegradation. *Water Res.* 26, 339–353.

OECD (1981) *OECD Guidelines for Testing of Chemicals.* Section 1: Physical-Chemical Properties. Organization for Economic Co-operation and Development. OECD, Paris.

Oehler, D.D., Ivie, G.W. (1980) Metabolic fate of the herbicide dicamba in a lactating cow. *J. Agric. Food Chem.* 28, 685–689.

Ohyama, H., Kawatsuka, S. (1978) Degradation of bifenox, a diphenylether herbicide, methyl-5-(2,4-dichlorophenoxy)-2-nitrobenzoate, in soils. *J. Pest. Sci.* 3, 401.

Otto, S., Riello, L., Düring, R.-A., Hummel, H.E. (1997) Herbicide dissipation and dynamics modelling in three different tillage system. *Chemosphere* 34, 163–178.

Pacakova, V., Stulik, K., Prihoda, M. (1988) High performance liquid chromatography of *s*-triazines and their degradation products using ultraviolet photometric and amperometric detection. *J. Chromatogr.* 442, 147–156.

Pait, A.S., De Souza, A.E., Farrow, D.R.G. (1992) *Agricultural Pesticide Use in Coastal Areas: A National Summary*, National Oceanic and Atmospheric Administration, Rockville, Maryland.

Paris, D.F., Steen, W.C., Baughman, G.L. (1978) Prediction of microbial transformation of pesticides in natural waters. (unpublished), presented before the American Chemical Society, Division of Pesticide Chemistry, Anaheim, California, Environmental Research Laboratory, U.S. Environmental Protection Agency, Athens, Georgia.

Paris, D.F., Steen, W.C., Baughman, G.L., Barnett, Jr., J.T. (1981) Second-order model to predict microbial degradation of organic compounds in natural waters. *Appl. Environ. Microbiol.* 41, 603–609.

Parr, J.F., Smith, S. (1973) Degradation of trifluralin under laboratory conditions and soil anaerobiosis. *Soil Sci.* 115, 55–63.

Paschke, A., Neitzel, P.L., Walther, W., Schüürumann. G. (2004) Octanol/water partition coefficient of selected herbicides: determination using shake-flask method and reversed-phase high performance liquid chromatography. *J. Chem. Eng. Data* 49, 1639–1642.

Patchett, G.G., Batchelder, G.H., Menn, J.J. (1964) In: *Analytical Methods for Pesticides and Plant Growth Regulators.* Vol. 4, Zweig, G., Editor, New York, Academic Press, pp. 117–123.

Patchett, G.G., Gray, R.A., Reed, A., Hyzak, D.L. (1983) Thiocarbamate sulfoxides protected against dry soil deactivation. U.S. Patent 4,389,237.

Patil, G.S. (1994) Prediction of aqueous solubility and octanol-water partition coefficient for pesticides based on their molecular structure. *J. Hazard. Materials* 36, 35–43.

Pavel, E.W., Lopez, A.R., Berry, D.F., Smith, E.P., Reneau, Jr., R.B., Mostagimi,. S. (1999) Anaerobic degradation of dicamba and metribuzin in riparian wetlands soils. *Water Res*. 33, 87–94.

Peck, D.E., Corwin, D.L., Farmer, W.J. (1980) Adsorption-desorption of diuron by fresh water sediments. *J. Environ. Qual.* 9, 101–106.

Pieuchot, M., Perrin-Ganier, C., Portal, J.M., Schiavon, M. (1996) Study on the mineralization and degradation of isoproturon in three soils. *Chemosphere* 33, 467–478.

Pinsuwan, S., Li, A., Yalkowsky, S.H. (1995) Correlation of octanol/water solubility ratios and partition coefficients. *J. Chem. Eng. Data* 40, 623–626.

Plato, C. (1972) Differential scanning calorimetry as a general method for the determining purity and heat of fusion of high-purity organic chemicals. Application to 64 compounds. *Anal. Chem.* 44(8), 1531–1534.

Plato, C., Glasgow, A.R., Jr. (1969) Differential scanning calorimetry as a general method for the determining purity and heat of fusion of high-purity organic chemicals. Application to 95 compounds. *Anal. Chem.* 41(2), 330–336.

Plimmer, J.R., Kearney, P.C., Chisaka, H. (1970) Microbial conversion of ^{14}C labelled propanil in Japanese soils. *Weed Sci. Soc. Am.*, Abst. No. 167.

Plimmer, J.R., Klingebiel, U I. (1974) Photochemistry of N-*sec*-butyl-4-*tert*-butyl-2,6-dinitroaniline. *J. Agric. Food Chem.* 22, 689–693.

Probst, G.W., Golab, T., Wright, W.L. (1975) Dinitroanilines. In: *Herbicides, Chemistry, Degradation and Mode of Action.* Vol. 1, Kearney, P.C., Kaufman, D.D., Editors, Marcel Dekker, New York.

Probst, G.W., Golab, T., Herberg, R.J., Holser, F.J., Parka, S.J., Van der Schans, C., Tepe, J.B. (1967) Fate of trifluralin in soils and plants. *J. Agric. Food Chem.* 15, 592–599.

Que Hee, S., Sutherland, R.G. (1981) *The Phenoxyalkanoic Herbicides. Volume 1: Chemistry, Analysis, and Environmental Pollution*. CRC Press, Inc., Boca Raton, Florida.

Quellette, R.P., King, J.A. (1977) *Chemical Week. Pesticide Register.* McGraw-Hill, New York.

Ramesh, A., Maheswari, S.T. (2004) Dissipation of alachlor in cotton plant, soil and water and its bioaccumulation in fish. *Chemosphere* 54, 647–652.

Rao, P.S.C., Davidson, J.M. (1979) Adsorption and movement of selected pesticides at high concentrations in soils. *Water Res.* 13, 375–380.

Rao, P.S.C., Davidson, J.M. (1980) Estimation of pesticide retention and transformation parameters required in nonpoint source pollution models. In: *Environmental Impact of Nonpoint Source Pollution.* Overcash, M.R., Davidson, J.M., Editors, Ann Arbor Science Publishers, Ann Arbor, Michigan.

Rao, P.S.C., Davidson, J.M. (1982) Retention and Transformation of Selected Pesticides and Phosphorus in Soil Water System: A Critical Review. U.S. EPA, EPA-600/3-82-060.

Reinert, K.H. (1989) Environmental behavior of aquatic herbicides in sediments. In: *Reactions and Movement of Organic Chemicals in Soils.* SSSA Special Publ. No.22, pp. 335–348, Soil Science Society of Ameroca and Society of Argonomy, Madison, Wisconsin.

Reinert, K.H., Rogers, J.H. (1984) Influence of sediment types on the sorption of endothall. *Bull. Environ. Contam. Toxicol.* 32, 557–564.

Reinert, K.H., Rogers, J.H. (1987) Fate and persistence of aquatic herbicides. *Rev. Environ. Contam. Toxicol.* 98, 69–91.

Reinhold, K.A. et al. (1979) Adsorption of Energy Related Organic Pollutants. U.S. EPA, EPA-600/3-79-086. p. 103.

Rekker, R.F. (1977) *The Hydrophobic Constants; Its Derivation and Application; A Means of Characterizing Membrane Systems.* Elsevier Scientific Publishing Company, New York.

Ribo, J.M. (1988) The octanol/water partition coefficient of the herbicide chlorsulfuron as a function of pH. *Chemosphere* 17, 709–715.

Rice, C., P., Chernyek, S.M., Hapeman, C.J., Bilboulian, S (1997) Air-water distribution of the endosulfan isomers. *J. Environ. Qual.* 26, 1101–1106.

Rice, C.P., Chernyak, S.M., McConnell, L.L. (1997) Henry's law constants for pesticides measured as a function of temperature and salinity. *J. Agric. Food Chem.* 45, 2291–2298.

Richards, R.P., Baker, D.B. (1993) Pesticide concentration patterns in agricultural drainage networks in the Lake Erie basin. *Environ. Toxicol. Chem*. 12, 13–26.

Riederer, M. (1990) Estimating partitioning and transport of organic chemicals in the foliage/atmosphere system: Discussion of a fugacity-based model. *Environ. Sci. Technol*. 24, 829–837.

Riise, G., Salbu, B. (1992) Mobility of dichlorprop in the soil-water system as a function of different environmental factors. I. A batch experiment. *Sci. Total Environ*. 123/124, 399–409.

Roberts, T.R. (1974) The fate of WL-6361 in a static aquatic system. *Proc. European Weed Res. Council*, 4th Int'l Symp. Aquat. Weeds, Vienna, Austria. pp. 232.

Romero, E., Dios, G., Mingorance, M.D., Matallo, M.B., Peña, A., Sánchez-Rasero, F. (1998) Photodegradation of mecoprop and dichlorprop on dry, moist and amended soil surfaces exposed to sunlight. *Chemosphere* 37, 577–589.

Rordorf, B.F. (1989) Unpublished data, private communication.

Rosen, J.D., Strusz, R.F., Still, C.C. (1969) Photolysis of phenylurea herbicides. *J. Agric. Food Chem.* 17, 206–207.

Roy, W.R., Krapac, I.G. (1994) Adsorption and desorption of atrazine and diethylatrazine by low organic carbon geologic materials. *J. Environ. Qual*. 23, 549–556.

Rüdel, H., Schmidt, S., Kördel, W., Klein, W. (1993) Degradation of pesticides in soil: comparison of laboratory experiments in a biometer system and outdoor lysimeter experiments. *Sci. Total Environ*. 132, 181–200.

Rueppel, M., Brightwell, B.B., Schaefer, J., Marvel, J.T. (1977) Metabolism and degradation of glyphosate in soil and water. *J. Agric. Food Chem.* 25, 517–528.

Ruzo, L.O., Casida, J.E. (1985) Photochemistry of thiocarbamate herbicides: Oxidative and free radical processes of thiobencarb and diallate. *J. Agric. Food Chem.* 33, 272.

Sabljic, A. (1984) Prediction of the nature and strength of soil sorption of organic pollutants by molecular topology. *J. Agric. Food Chem.* 32, 243–246.

Sabljic, A. (1987) On the prediction of soil sorption coefficients of organic pollutants from molecular structure: Application of molecular topology model. *Environ. Sci. Technol.* 21, 358–366.

Sabljic, A., Güsten, H., Verhaar, H., Hermens, J. (1995) QSAR modelling of soil sorption, improvement and systematics of log K_{OC} vs. log K_{OW} correlations. *Chemosphere* 31, 4489–4514.

Sagebiel, J.C., Seiber, J.N., Woodrow, J.E. (1992) Comparison of headspace and gas-stripping methods for determining the Henry's law constant (H) for organic compounds of low to intermediate H. *Chemosphere* 25(12), 1763–1768.

Saito, S., Koyasu, J., Yoshida, K., Shigeoka, T., Koike, S. (1993) Cytotoxicity of 109 chemicals to goldfish GFS cells and relationships with 1-octanol/water partition coefficients. *Chemosphere* 26(5), 1015–1028.

Sanborn, J.R., Francis, B.M., Metcalf, R.L. (1977) The Degradation of Selected Pesticides in Soil: A Review of the Published Literature. Prepared for the U.S. Environmental Protection Agency, Cincinnati, Ohio. Publication No. U.S. EPA-600/9-77-022.

Sanders, D.G., Mosier, J.W. (1983) Photolysis of the aquatic herbicide fluridone in aqueous solution. *J. Agric. Food Chem.* 31, 237–241.

Sangster, J. (1993) LOGKOW Data Bank. Sangster Research Laboratory, Montreal, Canada.

Sattar, M.A., Paasivirta, J. (1980) Fate of the herbicide MCPA in soil. Analysis of the residues of MCPA by an internal standard method. *Chemosphere* 9, 365–375.

Savage, K E. (1978) Persistence of several dinitroaniline herbicides as affected by soil moisture. *Weed Sci.* 26, 465.

Savage, K.E., Jordan, T.N. (1980) Persistence of three dinitroaniline herbicides on the soil surface. *Weed Sci.* 28, 105–110.

Savage, K.E., Wauchope, R.D. (1974) Flumeturon adsorption-desorption equilibria in soil. *Weed Sci.* 22, 106–110.

Schimmel, S.C., Garnas, R.L., Patrick, Jr., J.M., Moore, J. C. (1983) Acute toxicity, bioconcentration, and persistence of AC 222,705, benthiocarb, chlorpyrifos, fenvalerate, methyl parathion, and permethrin in the estuarine environment. *J. Agric. Food Chem.* 31, 104–113.

Schliebe, K A., Burnside, O.C., Lavy, T.L. (1965) Dissipation of amiben. *Weeds* 13, 321.

Schmidt, G. (1975) Von problematik der verhaltensprüfung von pflanzenschtzmitteln im ober-flächenwasser, schriftenr. des Ver Wasser-, Boden-, Lufthyg. *Berlin-Dahlem* 46, 155.

Schnoor, J.L., Editor (1992) *Fate of Pesticides and Chemicals in the Environment.* John Wiley & Sons, New York.

Schnoor, J.L. (1992) Chemical fate and transport in the environment. In: *Fate of Pesticides and Chemicals in the Environment.* Schnoor, J.L., Editor, pp. 1–24, John Wiley & Sons, New York.

Schnoor, J.L., McAvoy, D.C. (1981) Pesticide transport and bioconcentration model. *J. Environ. Eng. Div.* (*Am. Soc. Civ. Eng.*) 107(EE6), 1229–1246.

Schnoor, J.L., Rao, N.B., Cartwright, K.J., Noll, R.M. (1982) In: *Modeling the Fate of Chemicals in the Aquatic Environment.* Dickson, K.L., Maki, A.W., Cairns, Jr., J., Editors, pp. 145, Ann Arbor Science, Ann Arbor, Michigan.

Schwartz, H.J. (1967) Microbial degradation of pesticides in aqueous solutions. *J. Water Pollut. Control Fed.* 39, 1701.

Scifres, C.J., Allen, T.J., Leinweber, C.L., Pearson, K.H. (1973) Dissipation and phototoxicity of dicamba residues in water. *J. Environ. Qual.* 2, 306.

Scow, K.M. (1982) Rate of biodegradation. In: *Handbook on Chemical Property Estimation Methods. Environmental Behavior of Organic Compounds.* Lyman, W.J., Reehl, W.F., Rosenblatt, D.H., Editors, Chapter 9, McGraw-Hill, New York.

Segal, H.S., Sutherland, M.L. (1967) Amiben. In: *Analytical Methods for Pesticides, Plant Growth Regulators, and Food Additives*. Vol. VI., Zweig, G., Editor, pp. 321–334, Academic Press, New York.

Seiber, J.N., McChesney, M.M. (1987) Measurement and computer model simulation of the volatilization flux of molinate and methyl parathion from a flooded rice field. Final Report to the Department of Food and Agriculture, Sacramento, California.

Seiber, J.N., McChesney, M.M., Sanders, P.F., Woodrow, J.E. (1986) Models for assessing the volatilization of herbicides applied to flooded rice fields. *Chemosphere* 15, 127–138.

Seiber, J.N., McChesney, M.M., Sanders, P.F., Woodrow, J.E. (1989) Air borne residues resulting from use of methyl parathion, molinate and thiobencarb on rice in the Sacramento Valley, California. *Environ. Toxicol. Chem.* 8, 577–588.

Senseman, S.A., Lavy, T.L., Daniel, T.C. (1997) Monitoring groundwater for pesticides at selected mixing/loading sites in Arkansas. *Environ. Sci. Technol.* 31, 283–288.

Senseman, S.A., Lavy, T.L., Matice, J.D., Gbur, E.E. (1995) Influenced of dissolved humic acid and Ca-montmorilloinite clay on pesticide extraction efficiency from water using solid-phase extraction disks. *Environ. Sci. Technol.* 29, 2647–2653.

Sheets, T.J. (1963) Photochemical alteration and inactivation of amiben. *Weeds* 11, 186.

Shirmohammadi, A., Magette, W.L., Brinsfield, R.B., Staver, K. (1989) Ground water loading of pesticides in the Atlantic Coastal Plain. *Ground Water Monitor Rev.* 9, 141–148.

Shiu, W.Y., Ma, K.C., Mackay, D. (1990) Solubilities of pesticides in water. Part 1, Environmental physical chemistry and Part 2, Data compilation. *Rev. Environ. Contam. Toxicol.* 115, 1–187.

Sicbaldi, F., Finizio, A. (1993) K_{OW} estimation by combination of RP-HPLC and molecular connectivity indexes for a heterogeneous set of pesticide. In: *Proceedings IX Symposium Pesticide Chemistry, Mobility and Degradation of Xenobiotics*. Oct. 1993, Piacenza, Italy.

Sieber, J., Gottschild, D., Nolting, H.-G. (1994) Pesticides in precipitation in Northern Germany. *Chemosphere* 28, 1559–1570.

Simsiman, G.V., Chesters, G. (1976) Persistence of diquat in the aquatic environment. *Water Res.* 10, 105.

Skurlatov, Y I., Zepp, R.G., Baughman, G.L. (1983) Photolysis rates of (2,4,5-trichloro-phenoxy)acetic acid and 4-amino-3,5,6-trichloropicolinic acid in natural waters. *J. Agric. Food Chem.* 31, 1065–1071.

Slade, P., Smith, A.E. (1967) Photochemical degradation of diquat. *Nature* 213, 919.

Smalling, K.L., Aelion, C.M. (2004) Distribution pf atrazine into three chemical fractions: impart of sediment depth and organic carbon content. *Environ. Toxicol. Chem.* 23, 1164–1171.

Smith, A.E. (1969) Factors affecting the loss of tri-allate from soils. *Weeds Res.* 9, 306.

Smith, A.E. (1970) Degradation, adsorption, and volatility of di-allate and tri-allate in prairie soils. *Weed Res.* 10, 331–339.

Smith, A.E. (1973) Degradation of dicamba in prairie soils. *Weed Res.* 13, 373–378.

Smith, A.E. (1978) Relative persistence of di- and tri-chlorophenoxyalkanoic acid herbicides in Saskatchewan soils. *Weed Res.* 18, 275–279.

Smith, A.E. (1979) Soil persistence experiments with (^{14}C) 2,4-D in herbicidal mixtures and field persistence studies with triallate and trifluralin both singly and combined. *Weed Res.* 19, 165–170.

Smith, A.E., Biggs, G.G. (1978) The fate of the herbicide chlortoluron and its possible degradation products in soils. *Weed Res.* 18, 1–7.

Smith, A.E., Grove, J. (1969) Photochemical degradation of diquat in dilute aqueous solution and on silica gel. *J. Agric. Food Chem.* 17, 609–613.

Smith, A.E., Hayden, B.J. (1981) Relative persistence of MCPA and mecoprop in Saskatchewan soils and the identification of MCPA in MCPB-treated soil. *Weeds Sci.* 21, 179–183.

Soderquist, C.J., Bowers, J.B., Crosby, D.G. (1977) Dissipation of molinate in a rice field. *J. Agric. Food Chem.* 25, 940.

Soderquist, C.J., Crosby, D.G. (1975) Dissipation of 4-chloro-2-methyl-phneoxyacetic acid (MCPA) in a rice field. *Pest. Sci.* 6, 17.

Solomon, K.R., Baker, D.B., Richards, R.P., Kixon, K., Klaine, S.J., La Point, T.W., Kendall, R., Weisskopf, C.P., Giddings, J.M., Giesy, P., Hall, L.W., Williams, W.M. (1996) Ecological risk assessment of atrazine in North American surface waters. *Environ. Toxicol. Chem.* 15, 31–76.

Solomon, K.R., Bowhey, C.S., Liber, K., Stephenson, G.R. (1988) Persistence of hexazinone (Velpar), triclopyr (Garlon) and 2,4-D in a northern Ontario aquatic environment. *J. Agric. Food Chem.* 36, 1314–1318.

Somasundaram, L., Coats, J.R., Racke, K.D. (1991) Mobility of pesticides and their hydrolysis metabolites in soil. *Environ. Toxicol. Chem.* 10, 185–194.

Spacie, A., Hamelink, J.L. (1979) Dynamics of trifluralin accumulation in river fishes. *Environ. Sci. Technol.* 13(7), 817–822.

Spain, J.C., Van Veld, P.A. (1983) Adaptation of natural microbial communities to degradation of xenobiotic compounds: Effects of concentration, exposure time, inoculum and chemical structure. *Appl. Environ. Microbiol.* 45, 428.

Spencer, E.Y., Editor (1973) *Guide to the Chemicals Used in Crop Protection.* 6th edition, Research Branch Agriculture Canada, Ontario, Canada.

Spencer, E.Y., Editor (1981) *Guide to the Chemicals Used in Crop Protection.* 7th edition, Research Branch Agriculture Canada, Ontario, Canada.

Spencer, E.Y., Editor (1982) *Guide to the Chemicals Used in Crop Protection.* 8th edition, Research Branch Agriculture Canada, Ontario, Canada.

Spencer, W.F. (1976) Vapor pressure and vapor losses of benchmark pesticides. In: *A Literature Survey of Benchmark Pesticides.* pp. 72–165. The George Washington University Medical Center, Dept. of Medical and Public Affairs, Science Communication Division, Washington, DC.

Spencer, W.F., Cliath, M.M. (1990) Movement of pesticides from soil to the atmosphere. In: *Long Range Transport of Pesticides.* Kurtz, D.A., Editor, Chapter 1, Lewis Publishers, Ann Arbor, Michigan.

Spencer, W.F., Cliath, M.M. (1974) Factors affecting vapor loss of trifluralin from soil. *J. Agric. Food Chem.* 22, 987–991.

Spencer, W., Cliath, M.M. (1983) Measurement of pesticide vapor pressures. *Res. Rev.* 85, 57–71.

Spencer, W.F., Cliath, M.M., Jury, W.A., Zhang, L.Z. (1988) Volatilization of organic chemicals from soil as related to their Henry's law constants. *J. Environ. Qual.* 17(3), 504–509.

Spencer, W.F., Farmer, W.J., Cliath, M.M. (1973) Pesticide volatilization. *Res. Rev.* 49, 1–47.

Sprankle, P., Meggitt, W.F., Penner, D. (1975) Adsorption, mobility and microbial degradation of glyphosate in the soil. *Weed Sci.* 23, 229–234.

Spurlock, F.C. (1992) Thermodynamics of organic chemical partition in soils. Ph.D. Thesis, University of California at Davis, California.

Spurlock, F.C., Biggar, J.W. (1994a) Thermodynamics of organic chemical partition in soils. 2. Nonlinear partition of substituted phenylureas from aqueous solution. *Environ. Sci. Technol.* 28, 996–1002.

Spurlock, F.C., Biggar, J.W. (1994b) Thermodynamics of organic chemical partition in soils. 3. Nonlinear partition from water-miscible cosolvent solutions. *Environ. Sci. Technol.* 28, 1003–1009.

Staudinger, J., Roberts, P.V. (2001) A critical compilation of Henry's law constant temperature dependence relations for organic compounds in dilute aqueous solutions. *Chemosphere* 44, 561–576.

Steen, W.C., Collette, T.W. (1989) Microbial degradation of seven amides by suspended bacterial populations. *Appl. Environ. Microbiol.* 55, 2545–2549.

Steen, W.C., Paris, D.F., Baughman, G.L. (1979) Effects of sediment sorption on microbial degradation of toxic substances. in *Proc. 177th National Meeting of American Chemical Society*, April 1979, Honolulu, Hawaii.

Steen, W.C., Paris, D.F., Baughman, G.L. (1982) Effects of sediment sorption on microbial degradation of toxic substances. In: *Contaminants and Sediments: Fate and Transport, Case Studies, Modeling, Toxicity.* Vol. l, Baker, R.A., Editor, p. 477, Ann Arbor Science, Ann Arbor, Michigan.

Stephenson, R.M., Malanowski, S. (1987) *Handbook of the Thermodynamics of Organic Compounds.* Elsevier Science Publishing Co., Inc., New York.

Stepp, T.A., Camper, N.D., Paynter, M.J.B. (1985) Anaerobic microbial degradation of selected 3,4-dihalogenated aromatic compounds. *Pest. Biochem. Physiol*. 23, 256.

Stevens, P.J.G., Baker, E.A., Anderson, N.H. (1988) Factors affecting the foliar absorption and redistribution of pesticides. 2. Physicochemical properties of the active ingredient and the role of surfactant. *Pestic. Sci.* 24, 31–53.

Stewart, D.K.R., Gaul, S.O. (1977) Persistence of 2,4-D dichlorophenoxyacetic acid, 2,4,5-T, and dicamba in a Dykeland soil. *Bull. Environ. Contam. Toxicol.* 18, 210.

Subba-Rao, R.V., Rubin, H.E., Alexander, M. (1982) Kinetics and extent of mineralization of organic chemicals at trace levels in freshwater and sewage. *Appl. Environ. Microbiol.* 43, 1139.

Sukop, M., Cogger, C.G. (1992) Adsorption of carbofuran, metalaxyl, and simazine: KOC evaluation and relation to soil transport. *J. Environ. Sci. Health* B27(5), 565–590.

Suntio, L.R., Shiu, W.Y., Mackay, D., Seiber, J.N., Glotfelty, D. (1988) Critical review of Henry's law constants. *Rev. Environ. Contam. Toxicol.* 103, 1–59.

Swann, R.L., Laskowski, D.A., McCall, P., Vanderkuy, K., Dishburger, H. (1983) A rapid method for the estimation of the environmental parameters octanol/water partition coefficient, soil sorption constant, water to air ratio, and water solubility. *Residue Rev.* 85, 17–28.

Szabó, G., Guczi, J., Kördel, Zsonay, A., Major, V., Keresztes, P. (1999) Comparison of different HPLC stationary phases for determination of soil-water distribution coefficient. K_{OC}, values of organic chemicals in RP-HPLC system. *Chemosphere* 39, 431–442.

Swezey, A.W., Nex, R.W. (1961) Some physical and chemical properties of weed killers. *Suppl. I Weeds* 9, 209.

Takahashi, M., Kawamura, S., Miyakado, M., Sanemitsu, Y., Tanaka, S. (1993) Uptake and translocation of bleaching herbicidal compounds in radish seedlings. *Pestic. Sci*. 39, 159–177.

Tanaka, F.S., Wien, R.G., Mansager, E.R. (1979) Effects of nonionic surfactants on the photochemistry of 3-(4-chlorophenyl)-1,1-dimethylurea in aqueous solution. *J. Agric. Food Chem*. 27, 774–779.

Tanaka, F.S., Wien, R.G., Mansager, E.R. (1981) Survey for surfactant effects on the photodegradation of herbicides in aqueous media. *J. Agric. Food Chem*. 29, 227–230.

Tanaka, F.S., Wien, R.G., Mansager, E.R. (1982) Photolytic demethylation of monuron and demethylmonuron in aqueous solution. *Pest. Sci.* 13, 287.

Tanaka, F.S., Wien, R.G., Zaylskie, G. (1977) Photolysis of 3-(4-chlorophenyl)-1,1-dimethylurea in dilute aqueous solution. *J. Agric. Food Chem*. 25, 1068.

Taylor, A.W., Glotfelty, D.E. (1988) Evaporation from soils and crops. In: *Environmental Chemistry of Herbicides.* Vol. I, Grover, R., Editor, Chapter 4, pp. 89–130, CRC Press, Boca Raton, Florida.

Taylor, A.W., Spencer, W.F. (1990) Volatilization and vapor transport processes. In: *Pesticides in the Soil Environment: Processes, Impacts, and Modeling.* Cheng, H.H., Editor, Soil Science Society of America, Inc., Madison, Wisconsin.

Thomas, R.G. (1982) Chapter 15: Volatilization from water and Chapter 16: Volatilization from soil. In: *Handbook on Chemical Property Estimation Methods, Environmental Behavior of Organic Compounds.* Lyman, W.J., Reehl, W.F., Rosenblatt, D.H., Editors, McGraw-Hill, Inc., New York.

Thomas, V.M., Holt, C.L. (1980) The degradation of [^{14}C]-molinate in soil under flooded and non-flooded conditions. *J. Environ. Sci. Health* B15, 475.

Tomlin, C. (1994) *The Pesticide Manual*. (*A World Compendium*). 10th Edition. The British Crop Protection Council, Surrey, England and The Royal Society of Chemistry, Cambridge, England.

Traub-Eberhard, U., Kördel, W., Klein, W. (1994) Pesticide movement into subsurface drains on a loamy silt soil. *Chemosphere* 28, 273–284.

Travis, C.C., Arms, A.D. (1988) Bioconcentration of organics in beef, milk, and vegetation. *Environ. Sci. Technol.* 22, 271–274.

Trevisan, M., Montepiani, C., Ghebbioni, C., Del Re, A.A.M. (1991) Evaluation of potential hazard of propanil to groundwater. *Chemosphere* 22, 637–643.

Tucker, C.S., Boyd, C.E. (1981) Relationships between pond sediments and simazine loss from waters of laboratory systems. *J. Aquat. Plant Manag*. 19, 55.

Urosol, N.J., Hance, R.J. (1974) The effect of temperature and water contents on the rate of decomposition of the herbicide linuron. *Weed Sci.* 16, 19–21.

Ursin, C. (1985) Degradation of organic chemicals at trace levels in sea water and marine sediment. The effect of concentration on the initial fractional turnover rate. *Chemosphere* 14, 1539.

USDA (1989) Final environment impact statement, vegetation management in the Piedmont and Coastal Plain. Southern Region Management Bulletin R8-MB-23. U.S. Dept. of Agriculture, Forest Service, Atlanta, Georgia.

USEPA (1975) Substitute Chemical Program – Initial Scientific and Minieconomic Review of Bromocil. U.S. EPA-540/1-75-006. U.S. Government Printing Office, Washington DC.

USEPA (1988) Graphical Exposure Modeling System. (GEMS), CLOGP3, U.S. Environmental Protection Agency.

Van Zwieten, L., Kennedy, I.R. (1995) Rapid degradation of atrazine by *Rhodococcus* Sp. NI86/21 and by and atrazind-perfused soil. *J. Agric. Food Chem*. 43, 1377–1382.

Veeh, R.H., Inskeep, W.P., Camper, A.K. (1996) Soil depth and temperature effects on microbial degradation of 2,4-D. *J. Environ. Qual.* 25, 5–12.

Veith, G.D., Defoe, D.L., Bergstedt, B.V. (1979) Measuring and estimating the bioconcentration factor of chemicals in fish. *J. Fish Res. Board Can.* 26, 1040–1048.

Veith, G.D., Kosian, P. (1982) In: *Physical Behavior of PCBs in the Great Lakes.* Chapter 15, pp. 269–282, Ann Arbor Science, Michigan.

Veith, G.D., Macek, K.J., Petrocelli, S.R., Caroll, J. (1980) An evaluation of using partition coefficient and water solubilities to estimate bioconcentration factors for organic chemicals in fish. In: *Aquatic Toxicology.* Eaton, J.G., Parrish, P.R., Hendricks, A.C., Editors, ASTM STP 707, American Society for Testing and Materials. pp. 116–129.

Verloop, A. (1972) Fate of the herbicide diclobenil in plants and soil in relation to its biological activity. *Res. Rev.* 43, 55–103.

Verschueren, K. (1983) *Handbook of Environmental Data on Organic Chemicals.* 2nd. Edition, Van Nostrand Reinhold, New York, New York.

Virtanen, M., Hattula, M.L., Arstila, A.U. (1979) Behavior and fate of 4-chloro-2-methylphenoxyacetic acid (MCPA) and 2,6-dichloro-*o*-cresol as studied in an aquatic-terrestrial model ecosystem. *Chemosphere* 8, 431.

von Oepen, B., Kördel, W., Klein, W. (1991) Sorption of nonpolar and polar compounds to soils: Processes, measurements and experiences with the applicability of the modified OECD-guideline 106. *Chemosphere* 22, 285–304.

Vroumsia, T., Steiman, R., Seigle-Murandi, F., Benoit-Guyod, J.-L., Khadrani, A. (1996) Biodegradation of three substituted phenylurea herbicides (chlortolruon, diuron, and isoproturon) by soil fungi. A comparative study. *Chemosphere* 33, 2045–2056.

Yu, C.-C., Hansen, D.J., Booth, G.M. (1975) Fate of dicamba in a model ecosystem. *Bull. Environ. Contamin. Toxicol.* 13, 280–283.

Walker, A. (1976) Simulation of herbicide persistence in soil. III Propyzamide in different soil types. *Pest. Sci.* 7, 59–64.

Walker, A. (1978) Simulation of the persistence of eight soil applied herbicides. *Weed Res.* 18, 305–313.

Walker, A., Bond, W. (1977) Persistence of the herbicide AC-92, 553, N-(1-ethylpropyl)-2,6-dinitro-3,4-xylidine in soils. *Pestic. Sci.* 8, 359–369.

Walker, A., Brown, P.A. (1985) The relative persistence in soil of five acetanilide herbicides. *Bull. Environ. Contam. Toxicol.* 34, 143–149.

Walker, A., Cotterill, E.G., Welch, S.J. (1989) Adsorption and degradation of chlorsulfuron and metsulfuron-methyl in soils from different depths. *Weed Res.* 29, 281–287.

Walker, A., Welch, S.J. (1991) Enhanced degradation of some soil-applied herbicides. *Weed Res*. 31, 49–57.

Walker, A., Welch, S.J. (1992) Further studies of the enhanced biodegradation of some soil-applied herbicides. *Weed Res*. 32, 19–27.

Walker, A., Zimdahl, R.L. (1981) Simulation of the persistence of atrazine, linuron and metocholor in soil at different sites in U.S.A. *Weed Res.* 21, 255–265.

Walker, W.W. (1978) Insecticide persistence in natural seawater as affected by salinity, temperature and sterility. EPA-600/3-78-044. U.S. Environmental Protection Agency, Gulf Breeze, Florida.

Walker, W.W., Cripe, C.R., Pritchard, P.H., Bourquin, A.W. (1988) Biological and abiotic degradation of xenobiotic compounds in *in vitro* estuarine water and sediment/water systems. *Chemosphere* 17, 2255–2270.

Wang, S., Arnold, W.A. (2003) Abiotic reduction of dinitroaniline herbicides. *Water Res*. 37, 4191–4201.

Wang, Y.-S., Jaw, C.-G., Tang, H.-C., Lin, T.-S., Chen, Y.-L. (1992) Accumulation and release of herbicides butachlor, thiobencarb, and chlomethoxyfen by fish, clam, and shrimp. *Bull. environ. Contam. Toxicol*. 48, 474–480.

Wang, Y.-S., Madsen, E.L., Alexander, M. (1985) Microbial degradation by mineralization or cometabolism determined by chemical concentration and environment. *J. Agric. Food Chem*. 33, 495.

Wang, Y.-S., Subba-Rao, R.V., Alexander, M. (1984) Effect of substrate concentration and organic and inorganic compounds on the occurrence and rate of mineralization and cometabolism. *Appl. Environ. Microbiol.* 47, 1195.

Wang, X., Harada, S., Watanabe, M., Koshikawa, H., Geyer, P.R. (1996) Modelling the bioconcentration of hydrophobic organic organisms. *Chemosphere* 32, 1783–1793.

Ward, T.M., Weber, J.B. (1968) Aqueous solubility of alkylamino-*s*-triazines as a function of pH and molecular structure. *J. Agric. Food Chem.* 16, 959–961.

Wauchope, R.D. (1978) The pesticide content of surface water draining from agricultural fields – A review. *J. Environ. Qual.* 7, 459–472.

Wauchope, R.D. (1989) *ARS/SCS Pesticides Properties Database.* Version 1.9, preprint, August, 1989.

Wauchope, R.D., Buttler, T.M., Hornsby, A.G., Augustijn-Beckers, P.W.M., Burt, J.P. (1992) The SCS/ARS/SCS Pesticides Properties Database for Environmental Decision-Making. *Rev. Environ. Contam. Toxicol.* 123, 1–164.

Wauchope, R.D., Hornsby, A G., Goss, D.W., Burt, J.P. (1991) The SCS/ARS/SCS Pesticides Properties Database: A set of parameter values for first-tier comparative water pollution risk analysis. *Proceedings, National Pesticide Conference,* Brookfield, Virginia, November 8–9, 1990, pp. 455–470.

Wauchope, R.D., Myers, R.S. (1985) Adsorption-desorption kinetics of atrazine and linuron in freshwater-sediment aqueous slurries. *J. Environ. Qual.* 14, 132–137.

Weber, J.B. (1970) Mechanisms of adsorption of *s*-trazines by clay colloids and factors affecting plant availability. *Res. Rev.* 32, 93–130.

Weber, J.B. (1972) Interaction of organic pesticides with particulate matter in aquatic and soil systems. In: *Fate of Organic Pesticides in the Aquatic Environment. Adv. Chem. Ser.* 111. American Chemical Society, Washington, DC. p. 55.

Weber, J.B., Peter, C.J. (1982) Adsorption, bioactivity, and evaluation of soil tests for alachlor, acetochlor, and metolachlor. *Weed Sci*. 30, 14–20.

Weber, J.B., Shea, P.J., Strek, H.J. (1980) An evaluation of nonpoint sources of pesticide pollution in runoff. In: *Environmental Impact of Nonpoint Source Pollution.* Overcash, M., Davidson, J., Editors, Ann Arbor Science Publishers, Ann Arbor, Michigan.

Wiedemann, H.G. (1972) Applications of thermogravimetry of vapor pressure determination. *Thermochim. Acta* 3, 355–366.

Weidner, C.W. (1974) Degradation in ground water and mobility of herbicides. Report prepared for the Office of Water Research and Technology, U.S. Environmental Protection Agency, Washington DC. PB 239242.

Weinhold, B.J., Gish, T.J. (1994) Chemical properties influencing rate of release of starch encapsulated herbicides: Implications for modifying environmental fate. *Chemosphere* 28(5), 1035–1046.

Weinhold, B.J., Sadeghi, A.M., Gish, T.J. (1993) Organic chemicals in the environment. Effect of starch encapsulation and temperature on volatilization of atrazine and alachlor. *J. Environ. Qual*. 22, 162–166.

West, S.D., Burger, R.O., Poole, G.M., Mowrey, O.H. (1983) Bioconcentration and field dissipation of the aquatic herbicide fluridone and its degradation products in aquatic environments. *J. Agric. Food Chem*. 31, 579–585.

West, S.D., Day, E.W., Jr., Burger, R.O. (1979) Dissipation of the experimental aquatic herbicide fluridone from lakes and ponds. *J. Agric. Food Chem*. 27, 1067.

Willis, G.H., McDowell, L.L. (1982) Pesticides in agricultural runoff and their effects on downstream water quality. *Environ. Toxicol. Chem.* 1, 267–279.

Willis, G.H., Wander, R.C., Southwick, L.M. (1974) Degradation of trifluralin in soil suspensions as related to redox potential. *J. Environ. Qual.* 3, 262–265.

Wilson, R.G., Jr., Cheng, H.H. (1978) Fate of 2,4-D in a Naff silt loam soil. *J. Environ. Qual.* 7, 281.

Windholz, M., Editor (1983) *The Merck Index. An Encyclopedia of Chemicals, Drugs and Biologicals.* 10th Edition. The Merck & Co. Inc., Rahway, New Jersey.

Winkelmann, D.A., Klaine, S.J. (1991) Degradation and bound residue formation of atrazine in a western Tennessee soil. *Environ. Toxicol. Chem.* 10, 335–345.

Wolt, J.D. (1997) Environmental fate of ethalfluralin. *Rev. Environ. Contam. Toxicol*. 153, 65–90.

Wolf, D.C., Jackson, R.L. (1982) Atrazine degradation, sorption, and bioaccumulation in water systems. Arkansas Water Resources Center. NTIS PB83-150151.

Wolfe, N.L., Zepp, R.G., Baughman, G.L., Fincher, R.C., Gordon, J.A. (1976) Chemical and photochemical transformation of selected pesticides in aquatic systems. U.S. Environmental Protection Agency, Athens, Georgia. EPA-600/3-76-067.

Wolfe, N.L., Zepp, R.G., Paris, D.F. (1978) Carbaryl, propham, and chloropropham: A comparison of the rates of hydrolysis and photolysis with the rate of biolysis. *Water Res.* 12, 565–571.

Wood, A, Davidson, J.M. (1975) *Soil Science Society of America Proceedings* 39, 820–825.

Wood, M.J. et al. (1991) In: *Pesticides in Soil and Water: Current Perspectives.* Walker, A., Editor, (BCPC Monograph), 47, 175–182.

Woodburn, K.B., Batzer, F.R., White, F.H., Schultz, M.R. (1993) The aqueous photolysis of triclopyr. *Environ. Toxicol. Chem.* 12, 45–55.

Woodford, E.K., Evans, S.A., Editors (1963) *Weed Control Handbook: Properties of Herbicides.* Blackwell Scientific, Oxford, England.

Woodrow, J.E., Crosby, D.G., Mast, T., Moilanen, K.W., Seiber, J.N. (1978) Rates of transformation of trifluralin and parathion vapors in air. *J. Agric. Food Chem*. 26, 1312–1316.

Woodrow, J.E., Crosby, D.G., Seiber, J.N. (1983) Vapor-phase photochemistry of pesticides. *Residue Rev.* 85, 111–125.

Worthing, C.R., Editor (1983) *The Pesticide Manual*. (*A World Compendium*). 7th Edition, The British Crop Protection Council, Croydon, England.

Worthing, C.R., Walker, S.B., Editors (1987) *The Pesticide Manual*. (*A World Compendium*). 8th Edition, The British Crop Protection Council, Croydon, England.

Worthing, C.R., Hance, R., Editors (1991) *The Pesticide Manual*. (*A World Compendium*). 9th Edition, The British Crop Protection Council, Croydon, England.

Xu, F., Liang, X.-M., Su, F., Zhang, Z., Lin, B.-C., Wu, W.-Z., Yediler, A., Kettrup, A. (1999) A column method for determination of soil organic partition coefficients of eight pesticides. *Chemosphere* 39, 787–794.

Yalkowsky, S.H., Valvani, S.C., Kun, W.-Y., Dannenfelser, R.M., Editors (1987) *Arizona Database of Aqueous Solubility for Organic Compounds.* College of Pharmacy, University of Arizona, Tucson, Arizona.

Yao, C.C.D., Haag, W.R. (1991) Rate constants for direct reactions of ozone with several drinking water contaminants. *Water Res.* 25, 761–773.

Yockim, R.S., Isensee, A.R., Walker, E.A. (1980) Behavior of trifluralin in aquatic model ecosystems. *Bull. Environ. Contamin. Toxicol*. 24, 134–141.

Yoshioka, Y., Mizuno, T., Ose, Y., Sato, T. (1986) The estimation for toxicity of chemicals on fish by physico-chemical properties. *Chemosphere* 15(2), 195–203.

Yu, C-C., Hansen, D.J., Booth, G.M. (1975) Fate of dicamba in a model ecosystem. *Bull. Environ. Contam. Toxicol*. 13, 280–283.

Zandvoort, R., Van Dord, D.C., Leistra, M., Verlaat, J.G. (1979) The decline of propyzamide in soil under field conditions in the Netherlands. *Weed Res.* 19, 157.

Zepp, R.G. (1978) Quantum yields for reactions of pollutants in dilute aqueous solution. *Environ. Sci. Technol.* 12, 327–329.

Zepp, R.G. (1980). Assessing the photochemistry of organic pollutants in aquatic environments. In: *Dynamics, Exposure and Hazard Assessment of Toxic Chemicals.* Haque, R., Editor, pp. 60–110, Ann Arbor Science Publishers, Ann Arbor, Michigan.

Zepp, R.G. (1991) Photochemical fate of agrochemicals in natural waters. In: *Pesticide Chemistry. Advances in International Research, Development, and Legislation*. Frehse, H., Editor, pp. 329–345, VCH, New York, New York.

Zepp, R.G., Baughman, G.L. (1978) Prediction of photochemical transformation of pollutants in aquatic environment. In: *Aquatic Pollutants: Transformation and Biological Effects.* Hutzinger, O., Van Lelyveld, I.H., Zoeteman, B.C.J., Editors, pp. 237–264, Pergamon Press, Oxford, England.

Zepp, R.G., Cline, D.M. (1977) Rates of direct photolysis in aqueous environment. *Environ. Sci. Technol.* 11, 359–366.

Zepp, R.G., Schlotzhauer, P.F., Simmons, M.S., Miller, G.C., Baughman, G.L., Wolfe, N.L. (1984) Dynamics of pollutant photoreactions in the hydrosphere. *Fresenius Z. Anal. Chem.* 319, 119–125.

Zepp, R.G., Wolfe, N.L., Gordon, J.A., Baughman, G.L. (1975) Dynamics of 2,4-D esters in surface waters. Hydrolysis, photolysis and vaporization. *Environ. Sci. Technol.* 9, 1144.

Zhao, H., Jaynes, W.F., Vance, G.F. (1996) Sorption of the ionizable organic compound, dicamba (3,6-dichloro-2-methoxy benzoic acid), by organo-clays. *Chemosphere* 33, 2089–2100.

Zimdahl, R.L., Clark, S.K. (1982) Degradation of three acetanilide herbicides in soil. *Weed Sci*. 30, 545.

Zimdahl, R.L., Gwynn, S.M. (1977) Soil degradation of three dinitroanilines. *Weed Sci.* 25, 247–251.

Zitko, V., McLeese, D.W., Carson, W.G., Welch, H.E. (1976) Toxicity of alkyl-dinitrophenols to some aquatic organisms. *Bull. Environ. Contam. Toxicol*. 16, 508–515.

18 Insecticides

CONTENTS

18.1. List of Chemicals and Data Compilations (by Functional Group):

Organophosphorus compounds:

a) Phosphates:

b) Phosphorothioates:

c) Phosphorodithioates (Phosphorothiolothionates):

Carbamates:

Organochlorines:

Phenols:

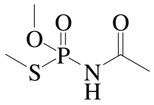
Synthetic pyrethroids:

Miscellaneous:

18.1 LIST OF CHEMICALS AND DATA COMPILATIONS

18.1.1 INSECTICIDES

18.1.1.1 Acephate



Common Name: Acephate
Synonym: Chevron RE 12420, ENT 27822, Orthene, Ortho 12420, Ortran, Ortril, RE 12420, 75 SP, Tornado
Chemical Name: acetylphosphoramidothioic acid *O,S*-dimethyl ester; *O,S*-dimethyl acetylphosphoramidothioate; *N*-[methoxy(methylthio)phosphinoyl]acetamide
Uses: systemic insecticide with contact and stomach action to control a wide range of chewing and sucking insects in fruit, cotton, hops, vines, soybeans, olives, groundnuts, beet, brassicas, celery, potatoes, rice ornamentals, forestry and other crops; also used as cholinesterase inhibitor.
CAS Registry No: 30560-19-1
Molecular Formula: $C_4H_{10}NO_3PS$
Molecular Weight: 183.166
Melting Point (°C):
88 (Lide 2003)
Boiling Point (°C):
Density (g/cm^3 at 20°C):
1.35 (Spencer 1982; Worthing & Hance 1991; Montgomery 1993; Tomlin 1994; Milne 1995)
Molar Volume (cm^3/mol):
135.7 (calculated from density)
Dissociation Constant, pK_a:
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
Entropy of Fusion, ΔS_{fus} (J/mol K):
Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F: 0.241 (mp at 88°C)

Water Solubility (g/m^3 or mg/L at 25°C or as indicated):
650000 (Spencer 1973, 1982; Martin & Worthing 1977; Worthing& Walker 1987, Worthing & Hance 1991)
> 5000 (20°C, shake flask-GC, Bowman & Sans 1983a)
790000 (20°C, Hartley & Kidd 1987)
818000 (Wauchope 1989)
818000 (20–25°C, selected, Wauchope et al. 1992; Hornsby et al. 1996)
790000 (20°C, Montgomery 1993; Tomlin 1994; Milne 1995)

Vapor Pressure (Pa at 25°C or as indicated):
2.26×10^{-4} (20°C, Hartley & Kidd 1987)
2.26×10^{-4} (24°C, Worthing & Walker 1987, Worthing & Hance 1991; Tomlin 1994)
2.27×10^{-4} (20–25°C, selected, Wauchope et al. 1992; Hornsby et al. 1996)
2.27×10^{-4} (20°C, Montgomery 1993)
0.513; 0.759, 0.457 (gradient GC method; estimation using modified Watson method: Sugden's parachor, McGowan's parachor, Tsuzuki 2000)

Henry's Law Constant (Pa·m^3/mol at 25°C or as indicated):
5.27×10^{-8} (20–25°C, calculated-P/C, Montgomery 1993)
6.37×10^{-8} (20–25°C, calculated-P/C as per Worthing & Walker 1987, Majewski & Capel 1995)
5.06×10^{-8} (calculated-P/C, this work)

Octanol/Water Partition Coefficient, log K_{OW}:
–0.85 (shake flask, Log P Database, Hansch & Leo 1987)
–1.87 (calculated, Montgomery 1993)

–0.85	(recommended, Sangster 1993)
–0.886	(Tomlin 1994)
1.12	(RP-HPLC-RT correlation, Finizio et al. 1997)

Bioconcentration Factor, log BCF:

–0.523	(calculated-S, Kenaga 1980)
0.053	(wet wt. basis, rainbow trout, Geen et al. 1984)

Sorption Partition Coefficient, log K_{OC}:

0.477	(calculated-S as per Kenaga & Goring 1978, Kenaga 1980)
0.30	(soil, 20–25°C, selected, Wauchope et al. 1992; Dowd et al. 1993; Hornsby et al. 1996)
0.48	(Montgomery 1993)
0.30	(estimated-chemical structure, Lohninger 1994)
3.50, 3.00	(soil, estimated-class-specific model, estimated-general model, Gramatica et al. 2000)

Environmental Fate Rate Constants or Half-Lives, $t_{½}$:

Volatilization:

Photolysis:

Oxidation: calculated rate constant k ~ 51×10^{-12} cm^3/molecules for the vapor phase reaction with hydroxyl radical in air (Winer & Atkinson 1990).

Hydrolysis: persistent to hydrolysis between pH 4.0 and 6.0 under laboratory condition at 20 and 30°C regardless of temperature while strongly affected by temperature at pH 8.2; and more persistent in pond than creek water (Szeto et al. 1979)

$t_{½}$ = 60 h at pH 9 and $t_{½}$ = 710 h at pH 3 both at 40°C (Montgomery 1993).

Biodegradation:

Biotransformation:

Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants:

Half-Lives in the Environment:

Air:

Surface water: resistant to hydrolysis in distilled, buffered water at pH 4.0 to 6.9, but not at pH 8.2; and more persistent in pond than creek water, 45% found after 50 d when incubated at 9°C in creek water (Szeto et al. 1979)

Ground water:

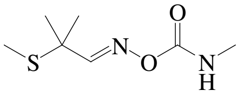
Sediment: degradation increased greatly when treated samples were incubated in the presence of sediments, ~ 20% recovered after 42 d and ~ 28% recovered after 58 d after incubating acephate-treated pond and creek water with their respective sediments (Szeto et al. 1979)

Soil: selected field $t_{½}$ = 3.0 d (Wauchope et al. 1992; Dowd et al. 1993; Hornsby et al. 1996);

$t_{½}$ = 7–10 d in soil (Tomlin 1994).

Biota:

18.1.1.2 Aldicarb



Common Name: Aldicarb

Synonym: Ambush, Carbanolate, ENT 27093, NCI-C08640, matadan, OMS 771, Pounce, Temik, Union Carbide 21149

Chemical Name: 2-methyl-2-(methylthio)propionaldehyde *O*-(methylcarbamoyl) oxime; 2-methyl-2-(methylthio)propanal *O*-(methylamino)carbonyl) oxime

Uses: systemic insecticide, acaricide, and nematocide with contact and stomach action; also used as cholinesterase inhibitor.

CAS Registry No: 116-06-3

Molecular Formula: $C_7H_{14}N_2O_2S$

Molecular Weight: 190.263

Melting Point (°C):
99 (Lide 2003)

Boiling Point (°C):
100 (decomposes above this temp., Howard 1991)

Density (g/cm^3 at 20°C):
1.195 (25°C, Hartley & Kidd 1987; Montgomery 1993; Tomlin 1994; Milne 1995)

Molar Volume (cm^3/mol):
224.3 (calculated-Compiled method at normal boiling point)

Dissociation Constant, pK_a:

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
25.94 (DSC method, Plato & Glasgow 1969)

Entropy of Fusion, ΔS_{fus} (J/mol K):

Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F: 0.188 (mp at 99°C)

Water Solubility (g/m^3 or mg/L at 25°C):
4000 (24°C, shake flask-GC, Felsot & Dahm 1979)
7800 (Kenaga 1980a; Kenaga & Goring 1980)
6000 (Khan 1980; Verschueren 1983)
6016, 6000 (exptl., corrected-mp, Briggs 1981)
6000 (20°C, shake flask-GC, Bowman & Sans 1983b)
6000 (Hartley & Kidd 1987; Worthing & Walker 1987, Worthing & Hance 1991; Budavari 1989; Montgomery 1993; Milne 1995)
5730 (Seiber 1987)
6000 (20–25°C, selected, Wauchope et al. 1992; Hornsby et al. 1996)
4930 (20°C at pH 7, Tomlin 1994)

Vapor Pressure (Pa at 25°C or as indicated and reported temperature dependence equations.):
6.67 (20°C, Khan 1980)
0.00707 (20°C, selected exptl. value, Kim 1985)
0.102, 0.016 (20°C, GC-RT correlation, GC-RT correlation with mp correction, Kim 1985)
0.013 (20°C, Hartley & Kidd 1987; Tomlin 1994)
0.013 (selected, Suntio et al. 1988)
0.013 (Worthing & Hance 1991)
0.004 (20–25°C, selected, Wauchope et al. 1992; Hornsby et al. 1996)
0.0046 (Montgomery 1993)

Henry's Law Constant (Pa·m^3/mol at 25°C):
2.48×10^{-4} (Jury et al. 1987a, Jury & Ghodrati 1989)
3.20×10^{-4} (calculated-P/C, Suntio et al. 1988)

1.47×10^{-4}	(20–25°C, calculated-P/C, Montgomery 1993)
1.27×10^{-4}	(calculated-P/C, this work)

Octanol/Water Partition Coefficient, log K_{OW}:

0.85	(shake flask, Felsot & Dahm 1979)
1.10	(Hansch & Leo 1979)
1.57	(shake flask-UV, Lord et al.1980)
0.70	(Rao & Davidson 1980)
1.57	(20°C, shake flask-UV, Briggs 1981)
1.13	(20°C, shake flask-GC, Bowman & Sans 1983b)
1.13	(Hansch & Leo 1985)
0.70, 1.13	(Montgomery 1993)
1.13	(recommended, Sangster 1993)
1.13	(recommended, Hansch et al. 1995)

Bioconcentration Factor, log BCF:

1.62	(fish in static water, Metcalf & Sanborn 1975; Kenaga & Goring 1980)
0.85	(vegetation, correlated-K_{OW}, Iwata et al. 1977; Maitlen & Powell 1982)
0.602	(calculated-S, Kenaga 1980; quoted, Howard 1991)
1.64	(earthworm, Lord et al. 1980; quoted, Connell & Markwell 1990)
1.00, 1.18	(log BCF_{lipid}, log $BCF_{protein}$, Briggs 1981)

Sorption Partition Coefficient, log K_{OC}:

1.36–1.57	(Felsot & Dahm 1979)
0.91, 1.20	(Bromilow & Leistra 1980)
1.51	(calculated-S as per Kenaga & Goring 1978, Kenaga 1980)
1.39	(reported as log K_{OM}, Briggs 1981)
1.51	(estimated, Kenaga 1980; quoted, Howard 1991)
1.30–1.40	(Bilkert & Rao 1985; quoted, Howard 1991)
1.56	(soil, screening model calculations, Jury et al. 1987a, b; Jury & Ghodrati 1989)
1.48	(soil, 20–25°C, selected, Wauchope et al. 1992; Dowd et al. 1993; Hornsby et al. 1996)
0.85–1.67	(Montgomery 1993)
1.48	(estimated-chemical structure, Lohninger 1994)
1.50	(soil, calculated-MCI $^1\chi$, Sabljic et al. 1995)
1.40, 1.97	(estimated-class-specific model, estimated-general model, Gramatica et al. 2000)
1.30	(soil: organic carbon OC ≥ 0.5%, average, Delle Site 2001)

Environmental Fate Rate Constants, k, or Half-Lives, $t_{½}$:

Volatilization:

Photolysis:

Oxidation: rate constant k, for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO3} with NO_3 radical and k_{O3} with O_3 or as indicated, *data at other temperatures see reference:

photooxidation $t_{½}$ = 1–9.5 h, based on an estimated rate constant for vapor-phase reaction with hydroxyl radical in air (Atkinson 1987; quoted, Howard et al. 1991)

$t_{½}$ = 1.7–12 d in soil for pH 1–10 with little change in rate between pH 4.4–10 (Lemley et al. 1988; quoted, Howard 1991)

k(aq.) = 5.9×10^9 M^{-1} s^{-1} for the reaction (Fenton with reference to acetophenone) with hydroxyl radical in aqueous solutions at pH 3.5 and at 24 ± 1°C (Buxton et al. 1988; quoted, Faust & Hoigné 1990; Haag & Yao 1992)

k(aq.) = $(4.4 \pm 0.1) \times 10^4$ M^{-1} s^{-1} for direct reaction with ozone in water at pH 2.1; k = $(4.3 \pm 0.2) \times 10^5$ M^{-1} s^{-1} at pH 7.0 and 24 ± 1°C, with $t_{½}$ = 0.08 s at pH 7 (Yao & Haag 1991).

k(aq.) = $(8.1 \pm 1.1) \times 10^9$ M^{-1} s^{-1} for the reaction (Fenton with reference to acetophenone) with hydroxyl radical in aqueous solutions at pH 3.5 and at 24 ± 1°C (Haag & Yao 1992)

Hydrolysis: $t_{1/2}$ = 23 d at pH 7.2 (Smelt et al. 1978; quoted, Howard 1991)

$t_{1/2}$ = 9.9 d at pH 6.3–7.0 at 15°C (Bromilow & Leistra 1980; quoted, Howard 1991)

$t_{1/2}$ = 4580 d, based on a first-order k = 1.51×10^{-4} d^{-1} at pH 5.5 and 5°C (Hansen & Spiegel 1983; quoted, Howard et al. 1991)

$t_{1/2}$ = 4.0 min at pH 12.9, $t_{1/2}$ = = 1.3 min at pH 13.39 and 15°C (Lemley & Zhong 1983)

$t_{1/2}$ = 0.4–3.2 d in soil at pH 4.5–4.9 and 25°C (Rao et al. 1984; quoted, Howard 1991)

Pseudo-first order k = 5.3×10^{-3} d^{-1} with $t_{1/2}$ = 131 d^{-1} at pH 3.95, k = 1.3×10^{-3} d^{-1} with $t_{1/2}$ = 559 d at pH 6.02, k = 2.1×10^{-3} d^{-1} with $t_{1/2}$ = 324 d at pH 7.96, k = 1.3×10^{-2} d^{-1} with $t_{1/2}$ = 55 d at pH 8.85 in period of 89 d; and k = 1.2×10^{-1} d^{-1} with $t_{1/2}$ = 6 d at pH 9.85 for period of 15 days at 20°C in pH-buffered distilled water (Given & Dierberg 1985; Mink et al. 1989)

For pH buffered distilled water at 20°C: $t_{1/2}$ = 131 d at pH 3.95, $t_{1/2}$ = 559 d at pH 6.02, $t_{1/2}$ = 324 d at pH 7.96, $t_{1/2}$ = 55 d at pH 8.85, and $t_{1/2}$ = 6 d at pH 9.85 (Montgomery 1993)

$t_{1/2}$ = 16 d in aqueous montmorillonite suspensions (10 g/L) at pH 3.7 (Wei et al. 2001).

Biodegradation:

k = 0.000222 h^{-1} for discharge rate of 30 cm/year and k = 0.000233 h^{-1} for discharge rate of 61 cm/year with $t_{1/2}$ = 30 d (Jones & Back 1984)

Aerobic mineralization k = (1.93–34.2) × 10^{-3} d^{-1} with $t_{1/2}$ = 20–361 d in surface soils and k = 2.97–5.28) × 10^{-3} d^{-1} with $t_{1/2}$ = 131–233 d in subsurface soils; anaerobic mineralization k = (8.09–31.1) × 10^{-4} d^{-1} with $t_{1/2}$ = 223–1130 d in surface soils after 63 d incubation (Ou et al. 1985)

$t_{1/2}$ = 70 d in 0–10 cm depth of soil (Jury et al. 1987a, b; Jury & Ghodrati 1989).

$t_{1/2}$(aq. aerobic) = 480–8664 h, based on unacclimated aerobic soil grab sample data; $t_{1/2}$(aq anaerobic) = 1488–15240 h, based on anaerobic ground water grab sample data (Howard et al. 1991)

Biotransformation:

Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants:

Half-Lives in the Environment:

Air: $t_{1/2}$ = 1–9.5 h, based on an estimated rate constant for vapor-phase reaction with hydroxyl radicals in air (Atkinson 1987; quoted, Howard 1991; Howard et al. 1991).

Surface water: $t_{1/2}$ = 5 d in pond water, $t_{1/2}$ = 6 d in lake water (Moorefield 1974; Mink et al. 1989)

Hydrolysis $t_{1/2}$ = 6 to 131 d in pH-buffered distilled water at 20°C (Given & Dierberg 1985)

$t_{1/2}$ = 480–8664 h, based on estimated aqueous aerobic biodegradation half-life (Howard et al. 1991); $t_{1/2}$ = 0.08 s for direct reaction with ozone in water at pH 7 and 24 ± 1°C (Yao & Haag 1991)

Ground water: $t_{1/2}$ = 960–15240 h, based on estimated aqueous aerobic biodegradation half-life and water grab sample data (Miles & Delfino 1985; quoted, Howard et al. 1991).

Sediment:

Soil: $t_{1/2}$ = 9, 7, and 12 d in clay, silty clay loam and fine sandy loam at an application rate of 20 ppm (Coppedge et al. 1967; quoted, Montgomery 1993);

hydrolysis $t_{1/2}$ = 23 d at pH 7.2 (Smelt et al. 1978; quoted, Howard 1991),

$t_{1/2}$ = 9.9 d at pH 6.3–7.0 at 15°C (Bromilow et al. 1980; Bromilow & Leistra 1980; quoted, Howard 1991; Montgomery 1993);

$t_{1/2}$ = 0.4–3.2 d at pH 4.5–4.9 and 25°C (Rao et al. 1984; quoted, Howard 1991);

degradation rate constants k = 0.000222 h^{-1} for discharge rate of 30 cm/year and k = 0.000233 h^{-1} for discharge rate of 61 cm/yr with $t_{1/2}$ = 30 d (Jones & Back 1984);

Mineralization $t_{1/2}$ = 20–361 d in surface soils and $t_{1/2}$ = 131–233 d in surface soils under aerobic condition, anaerobic $t_{1/2}$ = 223–1130 d in surface soils after 63 d incubation (Ou et al. 1985)

reported $t_{1/2}$ = 70 d from screening model calculations (Jury et al. 1987a, b; Jury & Ghodrati 1989; quoted, Montgomery 1993);

oxidation $t_{1/2}$ = 1.7–12 d for pH 1–10 with little change in rate between pH 4.4–10 (Lemley et al. 1988; quoted, Howard 1991);

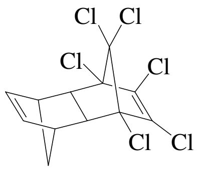
Rapidly oxidized to sulfoxide with $t_{1/2}$ ~ 7 d in some soils, much more slowly to sulfone, pH dependent with $t_{1/2}$ varying from a few minutes at a pH of > 12 to ~ 560 d at a pH of 6.0. $t_{1/2}$ from 2 to > 8 wk in laboratory experiment, and $t_{1/2}$ < 1 wk in field studies (Mink et al. 1989)

$t_{1/2}$ ≤ 2 wk, field study over 218–d period in the unsaturated zone beneath a citrus grove (Hornsby et al. 1990)

$t_{1/2}$ = 480–8664 h, based on unacclimated aerobic soil grab sample data (Howard 1991);
selected field $t_{1/2}$ = 30 d (Wauchope et al. 1992; Dowd et al. 1993; Hornsby et al. 1996);
$t_{1/2}$ between 0.3 and 3.5 months in surface soils (Jones & Norris 1998);
$t_{1/2}$ = 12.0 d in sterile soil, $t_{1/2}$ = 2.7 d in non–sterile soil; $t_{1/2}$ = 1.6, 1.4 and 1.7 d in soil grown with corn, mung bean and cowpea, respectively (Sun et al. 2004)

Biota: biochemical $t_{1/2}$ = 70 d from screening model calculations (Jury et al. 1987a, b; Jury & Ghodrati 1989).

18.1.1.3 Aldrin



Common Name: Aldrin
Synonym: Aldrec, Aldrex, Aldrite, Aldrosol, Altox, Compound 118, Drinox, ENT 15949, HHDN, NA 2761, NA 2762, Octalene, Seedrin
Chemical Name: 1,2,3,4,10,10-hexachloro-1,4,4a,5,8,8a-hexahydro-1,4-endoexo-5,8-dimethano-naphthalene
Uses: Insecticide/Fumigant
CAS Registry No: 309-00-2
Molecular Formula: $C_{12}H_8Cl_6$
Molecular Weight: 364.910
Melting Point (°C):
104 (Lide 2003)
Boiling Point (°C):
145 (at 2 mmHg, Hartley & Kidd 1987; Montgomery 1993; Milne 1995)
Density (g/cm^3 at 20°C):
1.70 (Montgomery 1993)
Molar Volume (cm^3/mol):
316.8 (calculated-Le Bas method at normal boiling point)
214.7 (calculated-density)
Dissociation Constant, pK_a:
80.20 (Rordorf 1989)
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
16.19 (Ruelle & Kesselring 1997)
Entropy of Fusion, ΔS_{fus} (J/mol K):
Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F: 0.168 (mp at 104°C)

Water Solubility (g/m^3 or mg/L at 25°C or as indicated. Additional data at other temperatures designated * are compiled at the end of this section):
0.20* (shake flask-GC/UV, measured range 25–45°C, Richardson & Miller 1960)
0.20 (Stephen & Stephen 1963)
0.027 (25–29°C, shake flask-GC/ECD, Park & Bruce 1968)
0.013*, 0.14*, 0.18* (particle size: 0.01, 0.05 and 5.0μ, shake flask-GC/ECD, Biggar & Riggs 1974)
0.017 (generator column-GC/ECD, Weil et al. 1974)
0.027 (Martin & Worthing 1977)
0.01–0.2 (20–25°C, Wauchope 1978; Willis & McDowell 1982)
0.013 (Kenaga 1980a, b; Kenaga & Goring 1980; Garten & Trabalka 1983)
0.027 (27°C, Spencer 1982; Worthing & Walker 1987)
< 0.05 (rm. temp., Hartley & Kidd 1987, Milne 1995)
0.017–0.18 (Montgomery 1993)
0.027 (20–25°C, selected, Augustijn-Beckers et al. 1994; Hornsby et al. 1996)
1.06, 0.985 (supercooled liquid: LDV derivation of literature-derived value, FAV final-adjusted value, Shen & Wania 2005)
$\log [C_L/(\text{mol m}^{-3})] = -1480/(T/K) + 2.42$ (supercooled liquid, linear regression of literature data, Shen & Wania 2005)

Vapor Pressure (Pa at 25°C or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):
0.00308 (Porter 1964a)
$\log (P/\text{mmHg})$ 2,351 – 2035.35/(T/K); temp range 20–50°C (Porter 1964a)

0.0008 (Günther & Günther 1971)
0.0031 (20°C, Martin 1972)
0.075 (20°C, Khan 1980)
0.001 (20°C, estimated-relative volatilization rate, Dobbs & Cull 1982)
0.0086* (20°C, extrapolated, gas saturation-GC, measured range 35.5–70°C, Grayson & Fosbracey 1982)
ln (P/Pa) = 32.9 – 11044/(T/K); temp range 35.5–70°C (Antoine eq., gas saturation-GC, Grayson & Fosbraey 1982)
0.023, 0.033 (P_{GC} by GC-RT correlation, different stationary phases, Bidleman 1984)
0.105 (supercooled liquid P_L, converted from literature P_S with ΔS_{fus} Bidleman 1984)
0.0092, 0.0071 (20°C, gas saturation-GC, gas saturation-mixed bed-GC, Kim 1985)
log (P/mmHg) = 10.4514 – 4281.065/(T/K); temp range 25–45°C (gas saturation, Kim 1985)
0.0086 (20°C, Hartley & Kidd 1987)
0.0010 (20°C, Budavari 1989)
0.0081* (gas saturation-GC, measured range 25–125°C, Rordorf 1989)
log (P_S/Pa) = 15.561 – 5262.3/(T/K); measured range 45–65.2°C (solid, gas saturation-GC, Rordorf 1989)
log (P_L/Pa) = 12.489 – 4189.8/(T/K); measured range 105–181°C (liquid, gas saturation-GC, Rordorf 1989)
0.105, 0.0757 (supercooled P_L, converted from literature P_S with different ΔS_{fus} values, Hinckley et al. 1990)
0.0231, 0.0202 (P_{GC} by GC-RT correlation with different reference standards, Hinckley et al. 1990)
log (P_L/Pa) = 12.04 – 3924/(T/K) (GC-RT correlation, Hinckley et al. 1990)
0.0031 (20°C, Montgomery 1993)
0.0009 (20–25°C, selected, Augustijn-Beckers et al. 1994; Hornsby et al. 1996)
0.061, 0.064 (supercooled liquid P_L: LDV literature derived value, FAV final adjusted value, Shen & Wania 2005)
log (P_L/Pa) = –4106/(T/K) + 12.56 (supercooled liquid, linear regression of literature data, Shen & Wania 2005)

Henry's Law Constant (Pa·m³/mol at 25°C or as indicated):
1.418 (calculated-P/C, Thomas 1982)
50.25 (20°C, gas stripping-GC, Warner et al. 1987)
91.23 (20°C, calculated-P/C, Suntio et al. 1988)
39.2 (calculated-bond contribution method LWAPC, Meylan & Howard 1991)
50.25 (calculated-P/C, Montgomery 1993)
50.8 (quoted from Howard 1989–1991, Capel & Larson 1995)
91.23 (calculated-P/C, this work)
4.46 (wetted wall column-GC, Altschuh et al. 1999)
15, 23 (LDV literature-derived value, FAV final adjusted value, Shen & Wania 2005)

Octanol/Water Partition Coefficient, log K_{OW}:
3.01 (Lu & Metcalf 1975)
5.67 (Callahan et al. 1979)
5.66 (calculated, Kenaga 1980a, b)
7.50 (RP-TLC-RT correlation, Lord et al. 1980)
7.40 (extrapolated from RP-TLC, Briggs 1981)
5.66 (shake flask, Geyer et al. 1984)
6.496 ± 0.035 (shake flask/slow-stirring-GC, De Bruijn et al. 1989)
5.17–7.40 (Montgomery 1993)
5.74 (RP-HPLC-RT correlation, Sicbaldi & Finizio 1993)
6.50 (selected, Hansch et al. 1995)
5.74, 5.49, 5.39 (RP-HPLC-RT correlation, CLOGP, calculated-S, Finizio et al. 1997)
6.50, 6.24 (LDV literature-derived value, FAV final-adjusted value, Shen & Wania 2005)

Octanol/Air Partition Coefficient, log K_{OA} at 25°C and reported temperature dependence equation. Additional data at other temperatures designated * are compiled at the end of this section:
8.08* (gas saturation-GC/MS, calculated, measured range 5–25°C, Shoeib & Harner 2002)
log K_{OA} = –4.37 + 3709/(T/K), temp range: 5–25°C (gas saturation-GC, Shoeib & Harner 2002)
8.08, 8.26 (LDV literature derived value, FAV final adjusted value, Shen & Wania 2005)

Bioconcentration Factor, log BCF:

0.398	(bioaccumulation factor log BF, adipose tissue in female Albino rats, Quaife et al. 1967)
3.56–4.88	(earthworms, Wheatley & Hardman 1968)
2.80	(lake bacteria, Leshniowsky et al. 1970)
4.36; 4.50; 5.15	(*Diptera*; *Epemeoptera*; *Cladocera*; non-steady-state, Johnson et al. 1971)
4.55	(*Daphnia magna*, wet wt. basis, Johnson et al. 1971)
3.56–4.60	(*Oedogonium sp.*, Metcalf et al. 1973)
3.50	(Metcalf 1974)
3.11	(*Anabaena cylindrica*, Schauberger & Wildman 1977)
2.30	(*Acacystis nidulans*, Schauberger & Wildman 1977; quoted, Baughman & Paris 1981)
2.99	(*Acacystis nidulans*, Schauberger & Wildman 1977; quoted, Baughman & Paris 1981)
4.03, 3.50	(fish: flow water, static water; Kenaga 1980b)
3.85, 1.34	(calculated-S, K_{OC}, Kenaga 1980a)
0.431	(average beef fat diet, Kenaga 1980b)
4.10	(*Chlorella fusca*, Geyer et al. 1981)
3.59	(golden orfe, Freitag et al. 1982)
4.10	(algae, Freitag et al. 1982)
4.26	(activated sludge, Freitag et al. 1982, 1984)
4.03	(Garten & Trabalka 1983; quoted, Howard 1991)
4.13	(clam fat, 60-d expt., Hartley & Johnson 1983)
4.09	(*Chlorella fusca*, Geyer et al. 1984)
4.09, 3.44, 4.26	(algae, golden ide, activated sludge, Freitag et al. 1985)
3.66	(molluscs, Hawker & Connell 1986; quoted, Howard 1991)
–1.07	(beef biotransfer factor log B_b, correlated-K_{OW} from Radeleff et al. 1952 & Kenaga 1980; Travis & Arms, 1988)
–1.62	(milk biotransfer factor log B_m, correlated-K_{OW} from Saha 1969; Travis Arms 1988)
–1.67	(vegetation, correlated-K_{OW} from Lichtenstein 1960 & Weisgerber et al. 1974; Travis & Arms, 1988)
4.09, 4.79	(algae *Chlorella*: wet wt basis, dry wt basis, Geyer et al. 2000)
4.55, 6.55	(*Daphnia*: wet wt basis, lipid wt basis, Geyer et al. 2000)
3.66, 5.66	(mussel *Mytilus edulis*: wet wt basis, lipid wt basis, Geyer et al. 2000)

Sorption Partition Coefficient, log K_{OC}:

2.61	(soil, Hamaker & Thompson 1972; quoted, Kenaga 1980a, b; Kenaga & Goring 1980)
4.68	(calculated-S as per Kenaga & Goring 1978, Kenaga 1980)
4.69	(soil, sorption isotherm, converted from K_{OM} multiplied by 1.724, Briggs 1981)
4.36	(calculated-K_{OW} as per Kenaga & Goring 1980, Chapman 1989)
4.69	(derived from exptl., Meylan et al. 1992)
5.02	(calculated-MCI χ, Meylan et al. 1992)
6.18	(estimated by QSAR & SPARC, Kollig 1993)
2.61, 4.69	(Montgomery 1993)
3.70	(20–25°C, selected, Augustijn-Beckers et al. 1994; Hornsby et al. 1996)
4.69; 4.68	(soil, quoted exptl.; estimated-general model, Gramatica et al. 2000)
6.50; 4.70	(soil, calculated-universal solvation model; quoted exptl., Winget et al. 2000)

Environmental Fate Rate Constants, k, or Half-Lives, $t_{1/2}$:

Volatilization: half-life of a few hours to a few days (Callahan et al. 1979);
calculated $t_{1/2}$ = 68 h from water (Thomas 1982).
Photolysis:
Oxidation: photooxidation $t_{1/2}$ = 0.9–9.1 h, based on an estimated rate constant for vapor-phase reaction with hydroxyl radicals in air (Atkinson 1987; quoted, Howard et al. 1991).
Hydrolysis: not readily hydrolyzable with $t_{1/2}$ > 4 yr (Callahan et al. 1979);
first-order $t_{1/2}$ = 760 d, based on a first-order rate constant $k = 3.8 \times 10^{-5}\ h^{-1}$ at pH 7.0 and 25°C (Ellington et al. 1987, 1988; quoted, Howard et al. 1991);
no disappearance in sealed glass ampoules after two weeks at pH 11 and 85°C (Kollig 1993)
$t_{1/2}$ = 760 d at pH 7 and 25°C (Montgomery 1993)

$t_{½}$ = 760 d at pH 7 in natural waters (Capel & Larson 1995).

Biodegradation: aqueous aerobic $t_{½}$ = 504–14200 h, based on unacclimated aerobic river die-away test data and soil field test data (Lichtenstein et al. 1971; quoted, Howard et al. 1991);

rate constant k = 0.013 d^{-1} by soil incubation studies from die-away tests (Rao & Davidson 1980; quoted, Scow 1982);

aqueous anaerobic $t_{½}$ = 24–168 h, based on soil and freshwater mud grab sample data (Maule et al. 1987; quoted, Howard et al. 1991);

$t_{½}$ = 43–63 d in a sandy loam soil incubated in the dark (McLean et al. 1988; quoted, Howard 1991)

$t_{½}$(aerobic) = 21 d, $t_{½}$(anaerobic) = 1 d in natural waters (Capel & Larson 1995).

Biotransformation:

Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants:

Half-Lives in the Environment:

Air: estimated $t_{½}$ ~ 35.5 min for the vapor phase reaction with hydroxyl radical in air (GEMS 1986; quoted, Howard 1991);

$t_{½}$ = 0.9–9.1 h, based on an estimated rate constant for vapor-phase reaction with hydroxyl radical in air (Atkinson 1987; quoted, Howard et al. 1991).

Surface water: $t_{½}$ = 504–14200 h, based on unacclimated aerobic river die-away test data (Eichelberger & Lichtenberg 1971; quoted, Howard et al. 1991) and soil field test data (Lichtenstein et al. 1971; quoted, Howard et al. 1991).

Biodegradation $t_{½}$(aerobic) = 21 d, $t_{½}$(anaerobic) = 1 d, hydrolysis $t_{½}$ = 760 d at pH 7 in natural waters (Capel & Larson 1995)

Ground water: $t_{½}$ = 24–28400 h, based on estimated aqueous aerobic and anaerobic biodegradation half-lives (Howard et al. 1991).

Sediment:

Soil: $t_{½}$ = 5–10 yr persistence in soil (Nash & Woolson 1967);

$t_{½}$ = 504–14200 h, based on unacclimated aerobic river die-away test data (Eichelberger & Lichtenberg 1971; quoted, Howard et al. 1991) and soil field test data (Lichtenstein et al. 1971; quoted, Howard et al. 1991);

persistence of 2 yr (Edwards 1973; quoted, Morrill et al. 1982);

more than 24 months of persistence in soil (Wauchope 1978);

estimated first-order k = 0.013 d^{-1} with $t_{½}$ = 53.3 d from biodegradation by soil incubation studies from die-away tests (Rao & Davidson 1980; quoted, Scow 1982);

moderately persistent with a $t_{½}$ = 20–100 d (Willis & McDowell 1982; quoted, Howard 1991);

$t_{½}$ = 43–63 d in a sandy loam soil incubated in the dark (McLean et al. 1988; quoted, Howard 1991);

selected field $t_{½}$ = 365 d (Augustijn-Beckers et al. 1994; Hornsby et al. 1996)

$t_{½}$ = 5–9 d (Geyer et al. 2000)

Biota:

TABLE 18.1.1.3.1
Reported aqueous solubilities and octanol-air partition coefficients of aldrin at various temperatures

Aqueous solubility						log K_{OA}	
Richardson & Miller 1960		**Biggar & Riggs 1974**				**Shoeib & Harner 2002**	
shake flask-UV spec.		**shake flask-GC**				**generator column-GC/MS**	
t/°C	**S/g·m^{-3}**	**t/°C**	**S/g·m^{-3}**	**S/g·m^{-3}**	**S/g·m^{-3}**	**t/°C**	**log K_{OA}**
		particle size	0.01μ	0.05μ	5.0μ		
25	0.20	15	0.0055	0.052	0.105	5	9.0091
35	0.39	25	0.0135	0.140	0.180	10	8.6780
45	0.79	35	0.030	0.235	0.350	15	8.5419
		45	0.065	0.455	0.600	20	8.2987
						25	8.0801
						25	8.080
						log K_{OA} = A + B/(T/K)	
						A	–4.366
						B	3709
						enthalpy of phase change	
						ΔH_{OA}/(kJ mol^{-1}) = 71.0	

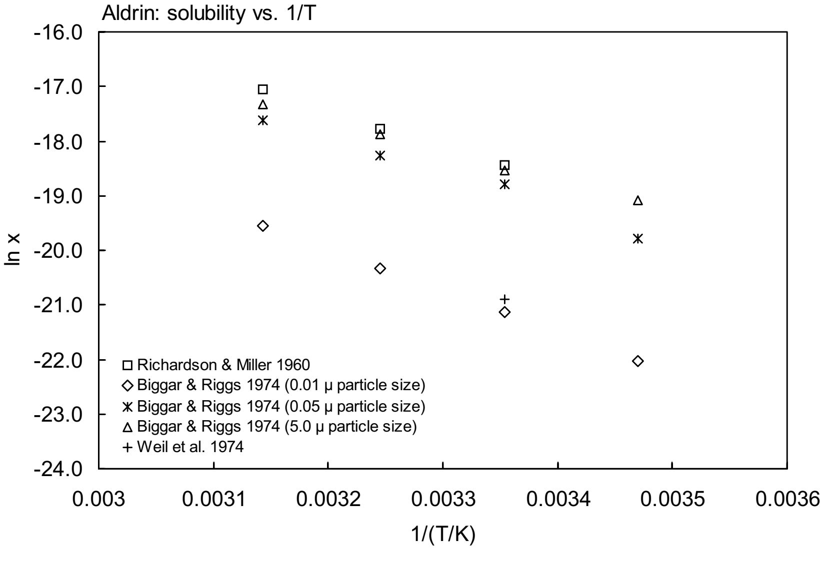


FIGURE 18.1.1.3.1 Logarithm of mole fraction solubility (ln *x*) versus reciprocal temperature for aldrin.

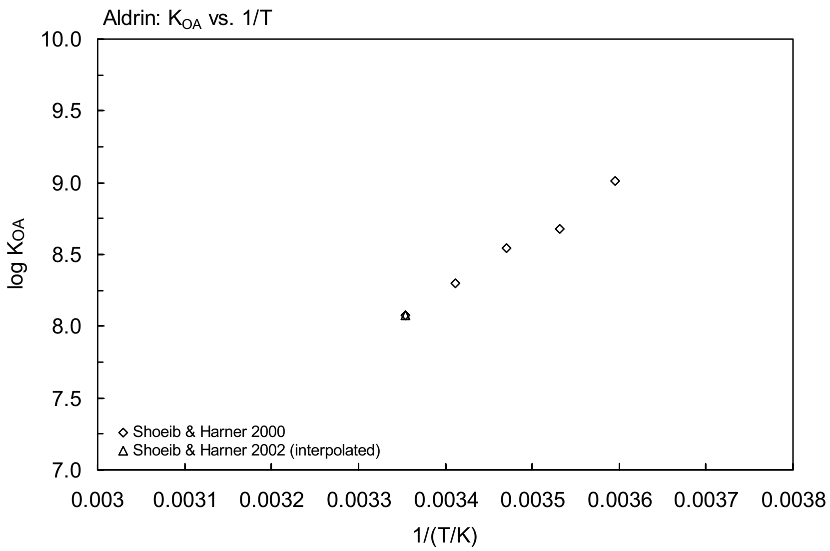


FIGURE 18.1.1.3.2 Logarithm of K_{OA} versus reciprocal temperature for aldrin.

TABLE 18.1.1.3.2
Reported vapor pressures of aldrin at various temperatures and the coefficients for the vapor pressure equations

$\log P = A - B/(T/K)$	(1)	$\ln P = A - B/(T/K)$	(1a)
$\log P = A - B/(C + t/°C)$	(2)	$\ln P = A - B/(C + t/°C)$	(2a)
$\log P = A - B/(C + T/K)$	(3)		
$\log P = A - B/(T/K) - C{\cdot}\log (T/K)$	(4)		

Grayson & Fosbracey 1982		Rordorf 1989	
gas saturation-GC		gas saturation-GC	
t/°C	P/Pa	t/°C	P/Pa
35.5	0.063	25	0.0081
41.0	0.101	50	0.19
41.6	0.112	75	2.80
45.6	0.163	100	29.0
50.8	0.329	125	220
63.3	1.033		
70.0	2.213	eq. 1	P_S/Pa
20	0.0086	A	15.561
		B	5262.3
eq. 1a	P/Pa		
A	11044		for liquid
B	32.9	eq 1	P_L/Pa
		A	12.489
		B	4189.8

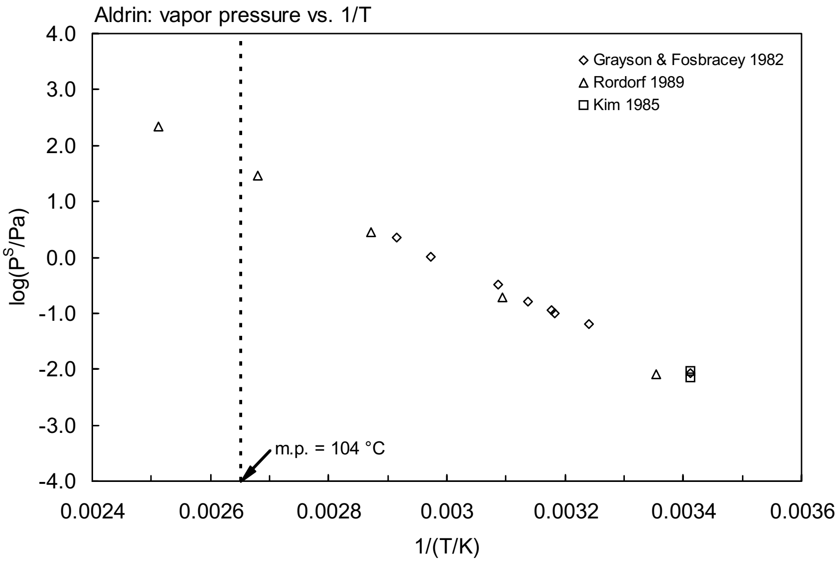
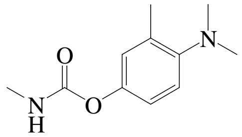


FIGURE 18.1.1.3.3 Logarithm of vapor pressure versus reciprocal temperature for aldrin.

18.1.1.4 Aminocarb



Common Name: Aminocarb
Synonym: A 363, Bay 44646, Bayer 5080, ENT 25784, Matacil, Mitacil
Chemical Name: 4-dimethylamino-*m*-tolyl methylcarbamate, 4-dimethylamino-3-methylphenol methylcarbamate
Uses: nonsystemic, broad-spectrum insecticide used to control the spruce budworm in forests and also as molluscicide.
CAS Registry No: 2032-59-9
Molecular Formula: $C_{11}H_{16}N_2O_2$
Molecular Weight: 208.257
Melting Point (°C):

94	(Lide 2003)

Boiling Point (°C):
Density (g/cm^3 at 20°C):
Molar Volume (cm^3/mol):

250.0	(calculated-Le Bas method at normal boiling point)

Dissociation Constant, pK$_a$:
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
Entropy of Fusion, ΔS_{fus} (J/mol K):
Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F: 0.210 (mp at 94°C)

Water Solubility (g/m^3 or mg/L at 25°C):

915	(20°C, shake flask-GC, Bowman & Sans 1983a, b)
915, 1360	(20°C, 30°C, Montgomery 1993)
915	(20–25°C, selected, Augustijn-Beckers et al. 1994; Hornsby et al. 1996)

Vapor Pressure (Pa at 25°C):

0.00227	(20–25°C, selected, Augustijn-Beckers et al. 1994; Hornsby et al. 1996)

Henry's Law Constant (Pa·m^3/mol):

5.17×10^{-4}	(20–25°C, calculated-P/C, this work)

Octanol/Water Partition Coefficient, log K_{OW}:

1.74	(Zitko & McLeese 1980)
1.73	(20°C, shake flask-GC, Bowman & Sans 1983b)
1.90	(22°C, shake flask-GC, pH 9, Bowman & Sans 1983b)
0.91, 1.90	(pH 5, pH 9, shake flask-GC, Weinberger & Greenhalgh 1983)
1.70	(Richardson & Qadri 1986)
1.73	(Montgomery 1993)
1.90	(recommended, Sangster 1993)
1.90	(pH 9, selected, Hansch et al. 1995)

Bioconcentration Factor, log BCF:

0.690	(mussel, McLeese et al. 1980)

Sorption Partition Coefficient, log K_{OC}:

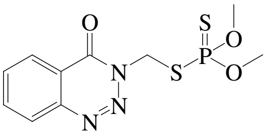
1.92	(calculated, Montgomery 1993)
2.00	(20–25°C, selected, Augustijn-Beckers et al. 1994; Hornsby et al. 1996)
2.52, 1.94	(soil, estimated-class-specific model, estimated-general model, Gramatica et al. 2000)

Environmental Fate Rate Constants, k, or Half-Lives, $t_{½}$:

Half-Lives in the Environment:

Soil: selected field $t_{½}$ = 6 d (Augustijn-Beckers et al. 1994; Hornsby et al. 1996).

18.1.1.5 Azinphos-methyl



Common Name: Azinphos-methyl
Synonym: Bay or Bayer 9027, Bay 17147, Carfene, Cotnion, Cotnion methyl, Crysthion 21, DBD, ENT 23233, Gothnion, Guthion, Gusathion, Metiltriazotion, R 1582
Chemical Name: *O,O*-dimethyl-*S*-[-4-*oxo*-1,2,3-benzotriazin-3(4*H*)-yl)methyl)] phosphorodithioate; *O,O*-dimethyl-*S*-[3,4-dihydro-4-keto-1,2,3-benzotriazinyl-3-methyl) dithiophosphate
Uses: nonsystemic insecticide and acaricide for control of insects and pests in blueberry, grape, maize, vegetable, cotton, and citrus crops.
CAS Registry No: 86-50-0
Molecular Formula: $C_{10}H_{12}N_3O_3PS_2$
Molecular Weight: 317.324
Melting Point (°C):
73 (Lide 2003)
Boiling Point (°C):
> 200 (dec., Montgomery 1993)
Density (g/cm^3 at 20°C):
1.518 (Tomlin 1994)
1.44 (Milne 1995; Montgomery 1993)
Molar Volume (cm^3/mol):
270.4 (calculated-Le Bas method at normal boiling point)
Dissociation Constant, pK_a:
Enthalpy of Vaporization, ΔH_V (kJ/mol):
96.65 (Rordorf 1989)
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
30.96 (DSC method, Plato & Glasgow 1969)
20.5 (Rordorf 1989)
Entropy of Fusion, ΔS_{fus} (J/mol K):
59 (Rordorf 1989)
Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F: 0.338 (mp at 73°C)

Water Solubility (g/m^3 or mg/L at 25°C or as indicated):
33 (rm. temp., Spencer 1973; Worthing 1979; Khan 1980; Budavari 1989)
30 (20°C, Melnikov 1971; Spencer 1982)
33 (20–25°C, Willis & McDowell 1982)
20.9 (20°C, shake flask-GC, Bowman & Sans 1983a, b)
29 (Hartley & Kidd 1987; Lohninger 1994)
28 (20°C, Worthing & Hance 1991; Tomlin 1994)
29 (20–25°C, selected, Wauchope et al. 1992; Hornsby et al. 1996)
30 (Milne 1995)

Vapor Pressure (Pa at 25°C or as indicated and reported temperature dependence equations):
2.93×10^{-5} (20°C, Melnikov 1971)
0.0510 (20°C, Khan 1980)
1.00×10^{-6} (20°C, Worthing & Walker 1983)
1.11×10^{-5} (20°C, GC-RT correlation without mp correction, Kim et al. 1984; Kim 1985)
3.10×10^{-6} (20°C, GC-RT correlation with mp correction, Kim et al. 1984; Kim 1985)
< 0.0010 (20°C, Hartley & Kidd 1987)
3.00×10^{-5} (20°C, selected, Suntio et al. 1988)
7.80×10^{-7}, 3.0×10^{-5}, 6.90×10^{-4}, 0.010, 0.11 (25, 50, 70, 100, 125°C, gas saturation-GC, Rordorf 1989)

log (P_S/Pa) = 14.416 – 6119.2/(T/K); measured range 80.3–145°C (solid, gas saturation-GC, Rordorf 1989)
log (P_L/Pa) = 11.327 – 5048.6/(T/K); measured range 80.3–145°C (liquid, gas saturation-GC, Rordorf 1989)
$<1.8 \times 10^{-4}$ (20°C, Worthing & Hance 1991)
1.80×10^{-4} (20°C, Tomlin 1994)
2.67×10^{-5} (20–25°C, selected, Wauchope et al. 1992; Hornsby et al. 1996)
2.13×10^{-4} (20°C, Montgomery 1993)

Henry's Law Constant (Pa·m^3/mol at 25°C):
0.0032 (20°C, calculated-P/C, Suntio et al. 1988)
1.52×10^{-5} (calculated-P/C, Howard 1991)
3.17×10^{-4} (calculated-P/C, this work)

Octanol/Water Partition Coefficient, log K_{OW}:
2.99 (Callahan et al. 1979)
2.69 (20°C, shake flask-GC, Bowman & Sans 1983b)
2.75 (Hansch & Leo 1985)
2.43 (HPLC-RT correlation, Moody et al. 1987)
2.69, 2.75 (Montgomery 1993)
2.75 (recommended, Sangster 1993)
2.96 (Tomlin 1994)
2.75 (recommended, Hansch et al. 1995)
2.62 (Pomona-database, Müller & Kördel 1996)

Bioconcentration Factor, log BCF:
1.96 (calculated-S as per Kenaga 1980, this work)
1.86 (calculated-K_{OW}, Lyman et al. 1982; quoted, Howard 1991)

Sorption Partition Coefficient, log K_{OC}:
2.61 (calculated-S, Lyman et al. 1982; quoted, Howard 1991)
2.28 (Fröbe et al. 1989)
1.30 (selected, USDA 1989; Neary et al. 1993)
2.28 (derived from exptl., Meylan et al. 1992)
1.84 (calculated-MCI χ, Meylan et al. 1992)
3.00 (soil, 20–25°C, selected, Wauchope et al. 1992; Hornsby et al. 1996)
2.47–3.53 (Montgomery 1993)
2.95 (soil, HPLC-screening method, mean value of different stationary and mobile phases, Kördel et al. 1993, 1995)
2.28 (soil, calculated- QSAR MCI $^1\chi$, Sabljic et al. 1995)
2.95; 1.84 (HPLC-screening method; calculated-PCKOC fragment method, Müller & Kördel 1996)
3.67, 3.69, 2.73, 2.74, 2.91 (first generation Eurosoils ES-1, ES-2, ES-3, ES-4, ES-5, shake flask/batch equilibrium-HPLC/UV, Gawlik et al. 1998, 1999)
3.30, 2.89, 2.75, 2.799, 3.231 (second generation Eurosoils ES-1, ES-2, ES-3, ES-4, ES-5, shake flask/batch equilibrium-HPLC/UV, Gawlik et al. 1999)
2.69 (sandy loam soil, column equilibrium method, 20°C, Xu et al. 1999)
3.299, 2.894, 2.755, 2.799, 3.231 (second generation Eurosoils ES-1, ES-2, ES-3, ES-4, ES-5, HPLC-k′ correlation, Gawlik et al. 2000)
2.28; 1.80, 2.04 (soil, quoted exptl.; estimated-class specific model, estimated-general model, Gramatica et al. 2000)

Environmental Fate Rate Constants, k, or Half-Lives, $t_{½}$:
Volatilization:
Photolysis:

Oxidation: photooxidation $t_{1/2}$ = 1.3 h, based on an estimated rate constant for the vapor-phase reaction with hydroxyl radical in air (Atkinson 1987; quoted, Howard et al. 1991).

Hydrolysis: first-order $t_{1/2}$ = 36.4, 27.9, 7.2 d in water at pH 8.6 and 6°C, 25°C and 40°C (Heuer et al. 1974; quoted, Howard 1991);
$t_{1/2}$ = 27.9 d at pH 8.6 and 25°C (Montgomery 1993);
$t_{1/2}$ = 87 d at pH 4, $t_{1/2}$ = 50 d at pH 7, and $t_{1/2}$ = 4 d at pH 9 at 22°C (Tomlin 1994).

Biodegradation: studies with aquatic water/sediment microorganisms at 5 mg/L and pH 6.7 indicate $t_{1/2}$ = 3.3 d in microcosms compared to $t_{1/2}$ = 2.7 d in field studies (Portier 1985; quoted, Howard 1991).

Biotransformation:

Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants:

Half-Lives in the Environment:

Air: $t_{1/2}$ = 1.3 h, based on an estimated rate constant for the vapor-phase reaction with hydroxyl radical in air (Atkinson 1987; quoted, Howard et al. 1991).

Surface water: $t_{1/2}$ = 415 d at 6°C, $t_{1/2}$ = 115 d at 22°C in darkness for Milli-Q water; $t_{1/2}$ = 278 d at 6°C, $t_{1/2}$ = 42 d at 22°C in darkness, 8 d under sunlight conditions for river water at pH 7.3; $t_{1/2}$ = 506 d at 6°C, $t_{1/2}$ = 35 d at 22°C in darkness for filtered river water at pH 7.3; $t_{1/2}$ = 26 d at 22°C in darkness, $t_{1/2}$ = 11 d under sunlight conditions for seawater at pH 8.1 (Lartiges & Garrigues 1995).

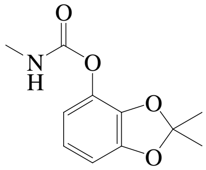
Ground water:

Sediment:

Soil: for dry soil with 2–3% moisture, $t_{1/2}$ = 484, 88, and 32 d at 6, 25, and 40°C, respectively; while for moist soil with 50% moisture content, half-lives were much shorter: 64, 13, and 5 d at 6, 25, and 40°C, respectively (Yaron et al. 1974; quoted, Montgomery 1993);
selected field $t_{1/2}$ = 10 d (Wauchope et al. 1992; Hornsby et al. 1996);
average $t_{1/2}$ = 40 d (Dowd et al. 1993);
half-life in soil ranges from a few days to many weeks, depending on soil type (Tomlin 1994);
$t_{1/2}$ = 10 d (selected, Halfon et al. 1996).

Biota: average $t_{1/2}$ = 30 d in forest (selected, USDA 1989; quoted, Neary et al. 1993).

18.1.1.6 Bendiocarb



Common Name: Bendiocarb
Synonym: Bencarbate, Dycarb, Ficam, Garvox, Multamat, Multimet, NC 6897, Niomil, Rotate, Seedox, Tatto, Turcam
Chemical Name: 2,3-isopropylidenedioxyphenyl methylcarbamate; 2,2-dimethyl-1,3-benzodioxol-4-yl methyl-carbamate
Uses: contact insecticide used to control beetles, wireworms, flies, wasps, and mosquitoes in beets and maize.
CAS Registry No: 22781-23-3
Molecular Formula: $C_{11}H_{13}NO_4$
Molecular Weight: 223.226
Melting Point (°C):

130	(Lide 2003)

Boiling Point (°C):
Density (g/cm^3 at 20°C):

1.25	(Worthing & Hance 1991; Montgomery 1993; Tomlin 1994; Milne 1995)

Molar Volume (cm^3/mol):

231.7	(calculated-Le Bas method at normal boiling point)
178.6	(calculated-density)

Dissociation Constant, pK_a:

8.80	(Worthing & Hance 1991; Wauchope et al. 1992; Montgomery 1993; Tomlin 1994)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
Entropy of Fusion, ΔS_{fus} (J/mol K):
Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F: 0.0933 (mp at 130°C)

Water Solubility (g/m^3 or mg/L at 25°C or as indicated):

40	(Spencer 1973, 1982)
40	(Martin & Worthing 1977; Worthing & Walker 1987; Kenaga 1980;)
40	(20°C, Hartley & Kidd 1987; Montgomery 1993; Milne 1995)
40	(20–25°C, selected, Wauchope et al. 1992; Hornsby et al. 1996)
40	(Lohninger 1994)
280	(20°C at pH 7, Tomlin 1994)

Vapor Pressure (Pa at 25°C or as indicated):

6.6×10^{-4}	(Hartley & Kidd 1987)
0.00467	(20–25°C, selected, Wauchope et al. 1992; Hornsby et al. 1996)
6.6×10^{-4}	(20°C, Montgomery 1993)
0.0046	(quoted, gas saturation-GC, Tomlin 1994)

Henry's Law Constant (Pa·m^3/mol at 25°C or as indicated):

0.365	(20°C, calculated-P/C, Montgomery 1993)

Octanol/Water Partition Coefficient, log K_{OW}:

5.29	(selected, Dao et al. 1983)
1.70	(Worthing & Hance 1991; Montgomery 1993; Milne 1995)
1.72	(at pH 6.55, Tomlin 1994)
1.70	(recommended, Hansch et al. 1995)

Bioconcentration Factor, log BCF:

1.89	(calculated-S, Kenaga 1980)

Sorption Partition Coefficient, log K_{OC}:

2.76	(calculated-S, Kenaga 1980)
2.76	(soil, 20–25°C, selected, Wauchope et al. 1992; Hornsby et al. 1996)
2.76	(Montgomery 1993)
2.76	(estimated-chemical structure, Lohninger 1994)
1.45–1.60	(Tomlin 1994)
1.30, 1.83	(soil, estimated-class-specific model, estimated-general model, Gramatica et al. 2000)

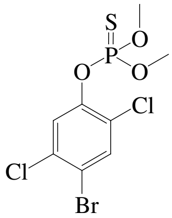
Environmental Fate Rate Constants, k, or Half-Lives, $t_{1/2}$:

Hydrolysis: $t_{1/2}$ = 4 d at pH 7 and 25°C (Spencer 1982; Montgomery 1993; Tomlin 1994).

Half-Lives in the Environment:

Air:
Surface water: hydrolysis half-life of 4 d at 25°C and pH 7 under EPA guidelines (Spencer 1982)
Ground water:
Sediment:
Soil: half-life of several days to a few weeks (Hartley & Kidd 1987; quoted, Montgomery 1993); selected field $t_{1/2}$ = 5.0 d (Wauchope et al. 1992; Hornsby et al. 1996).
Biota:

18.1.1.7 Bromophos



Common Name: Bromophos
Synonym: Nexion, S-1942, Omexan, Brofene
Chemical Name: *o*-4-bromo-2,5-dichlorophenyl *O,O*-dimethyl phosphorothioate
CAS Registry No: 2104-96-3
Uses: insecticide
Molecular Formula: $C_8H_8BrCl_2PS$
Molecular Weight: 317.999
Melting Point (°C):
54 (Lide 2003)
Boiling Point (°C):
140–142 at 0.01 mmHg (Hartley & Kidd 1987; Worthing & Walker 1987)
Density (g/cm^3 at 20°C):
Molar Volume (cm^3/mol):
Dissociation Constant, pK_a:
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
Entropy of Fusion, ΔS_{fus} (J/mol K):
Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F: 0.519 (mp at 54°C)

Water Solubility (g/m^3 or mg/L at 25°C):

40	(Kenaga 1980b; Spencer 1982; Hartley & Kidd 1987)
0.30	(20°C, shake flask-GC, Bowman & Sans 1979)
0.652	(20°C, correlated, Bowman & Sans 1983b)
0.70	(20°C, Worthing & Walker 1987)

Vapor Pressure (Pa at 25°C):

0.017	(20°C, Hartley & Kidd 1987; Worthing & Walker 1987)

Henry's Law Constant (Pa·m^3/mol):

Octanol/Water Partition Coefficient, log K_{OW}:

4.88	(shake flask-concn ratio-GC, Bowman & Sans 1983b)
5.208 ± 0.009	(slow stirring-GC, De Bruijn et al. 1989; De Bruijn & Hermens 1991)
4.88	(recommended, Sangster 1993)
5.21	(recommended, Hansch et al. 1995)

Octanol/Air Partition Coefficient, log K_{OA}:

Bioconcentration Factor, log BCF or log K_B:

1.89	(calculated, Kenaga 1980b)
4.65 ± 0.06	(guppy, calculated on an extractable liquid wt basis, De Bruijn & Hermens 1991)

Sorption Partition Coefficient, log K_{OC}:

2.76	(calculated-solubility, Kenaga 1980b)

Environmental Fate Rate Constants, k, or Half-Lives, $t_{½}$:

Volatilization:

Photolysis:

Oxidation:

Hydrolysis: hydrolyzed in alkaline media (Worthing 1987).

Biodegradation:

Biotransformation:

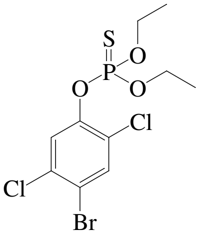
Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants:

k_1 = 0.01307 mL g^{-1} d^{-1}; k_2 = 0.33 d^{-1} (guppy, De Bruijn & Hermens 1991)

k_2 = 12 d^{-1} (guppy, calculated-K_{OW}, De Bruijn & Hermens 1991)

Half-Lives in the Environment:

18.1.1.8 Bromophos-ethyl



Common Name: Bromophos-ethyl
Synonym: Nexagan, Filariol
Chemical Name: *O*-(4-bromo-2,5-dichlorophenyl) *O*,*O*-diethyl phosphorothioate
CAS Registry No: 4824-78-6
Uses: insecticide, acaricide
Molecular Formula: $C_{10}H_{12}Cl_2O_3PS$
Molecular Weight: 394.049
Melting Point (°C):
colorless liquid (Spencer 1982)
Boiling Point (°C):

122–123	(at 0.001 mmHg, Hartley & Kidd 1987; Worthing & Walker 1987)

Density (g/cm^3 at 20°C):

1.52–1.55	(Hartley & Kidd 1987; Worthing & Walker 1987)

Molar Volume (cm^3/mol):
Dissociation Constant, pK_a:
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
Entropy of Fusion, ΔS_{fus} (J/mol K):
Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F: 1.0

Water Solubility (g/m^3 or mg/L at 25°C):

2.0	(Kenaga 1980b; Spencer 1982; Hartley & Kidd 1987)
0.44	(20°C, Bowman & Sans 1983b)
0.14	(20°C, Worthing & Walker 1987)

Vapor Pressure (Pa at 25°C):

6.1×10^{-3}	(30°C, Spencer 1982; Hartley & Kidd 1987; Worthing & Walker 1987)

Henry's Law Constant (Pa·m^3/mol):

Octanol/Water Partition Coefficient, log K_{OW}:

5.68	(shake flask-concn-ration, Bowman & Sans 1983b)
6.149 ± 0.019	(slow-stirring-GC; De Bruijn et al. 1989)
5.68	(recommended, Sangster 1993)
6.15	(recommended, Hansch et al. 1995)

Octanol/Air Partition Coefficient, log K_{OA}:

Bioconcentration Factor, log BCF or log K_B:

2.62	(fish, calculated, Kenaga 1980b)

Sorption Partition Coefficient, log K_{OC}:

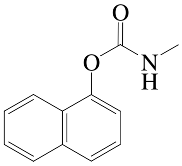
3.48	(soil, calculated-solubility, Kenaga 1980b)

Environmental Fate Rate Constants, k, or Half-Lives, $t_{½}$:

Hydrolysis: at room temp., stable in aqueous suspension at pH < 9, hydrolysed at pH > 9, particularly at higher temperature (Worthing & Walker 1987).

Half-Lives in the Environment:

18.1.1.9 Carbaryl



Common Name: Carbaryl

Synonym: Arylam, Atoxan, Caproline, Carbamine, Carbatox, Carpolin, Carylderm, Cekubaryl, Crag sevin, Denapon, Devicarb, Dicarbam, ENT 23969, Gamonil, Germain's, Hexavin, Karbaspray, Karbatox, Karbosep, OMS 29, naphthyl carbamate, Panam, Ravyon, Rylam, Seffein, Septene, Sevimol, Sevin, Sok, Tercyl, Toxan, Union Carbide 7744

Chemical Name: carbamic acid, methyl-, 1-naphthyl ester; 1-naphthalenol, methyl carbamate; 1-naphthyl-*N*-methyl carbamate; 1-naphthyl methylcarbamate; 1-naphthalenyl methylcarbamate

Uses: contact insecticide used to control most insects on fruits, vegetables, and ornamentals; also used as growth regulator for fruit thinning of apples.

CAS Registry No: 63-25-2

Molecular Formula: $C_{12}H_{11}NO_2$

Molecular Weight: 201.221

Melting Point (°C):

145	(Lide 2003)

Boiling Point (°C): dec. on distillation

Density (g/cm^3 at 20°C):

1.232	(Spencer 1982; Hartley & Kidd 1987; Montgomery 1993; Tomlin 1994; Milne 1995)
0.52–0.61	(Worthing & Hance 1991)

Molar Volume (cm^3/mol):

218.7	(calculated-Le Bas method at normal boiling point)

Dissociation Constant, pK_a:

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

24.27	(DSC method, Plato & Glasgow 1969)

Entropy of Fusion ΔS_{fus} (J/mol K):

Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F: 0.0665 (mp at 145°C)

Water Solubility (g/m^3 or mg/L at 25°C or as indicated):

40	(shake flask, David et al. 1960)
40	(30°C, Spencer 1973; Worthing & Hance 1991)
40	(Martin & Worthing 1977)
34	(20–25°C, shake flask-GC, Kanazawa 1981)
50	(20°C, Spencer 1982)
104	(20°C, shake flask-GC, Bowman & Sans 1983a, b)
82.6	(generator column-GC, Swann et al. 1983)
590	(RP-HPLC-RT correlation, Swann et al. 1983)
120	(30°C, Hartley & Kidd 1987; Worthing & Walker 1987; Tomlin 1994)
120	(20–25°C, selected, Wauchope et al. 1992; Hornsby et al. 1996)
104, 130	(20°C, 30°C, Montgomery 1993)
40, 1000	(Milne 1995)

Vapor Pressure (Pa at 25°C or as indicated):

<0.665	(26°C, Melnikov 1971)
2.80×10^{-3}	(20°C, Hartley & Graham-Bryce 1980)
<0.133	(20–25°C, Weber et al. 1980)
1.81×10^{-4}	(Ferreira & Seiber 1981)
7.75×10^{-3}, 5.39×10^{-4}	(20°C, GC-RT correlation, GC-RT correlation with mp correction, Kim 1985)

< 0.665 (26°C, Hartley & Kidd 1987)
< 0.0053 (Worthing & Hance 1991)
1.60×10^{-4} (20–25°C, selected, Wauchope et al. 1992; Hornsby et al. 1996)
8.77×10^{-4} (Montgomery 1993)
2.00×10^{-4} (23.5°C, Tomlin 1994)

Henry's Law Constant (Pa m^3/mol):
0.0013 (calculated-P/C, Suntio et al. 1988;)
4.41×10^{-4} (calculated-P/C as known LWAPC, Meylan & Howard 1991)
3.18×10^{-4} (calculated-bond contribution method LWAPC, Meylan & Howard 1991)
1.287 (20°C, calculated-P/C, Montgomery 1993)
< 0.010 (estimated, Mabury & Crosby 1996)
4.48×10^{-5} (calculated-P/C, this work)

Octanol/Water Partition Coefficient, log K_{OW}:
2.36 (shake flask-UV, Fujita et al. 1974)
2.36 (Freed et al. 1976)
2.81 (Hansch & Leo 1979; Rao & Davidson 1980)
2.32 (shake flask-UV, Lord et al. 1980)
2.32 (20°C, shake flask-UV, Briggs 1981)
2.29 (20°C, shake flask-GC, Kanazawa 1981)
2.36 (Lyman et al. 1982; Magee 1991; Trapp & Pussemier 1991)
2.31 (22°C, shake flask-GC, Bowman & Sans 1983b)
2.36 (Hansch & Leo 1985)
2.14 (RP-HPLC-RT correlation, Trapp & Pussemier 1991)
2.63 (HPLC-RT correlation, average, Hu & Leng 1992)
2.31–2.81 (Montgomery 1993)
1.99 (RP-HPLC-RT correlation, Saito et al. 1993)
1.59 (Tomlin 1994)
2.36 (recommended, Hansch et al. 1995)
2.24 (RP-HPLC-RT correlation, Nakamura et al. 2001)

Bioconcentration Factor, log BCF:
< 0.0 (fish in static water, Metcalf & Sanborn 1975; Freed et al. 1976)
1.89 (calculated-S, Kenaga 1980)
1.08 (calculated-K_{OC}, Kenaga 1980)
1.64 (earthworm, Lord et al. 1980)
0.95 (*Pseudorasbora parva*, Kanazawa 1981)
1.86 (algae, Freitag et al. 1982)
1.53 (golden orfe, Freitag et al. 1982)
1.95 (activated sludge, Freitag et al. 1982, 1984)
0.954 (topmouth gudgeon, Kanazawa 1983)
1.45 (golden ide, Freitag et al. 1984)
1.85, 1.48, 1.95 (algae, golden ide, activated sludge, Freitag et al. 1985)

Sorption Partition Coefficient, log K_{OC}:
2.36 (soil, Leenheer & Atrichs 1971; LaFleur 1976)
2.36 (Kenaga 1980; Kenaga & Goring 1978)
2.76 (calculated-S as per Kenaga & Goring 1978, Kenaga 1980)
2.49 (average of 3 soils, McCall et al. 1980)
2.49 (average of 3 soils, HPLC-RT correlation, McCall et al. 1980)
2.02 (soil slurry/shake flask-UV method, converted form reported as log K_{OM} of 1.78, Briggs. 1981)
3.04, 2.50, 2.42 (estimated-S, calculated-S and mp, estimated-K_{OW}, Karickhoff 1981)

2.76, 2.66	(estimated-S, K_{OW}, Lyman 1982)
2.59	(soil slurry method, Swann et al. 1983)
2.57	(reverse phase HPLC-RT correlation, Swann et al. 1983)
2.14	(calculated- MCI χ, Gerstl & Helling 1987)
2.36	(soil, screening model calculations, Jury et al. 1987b)
2.23	(calculated-MCI χ, Bahnick & Doucette 1988)
2.30	(RP-HPLC-k′ correlation, cyanopropyl column, Hodson & Williams 1988)
2.04	(estimated as log K_{OM}, Magee 1991)
2.48	(soil, 20–25°C, selected, Wauchope et al. 1992; Hornsby et al. 1996)
2.30	(soil, Dowd et al. 1993)
2.02–2.59	(Montgomery 1993)
2.71	(estimated-chemical structure, Lohninger 1994)
2.40	(soil, calculated-MCI $^1\chi$, Sabljic et al. 1995)
2.21, 2.39	(soil, estimated-class-specific model, estimated-general model, Gramatica et al. 2000)
2.49–2.62	(sediments of San Diego Creek and Bonita Creek, shake flask-GC, Bondarenko & Gan 2004)

Environmental Fate Rate Constants, k, or Half-Lives, $t_{1/2}$:

Volatilization: $t_{1/2}$ = 3000 d estimated from Henry's law constant for a body of water 1 m deep, flowing at 1 m/s and with a wind speed of 3 m/s (Howard 1991).

Photolysis: $t_{1/2}$ = 6.6 d for a mid-summer day at latitude 40°, photolysis is about 4 times faster than in the winter months (Wolfe et al. 1978)

$t_{1/2}$(air) = 52–200 h in the atmosphere, based on aqueous photolysis data; $t_{1/2}$(aq.) = 52–200 h, based on reported photolysis half-life for summer and winter sunlight at 40°N (Howard et al. 1991)

k(aq.) = 6.4×10^{-4} h^{-1} (Armbrust 2000)

k(aq.) = $(5.6 \pm 0.3) \times 10^{-5}$ s^{-1} in the presence of UV light, a 30 ppm carbaryl solution at 298 K; in the presence of silver-doped zeolite Y catalyst with 2.42% Ag by weight, the photodecomposition rate becomes 80 times faster. The addition of Suwannee River natural organic matter had a minimal effect on this system, increases or decreases the catalytic photodecomposition rate by a factor of 3 at most (Kanan et al. 2003).

Oxidation: photooxidation $t_{1/2}$ = 4.5–7.4 h, based on estimated rate constant for the vapor-phase reaction with hydroxyl radical in air (Howard et al. 1991)

k_{OH}(aq.) = 3.40×10^9 M^{-1} s^{-1} in irradiated field water both in the laboratory and sunlit rice paddies and the field dissipation $t_{1/2}$ = 8.8 h (Mabury & Crosby 1996).

Hydrolysis: k(alkaline) = (5.02 ± 0.03) M^{-1} h^{-1} with $t_{1/2}$ = 1500 d at pH 5, $t_{1/2}$ = 15 d at pH 7 and $t_{1/2}$ = 0.15 d at pH 9 and 28°C (Wolfe et al. 1978)

$t_{1/2}$ = 312 h, based on base rate constant at pH 7 and 25°C (Howard et al. 1991)

$t_{1/2}$ = 1500 d at pH 5, $t_{1/2}$ = 15 d at pH 7, and $t_{1/2}$ = 0.15 d at pH 9 at 27°C (Montgomery 1993)

$t_{1/2}$ = 12 d at pH 7 and $t_{1/2}$ = 3.2 h at pH 9 (Tomlin 1994)

$t_{1/2}$ = 1500 d at pH 2, $t_{1/2}$ = 13 d at pH 7 and $t_{1/2}$ = 0.00013 d at pH 12 in natural waters (Capel & Larson 1995)

k = 0.066 d^{-1} at pH 7, k = 5.2 d^{-1} at pH 9; dissipation by hydrolysis from a simulated aquatic system after 30 d: 53.9%, 59.1% of depth of 10 cm, 1 m, respectively, at pH 6; 64.2%, 70.7% of depth of 10 cm, 1 m, respectively, at pH 7; and 85.7%, 81.0% of depth of 10 cm, 1 m, respectively, at pH 7 (Armbrust 2000) Biodegradation:

$t_{1/2}$(aerobic) = 40–720 h, based on unacclimated aerobic river die-away test data and freshwater grab sample data (Eichelberger & Lichtenberg 1971; quoted, Howard et al. 1991)

$t_{1/2}$ > 3×10^4 d, assuming a bacterial population of 0.1 mg/L (Wolfe et al. 1978b)

k(aq.) = 2.4×10^{-10} mL $cell^{-1}$ d^{-1} in aquatic system (Scow 1982)

$t_{1/2}$(anaerobic) = 160–2880 h, based on unacclimated aerobic biodegradation (Howard et al. 1991)

$t_{1/2}$(aerobic) = 1.7 d, $t_{1/2}$(anaerobic) = 6.7 d in natural waters (Capel & Larson 1995)

k(aerobic) = 1.70×10^{-3} h^{-1} (Armbrust 2000) .

Biotransformation:

Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants:

Half-Lives or Fate Rate Constants in the Environment:

Air: $t_{1/2}$ = 12.6 h, based on estimated rate constant for the vapor-phase reaction with photochemically produced hydroxyl radical in the atmosphere (Howard 1991);

$t_{1/2}$ = 4.5–7.4 h, based on estimated rate constant for the vapor-phase reaction with hydroxyl radical in air (Howard et al. 1991);

atmospheric transformation lifetime was estimated to be <1 d (Kelly et al. 1994).

Surface water: hydrolysis $t_{1/2}$ = 1500 d at pH 5, $t_{1/2}$ = 15 d at pH 7 and $t_{1/2}$ = 0.15 d at pH 9; direct photolysis $t_{1/2}$ = 6.6 d; and biolysis $t_{1/2} > 3 \times 10^4$ d assuming a bacterial population of 0.1 mg/L (Wolfe et al. 1978b);

18–20% recovered from pond water after 42 d, 37–42% recovered after 50 d from creek water (Szeto et al. 1979)

$t_{1/2}$ = 3.2–200 h, based on aqueous hydrolysis half-life at pH 9 and 28°C and photolysis half-life for winter sunlight at 40°N (Howard et al. 1991)

Biodegradation $t_{1/2}$(aerobic) = 1.7 d, $t_{1/2}$(anaerobic) = 6.7 d, hydrolysis $t_{1/2}$ = 1500 d at pH 2, $t_{1/2}$ = 13 d at pH 7 and $t_{1/2}$ = 0.00013 d at pH 12 in natural waters (Capel & Larson 1995)

$t_{1/2}$ = 37 d at 22°C for Milli-Q water at pH 6.1; $t_{1/2}$ = 31 d at 6°C, $t_{1/2}$ = 11 d at 22°C in darkness, $t_{1/2}$ = 9 d under sunlight conditions for river water at pH 7.3; $t_{1/2}$ = 45 d at 6°C, $t_{1/2}$ < 2 d at 22°C in darkness for filtered river water at pH 7.3; $t_{1/2}$ = 22 d at 6°C, $t_{1/2}$ < 2 d at 22°C in darkness and $t_{1/2}$ = 13 d under sunlight conditions for seawater at pH 8.1 (Lartiges & Garrigues 1995);

dissipation by hydrolysis from a simulated aquatic system after 30 d, 53.9%, 59.1% of depth of 10 cm, 1 m, respectively, at pH 6, 64.2%, 70.7% of depth of 10 cm, 1 m, respectively, at pH 7 and 85.7%, 81.0% of depth of 10 cm, 1 m, respectively, at pH 7 (Armbrust 2000).

Ground water: $t_{1/2}$ = 3.2–1440 h, based on aqueous hydrolysis half-life at pH 9 and 28°C, and unacclimated aerobic biodegradation half-life (Howard et al. 1991).

Sediment: ~ 55% recovered after 50 d in autoclaved water and sediment samples (Szeto et al. 1979)

first-order degradation k = 0.392 d^{-1} with $t_{1/2}$ = 1.8 d under aerobic conditions, k = 0.005 d^{-1} with $t_{1/2}$ = 125 d under anaerobic conditions in sediment from San Diego Creek, Orange County, CA; first-order degradation k = 0.141 d^{-1} with $t_{1/2}$ = 4.9 d under aerobic conditions, k = 0.0009 d^{-1} with $t_{1/2}$ = 746 d under anaerobic conditions in sediment from Bonita Creek, Orange County, CA (Bondarendo & Gan 2004)

Soil: $t_{1/2}$ = 97–251 h in dry soil and 4458–688 h in wet or saturated soil (Hautala 1978; quoted, Howard 1991);

persistence of less than one month (Wauchope 1978);

$t_{1/2}$ = 3.2–720 h, based on aqueous hydrolysis half-life at pH 9 and 28°C and unacclimated aerobic biodegradation half-life (Howard et al. 1991);

biodegradation rate constant k = 0.037 d^{-1} in soil by die-away test (Rao & Davidson 1980; quoted, Scow 1982);

moderately persistent in soils with $t_{1/2}$ = 20–100 d (Willis & McDowell 1982);

$t_{1/2}$ = 22 d from screening model calculations (Jury et al. 1987b);

selected field $t_{1/2}$ = 10 d (Wauchope et al. 1992; Dowd et al. 1993; Hornsby et al. 1996);

$t_{1/2}$ = 8 d (Pait et al. 1992);

degradation $t_{1/2}$ = 7–14 d in a sandy loam and $t_{1/2}$ = 14–28 d in a clay loam under aerobic conditions for concn. at 1 ppm (Tomlin 1994);

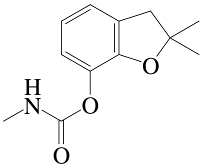
$t_{1/2}$ = 10 d (selected, Halfon et al. 1996)

Field dissipation $t_{1/2}$ = 8.8 h (Mabury & Crosby 1996)

$t_{1/2}$ = 14 d in an aerobic soil, $t_{1/2}$ = 72 d in an anaerobic aquatic soil (quoted, Bondarenko & Gan 2004)

Biota: biochemical $t_{1/2}$ = 22 d from screening model calculations (Jury et al. 1987b).

18.1.1.10 Carbofuran



Common Name: Carbofuran
Synonym: Bay 70143, Curaterr, ENT 27164, Furadan, NIA 10242, Niagara 10242, Yaltox
Chemical Name: 2,3-dihydro-2,2-dimethylbenzofuran-7-yl methylcarbamate; 2,3-dihydro-2,2-dimethyl-7-benzo-furanyl methylcarbamate
Uses: broad-spectrum systemic insecticide, nematocide and acaricide applied in soil to control insects and nematodes; also to control insects and mites on foliage.
CAS Registry No: 1563-66-2
Molecular Formula: $C_{12}H_{15}NO_3$
Molecular Weight: 221.252
Melting Point (°C):
151 (Lide 2003)
Boiling Point (°C):
Density (g/cm^3 at 20°C):
1.18 (Hartley & Kidd 1987; Trotter et al. 1991; Montgomery 1993; Tomlin 1994; Milne 1995)
Molar Volume (cm^3/mol):
240.8 (calculated-Le Bas method at normal boiling point)
187.5 (calculated-density)
Dissociation Constant, pK$_a$:
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
Entropy of Fusion, ΔS_{fus} (J/mol K):
Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F: 0.0580 (mp at 151°C)

Water Solubility (g/m^3 or mg/L at 25°C or as indicated):
700 (Spencer 1973, 1982; Khan 1980; Weber et al. 1980)
250 (Caro et al. 1976)
415 (Martin & Worthing 1977; Herbicide Handbook 1978, 1983)
320 (19°C, shake flask-GC, Bowman & Sans 1979, 1983b)
700 (Verschueren 1983; Windholz 1983, Budavari 1989)
480 (generator column-HPLC/RI, Swann et al. 1983)
670 (RP-HPLC-RT correlation, Swann et al. 1983)
700 (Hartley & Kidd 1987; Worthing & Walker 1987; Milne 1995)
351 (20–25°C, selected, Wauchope 1989; Wauchope et al. 1992; Hornsby et al. 1996)
320 (20°C, Montgomery 1993; Tomlin 1994; Milne 1995)
375 (30°C, Montgomery 1993)

Vapor Pressure (Pa at 25°C or as indicated):
1.12×10^{-3} (Knudsen effusion method, Cook 1973)
1.11×10^{-3} (Caro et al. 1976; Fuhrmann & Lichtenstein 1980)
8.67×10^{-4} (20°C, Hartley & Graham-Bryce 1980)
2.70×10^{-3} (33°C, Khan 1980)
2.67×10^{-3} (20–25°C, Weber et al. 1980)
2.70×10^{-4} (Thomas 1982)
2.20×10^{-3}, 1.08×10^{-4} (20°C, GC-RT correlation, GC-RT correlation with mp correction, Kim 1985)
2.70×10^{-3} (33°C, Hartley & Kidd 1987)
8.00×10^{-5} (20–25°C, selected, Wauchope et al. 1992; Hornsby et al. 1996)
3.10×10^{-5}, 7.20×10^{-5} (20, 25°C, Tomlin 1994)

Henry's Law Constant (Pa·m^3/mol at 25°C):
3.95×10^{-4} (calculated-P/C, Lyman et al. 1982; quoted, Howard 1991)
7.69×10^{-4} (Jury et al. 1984)
9.42×10^{-6} (Jury et al. 1987a, b; Jury & Ghodrati 1989)
5.10×10^{-4} (calculated-P/C, Suntio et al. 1988)
7.69×10^{-4} (calculated-P/C, Taylor & Glotfelty 1988)
< 0.010 (estimated, Mabury & Crosby 1996)
5.04×10^{-5} (calculated-P/C, this work)

Octanol/Water Partition Coefficient, log K_{OW}:
2.32 (Hansch & Leo 1979, 1985)
1.60 (from Dow Chemical data, Kenaga & Goring 1980)
2.88 (Belluck & Felsot 1981)
2.07 (quoted, Karickhoff 1981)
1.60 (calculated, Lyman 1982)
1.82 (RP-HPLC-RT correlation, Trapp & Pussemier 1991)
1.60–2.32 (Montgomery 1993)
1.60 (RP-HPLC-RT correlation, Saito et al. 1993)
2.32 (recommended, Sangster 1993)
1.52 (20°C, Tomlin 1994)
1.23–1.42 (Milne 1995)
2.32 (recommended, Hansch et al. 1995)

Bioconcentration Factor, log BCF:
1.00 (estimated-log K_{OW}, Neely et al. 1974)
1.32 (calculated-S, Kenaga 1980)
0.60 (*Triaenodes tardus*, Belluck & Felsot 1981)
1.00 (selected, Schnoor & McAvoy 1981;, Schnoor 1992)
1.53 (calculated-log K_{OW}, Lyman et al. 1982; quoted, Howard 1991)
1.18 (calculated-S, Lyman et al. 1982; quoted, Howard 1991)
2.07 (*Tilapia nilotica,* Tejada & Magallona 1985)
1.00 (*Pila luzonica,* Tejada & Magallona 1985)
2.07 (paddy field fish, Tejada 1995)

Sorption Partition Coefficient, log K_{OC}:
2.20 (calculated-S as per Kenaga & Goring 1978, Kenaga 1980)
1.67 (calculated values for 6 samples while high organic carbon >15% were omitted from calculation by Felsot & Wilson 1980)
1.78–2.20 (3 soils of org. content 0.68–2.01, McCall et al. 1980)
2.02 (average of 3 soils, McCall et al. 1980)
1.46 (soil/sediments, Rao & Davidson 1980)
2.46; 1.51; 1.68 (estimated-S; estimated-S and mp; estimated-K_{OW}, Karickhoff 1981)
2.70 (selected, sediment/water, Schnoor & McAvoy 1981; Schnoor 1992)
2.25 (calculated-S, Lyman 1982)
1.47 (average of 5 different soils, Rao & Davidson 1982)
2.11 (retention times of RP-HPLC-RT correlation, Swann et al. 1983)
2.00 (soil slurry/shake flask method, Swann et al. 1983; quoted, Howard 1991)
1.45 (soil, screening model calculations, Jury et al. 1987a, b; Jury & Ghodrati 1989)
1.73 (calculated-Freund isotherm linearized for 12 samples, Sukop & Cogger 1992)
0.903 (selected, USDA 1989)
1.34 (soil, 20–25°C, selected, Wauchope et al. 1992; Tomlin 1994; Hornsby et al. 1996)
1.98–2.32 (Montgomery 1993)
1.80, 2.01 (soil, estimated-class specific model, estimated-general model, Gramatica et al. 2000)

1.63, 1.64 (soils: organic carbon OC ≥ 0.1%, OC ≥ 0.5%, average, Delle Site 2001)
1.55 (sediment: organic carbon OC ≥ 0.5%, average, Delle Site 2001)

Environmental Fate Rate Constants, k, or Half-Lives, $t_{½}$:

Volatilization: initial rate constant $k = 1.2 \times 10^{-3}\ h^{-1}$ and a predicted rate constant $k = 2.9 \times 10^{-4}\ h^{-1}$ from soil with $t_{½} = 2390$ h (Thomas 1982).

Photolysis: near surface direct sunlight photolysis rate constant $k = 0.003\ d^{-1}$ with $t_{½} \sim 200$ d (Schnoor & McAvoy 1981; Schnoor 1992);

$t_{½} \sim 2, 6, 12$ h for degradation in river, lake and seawater, respectively, from Greece which were irradiated with sunlight (Samanidou et al. 1988; quoted, Howard 1991)

Photodegradation ($\lambda > 290$ nm) half-lives in aqueous carbofuran solutions: $t_{½} \sim 50$ min with TiO_2 (160 mg/L) + O_2, $t_{½} \sim 40$ min with H_2O_2 (6×10^{-3} mg/L); $t_{½} \sim 30$ min with O_3 (10^{-3} mg/L) and $t_{½} \sim 65$ h in water/oil suspension. (Mansour et al. 1997)

Oxidation: photooxidation $t_{½} = 4.6$ h, based on estimated rate constant for the vapor-phase reaction with hydroxyl radical in air (Atkinson 1987; quoted, Howard et al. 1991)

k(aq.) = (620 ± 60) $M^{-1}\ s^{-1}$ for direct reaction with ozone in water at pH 3.7 and 21°C, with $t_{½} = 54$ s at pH 7 (Yao & Haag 1991).

k(aq.) = $7 \times 10^9\ M^{-1}\ s^{-1}$ for the reaction with hydroxyl radical in aqueous solutions at 24 ± 1°C (Haag & Yao 1992);

k_{OH}(aq.) = $2.20 \times 10^9\ M^{-1}\ s^{-1}$ in irradiated field water both in the laboratory and sunlit rice paddies with field dissipation $t_{½} = 16.3$ h (Mabury & Crosby 1996).

Hydrolysis: aqueous hydrolysis $t_{½} = 5.1$ wk at pH 7.0 and at 27°C and $t_{½} = 1.2$ h at pH 10 (Seiber et al. 1978; quoted, Howard 1991);

alkaline chemical hydrolysis rate constant $k = 6 \times 10^{-5}\ M^{-1}\cdot s^{-1}$ with $t_{½} > 10{,}000$ d (Schnoor & McAvoy 1981; Schnoor 1992);

$t_{½} = 690$, 8.2, and 1.0 wk in water at 25°C and pH 6.0, 7.0 and 8.0, respectively (Chapman & Cole 1982; quoted, Howard 1991);

hydrolysis rate constants: k = (30.6 ± 0.6) L $min^{-1}\ mol^{-1}$ at 15°C, k = (67.0 ± 0.4) L/min·mol at 25°C and k = (163 ± 1.0) L $min^{-1}\ mol^{-1}$ at 35°C (Trotter et al. 1991);

$t_{½} = 170$ wk at pH 4.5, $t_{½} = 690$ wk at pH 5–6, $t_{½} = 8.2$ wk at ph 7 and $t_{½} = 1$ wk at pH 8.0 at 25°C (Montgomery 1993);

$t_{½} > 1$ yr at pH 4, $t_{½} = 121$ d at pH 7, and $t_{½} = 31$ d at pH 9 at 22°C (Tomlin 1994);

rate constant $k = 5.0 \times 10^{-3}\ M^{-1}\ h^{-1}$ at 24°C; $t_{½} = 737$ h at pH 7.0, $t_{½} = 93.7$ h at pH 8.0 and $t_{½} = 1.17$ h at pH 10.0 in aqueous solutions; $t_{½} = 630$ d at pH 7, $t_{½} = 133$ d at pH 8, and $t_{½} = 0.87$ d at pH 10 in aqueous solutions with montmorillonite suspensions (23.9 g/L); $t_{½} = 937$ d at pH 7, $t_{½} = 76.2$ d at pH 8, $t_{½} = 0.98$ d at pH 10 in aqueous solutions with beidellite suspensions (4.9 g/L); $t_{½} = 889$ d at pH 7, $t_{½} = 113$ d at pH 8, $t_{½} = 0.78$ d at pH 10 in aqueous solutions with illite suspensions (9.2 g/L); and $t_{½} = 753$ d at pH 7, $t_{½} = 80.6$ d at pH 8, $t_{½} = 0.91$ d at pH 10 in aqueous solutions with vermiculite suspensions (8.5 g/L) with an initial carbofuran concentration of 1.0×10^{-4} M (Wei et al. 2001).

Biodegradation: rate constants $k = 0.047\ d^{-1}$ from soil incubation studies and $k = 0.026\ d^{-1}$ in anaerobic system from flooded soil incubation studies both by die-away test (Rao & Davidson 1980; quoted, Scow 1982);

$t_{½} = 40$ d in 0 to 10 cm depth of soil (Rao & Davidson 1980; quoted, Jury et al. 1983, 1984, 1987a, b; Jury & Ghodrati 1989)

Biotransformation:

Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants:

Half-Lives in the Environment:

Air: $t_{½} = 4.6$ h, based on estimated rate constant for the vapor-phase reaction with photochemically produced hydroxyl radical in the atmosphere (Atkinson 1987; quoted, Howard 1991).

Surface water: average $t_{½} = 57$ h in rice paddy water, but pH dependent, e.g., $t_{½} = 1.2$ h at pH 10 and $t_{½} = 864$ h at pH 7; $t_{½} = 48$ and 55 h for two farm ponds (Seiber et al. 1978);

$t_{½} = 2, 6, 12$ h for degradation in river, lake and seawater, respectively, from Greece which were irradiated with sunlight (Samanidou et al. 1988; quoted, Howard 1991);

measured rate constant k = (620 ± 60) $M^{-1}\ s^{-1}$ for direct reaction with ozone in water at pH 3.7 and 21°C, with $t_{½} = 54$ s at pH 7 (Yao & Haag 1991).

Ground water:

Sediment:

Soil: persistence of less than one month (Wauchope 1978);

$t_{1/2}$ = 11–13 d at pH 6.5, and $t_{1/2}$ = 60–75 d for a granular formulation (Ahmad et al. 1979; quoted, Montgomery 1993);

estimated first-order $t_{1/2}$ = 15 d in soil from biodegradation rate constant $k = 0.047\ d^{-1}$ by die-away test from soil incubation studies and $t_{1/2}$ = 26 d from biodegradation rate constant $k = 0.026\ d^{-1}$ in anaerobic system from flooded soil incubation studies by die-away test (Rao & Davidson 1980; quoted, Scow 1982);

moderately persistent in soils with $t_{1/2}$ = 20–100 d (Willis & McDowell 1982);

$t_{1/2}$ = 1–2 months (Hartley & Kidd 1987; quoted, Montgomery 1993);

$t_{1/2}$ = 40 d from screening model calculations (Jury et al. 1987a, b; Jury & Ghodrati 1989);

selected field $t_{1/2}$ = 50 d (Wauchope et al. 1992; Dowd et al. 1993; Hornsby et al. 1996);

soil $t_{1/2}$ = 81 d (Pait et al. 1992);

$t_{1/2}$ = 30 d for soil depth <5 cm, $t_{1/2}$ = 60 d for soil depth 5–20 cm and $t_{1/2}$ = 120 d for soil depth > 20 cm (Dowd et al. 1993);

$t_{1/2}$ = 60 d in forest soil (Neary et al. 1993);

$t_{1/2}$ = 42.4 d in loam and $t_{1/2}$ = 95.5 d in sand (Behrendt & Brüggemann 1993);

$t_{1/2}$ = 30–60 d in soil (Tomlin 1994)

Disappearance rate constants $k = (1.33–5.16) \times 10^{-2}\ h^{-1}$ and $k = (0.36–1.13) \times 10^{-2}\ h^{-1}$ in non-sterile soil suspensions; $k = (1.20–5.07) \times 10^{-2}\ h^{-1}$ in sterile soil suspension at 30°C for 5 Spanish soils. Kinetic profiles in 3 consecutive steps assumed as sorption and fast and slow degradation. Disappearance $t_{1/2}$ = 24 h at 30 and $t_{1/2}$ = 5 h at 40°C for all 5 soil suspensions; $t_{1/2}$ = 48 h at 30°C and $t_{1/2}$ = 12 h at 40°C in Soil 3 (Mora et al. 1996)

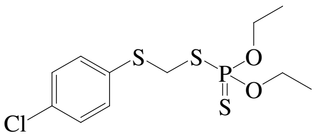
First order rate constants for photolytic decline in sandy soil: $k = 1.88 \times 10^{-3}\ h^{-1}$ with $t_{1/2}$ = 370 h irradiated in moisture-maintained soil, $k = 0.86 \times 10^{-3}\ h^{-1}$ with $t_{1/2}$ = 800 h, irradiated in air-dried soil, $k = 1.15 \times 10^{-3}\ h^{-1}$ with $t_{1/2}$ = 600 h in dark control moist sandy soil, but not degraded in the dark control air-dry system. The photolytic $k = 7.31 \times 10^{-4}\ h^{-1}$ with $t_{1/2}$ = 950 h in moist soil and the contribution of moisture to irradiated metabolism $k = 1.02 \times 10^{-3}\ h^{-1}$ with $t_{1/2}$ = 680 h (Graebing & Chib 2004)

Biota: biochemical $t_{1/2}$ = 40 d from screening model calculations (Jury et al. 1987a, b; Jury & Ghodrati 1989);

$t_{1/2}$ = 4 d in wheat/barley (Behrendt & Brüggemann 1993);

average $t_{1/2}$ = 60 d in the forest (USDA 1989; quoted, Neary et al. 1993)

18.1.1.11 Carbophenothion



Common Name: Carbophenothion
Synonym: Carbofenotion, Acarithion, Akarithion, Trithion, Garrathion, Nephocarb, Dagadip
Chemical Name: *S*-chlorophenylthio methyl *O,O*-diethyl phosphorothioate
Uses: insecticide/acaricide
CAS Registry No: 786-19-6
Molecular Formula: $C_{11}H_{16}ClO_2PS_3$
Molecular Weight: 342.866
Melting Point (°C):
  colorless liquid (Spencer 1982, Hartley & Kidd 1987, Tomlin 1994)
  < 25 (Montgomery 1993)
Boiling Point (°C):
  82 (at 0.01 mmHg, Spencer 1982; Hartley & Kidd 1987; Montgomery 1993; Milne 1995)
Density (g/cm^3):
  1.274 (Spencer 1982)
  1.271 (20°C, Hartley & Kidd 1987; Montgomery 1993, Milne 1995)
Acid Dissociation Constant, pK_a:
Molar Volume (cm^3/mol):
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
Entropy of Fusion, ΔS_{fus} (J/mol K):
Fugacity Ratio at 25°C, F: 1.0

Water Solubility (g/m^3 or mg/L at 25°C):
  < 2.0 (Martin 1961; Spencer 1982)
  0.34 (Gunther et al. 1968; Kenaga 1980b; Kenaga & Goring 1980)
  < 40 (Verschueren 1983)
  0.63 (20°C, shake flask-GC, Bowman & Sans 1983a, b)
  < 1.0 (room temp., Hartley & Kidd 1987, Worthing & Walker 1987)
  0.61, 0.63, 0.73 (10, 20, 30°C, Montgomery 1993)
  0.34 (selected, Augustijn-Beckers et al. 1994; Hornsby et al. 1996)
  40, < 1 (Milne 1995)

Vapor Pressure (Pa at 25°C or as indicated):
  0.40 (Menn et al. 1964)
  4.13×10^{-5} (20°C, Eichler 1965)
  4.07×10^{-5} (20°C, Melnikov 1971)
  4.0×10^{-5} (20°C, Hartley & Graham-Bryce 1980)
  1.07 (Spencer 1982)
  7.73×10^{-5} (20°C, GC-RT correlation, Kim et al. 1984, Kim 1985)
  1.07×10^{-3} (Hartley & Kidd 1987; Montgomery 1993)
  1.107×10^{-3} (selected, Augustijn-Beckers et al. 1994, Hornsby et al. 1996)

Henry's Law Constant (Pa·m^3/mol):
  0.046 (20°C, Montgomery 1993)

Octanol/Water Partition Coefficient, log K_{OW}:
  4.53 (Callahan et al. 1979)
  5.12 (shake flask-concn ratio-GC, Bowman & Sans 1983b)

5.66 (shake flask-GC, De Bruijn et al. 1989)
5.50 (recommended, 1993)
5.33 (recommended, Hansch et al. 1995)

Octanol/Air Partition Coefficient, log K_{OA}:

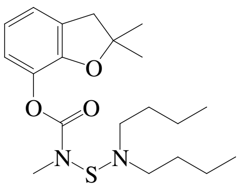
Bioconcentration Factor, log BCF or log K_B:
3.07, 3.63 (calculated-solubility, K_{OW}, Kenaga 1980b)

Sorption Partition Coefficient, log K_{OC}:
4.66 (Kenaga & Goring 1980)
3.90 (calculated, Kenaga 1980b)
4,98, 4.72, 3.92, 4.48 (Elkhorn sandy loam at pH 6.0, Hugo gravelly sandy loam at pH 5.5, Sweeney sandy clay loam at pH 6.3 and Tierra clay loam at pH 6.2, Rao & Davidson 1982)
3.56 (calculated-MCI χ, Gerstl & Helling 1987)
3.92–4.98 (Montgomery 1993)
5.10, 4.66, 5,07, 4.76, 5.09, 4.69, 4.90 (mg/L, quoted, Augustijn-Beckers et al. 1994)
4.70 (recommended, soil, Augustijn & Beckers 1994; Hornsby et al. 1996)
4.66 (calculated-MCI $^1\chi$, Sabljic et al. 1995)
4.47, 4.08 (soil, estimated-class-specific model, estimated-general model using molecular descriptors, Gramatica et al. 2000)

Environmental Fate Rate Constants, k, and Half-Lives, $t_{½}$:
Volatilization:
Photolysis:
Photooxidation:
Hydrolysis:
Biodegradation:
Biotransformation: $t_{½} \geq 100$ d in soil (Verschueren 1983; quoted, Montgomery 1993).
Bioconcentration and Uptake and Elimination Rate Constants (k_1 and k_2):

Half-Lives in the Environment:
Soil: $t_{½} \geq 100$ d (Verschueren 1983; quoted, Montgomery 1993);
field $t_{½} = 30$ d (selected, Augustijn-Beckers et al. 1994; Hornsby et al. 1996).

18.1.1.12 Carbosulfan



Common Name: Carbosulfan
Synonym: Marshal, Adventage, Posse, FMC 35001
Chemical Name: 2,3-dihydro-2,2-dimethylbenzofuran-7-yl(dibutylaminothio) methylcarbamate
Uses: insecticide/acarrcide/nematicide
CAS Registry No: 55285-14-8
Molecular Formula: $C_{20}H_{32}N_2O_3S$
Molecular Weight: 380.544
Melting Point (°C):
  viscous brown liquid (Hartley & Kidd 1987)
Boiling Point (°C):
  124–128 (Tomlin 1994; Milne 1995)
Density (g/cm^3):
  1.056 (20°C, Hartley & Kidd 1987; Tomlin 1994; Milne 1995)
Acid Dissociation Constant, pK_a:
Molar Volume (cm^3/mol):
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
Entropy of Fusion, ΔS_{fus} (J/mol K):
Fugacity Ratio at 25°C, F: 1.0

Water Solubility (g/m^3 or mg/L at 25°C):
  0.30 (Hartley & Kidd 1987; Tomlin 1994)
  0.03 (Milne 1995)

Vapor Pressure (Pa at 25°C):
  0.041×10^{-3} (Hartley & Kidd 1987, Tomlin 1994)

Henry's Law Constant (Pa·m^3/mol at 25°C):

Octanol/Water Partition Coefficient, log K_{OW}:
  3.30 (Tomlin 1994)
  2.20 (Milne 1995)

Octanol/Air Partition Coefficient, log K_{OA}:

Bioconcentration Factor, log BCF or log K_B:

Sorption Partition Coefficient, log K_{OC}:

Environmental Fate Rate Constants, k, and Half-Lives. $t_{½}$:
  Volatilization:
  Photolysis:
  Oxidation:
  Hydrolysis: hydrolyzed in aqueous media with $t_{½} < 1$ h in pure water at pH 4; $t_{½} = 22$ h at pH 6, $t_{½} = 7.6$ d at pH 7, $t_{½} = 14.2$ d at pH 8 and $t_{½} > 58.3$ d at pH 9 (Haretly & Kidd 1987; Tomlin 1994)

Biodegradation: in soil, rapidly degraded under both aerobic and anaerobic conditions with $t_{½}$ = 2–3 d (Hartley & Kidd 1987).

Biotransformation:

Bioconcentration and Uptake and Elimination Rate Constants (k_1 and k_2):

Half-Lives in the Environment:

Air:

Surface water: hydrolyzed in aqueous media with half-lives at 25°C are, $t_{½}$ < 1 h in pure water at pH 4; $t_{½}$ = 22 h at pH 6, $t_{½}$ = 7.6 d at pH 7, $t_{½}$ = 14.2 d at pH 8 and $t_{½}$ > 58.3 d at pH 9 (Hartley & Kidd 1987; Tomlin 1994)

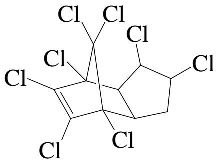
Ground water:

Sediment:

Soil: rapidly degraded under both aerobic and anaerobic conditions with $t_{½}$ = 2–3 d (Hartley & Kidd 1987).

Biota:

18.1.1.13 Chlordane



Common Name: Chlordane

Synonym: A 1068, Aspon-chlordane, Belt, beta-chlordane, CD-68, Chlorindan, Chlor-Kill, Chlortox, Corodane, Cortilan-neu, Dichlorochlordene, Dowchlor, ENT 9932, ENT 25552, HCS 3260, Kypchlor, M 140, Octachlor, Octaterr, Orthoklor, Shell SD 5532, Synklor, Tat chlor 4, Topichlor, Toxichlor, Velsicol

Chemical Name: 1,2,4,5,6,7,8,8-octachloro-3*a*,4,7,7*a*-tetrahydro-4,7-methano-1*H*-indane; 1,2,4,5,6,7,8,8-octa-chloro-3*a*,4,7,7*a*-tetrahydro-4,7-methanoindane

Uses: nonsystemic insecticide with contact, stomach, and respiratory action and also used as fumigant.

CAS Registry No: 57-74-9 (nonstereospecific chlordane); 5103-71-9 (*cis*- or α-isomer); 5103-74-2 (*trans*- or β-isomer); 5564-34-7 (γ-isomer); 12789-03-6 (technical grade chlordane)

Molecular Formula: $C_{10}H_6Cl_8$

Molecular Weight: 409.779

Melting Point (°C):

107–108.8 (*cis*-isomer, Callahan et al. 1979; Howard 1991)
103–105 (*trans*-isomer, Callahan et al. 1979; Howard 1991)
106–107, 104–105 (*cis*-isomer, *trans*-isomer, Hartley & Kidd 1987; Tomlin 1994)

Boiling Point (°C):

175 (at 2 mmHg, Roark 1951; Callahan et al. 1979; Howard 1991; Montgomery 1993)
262, 363, 365 (estimated from structure, Tucker et al. 1983)
175 (at 1 mmHg, Hartley & Kidd 1987; Tomlin 1994; Milne 1995)

Density (g/cm^3 at 20°C):

1.59–1.63 (25°C, Worthing & Walker 1987, Worthing & Hance 1991; Tomlin 1994; Milne 1995)
1.59–1.63 (Montgomery 1993)

Molar Volume (cm^3/mol):

340.5 (calculated-Le Bas method at normal boiling point)

Dissociation Constant, pK_a:

Enthalpy of Vaporization, ΔH_V (kJ/mol):

77.22, 80.26, 82.92 (mixture, α-chlordane, β-chlordane, Rordorf 1989)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

28.033 (*cis*-isomer, DSC method, Plato 1972)
16.45 (*trans*-isomer, DSC method, Plato 1972)

Entropy of Fusion, ΔS_{fus} (J/mol K):

56.4 (Passivirta et al. 1999)

Fugacity Ratio at 25°C, F:

0.162 (assuming ΔS_{fus} = 56 J/mol K, Mackay et al. 1986)
0.140 (20°C, assuming ΔS_{fus} = 56 J/mol K, Suntio et al. 1988)

Water Solubility (g/m^3 or mg/L at 25°C and reported temperature dependence equations):

1.850 (generator column-GC/ECD, Weil et al. 1974)
0.056 (shake flask-LSC, Sanborn et al. 1976)
0.056 (Martin & Worthing 1977)
0.10 (Hartley & Kidd 1987; Worthing & Walker 1987, 1991)
0.56 (Agency for Toxic Substances and Disease Registry 1988; quoted, Burmaster et al. 1991)
0.05 (20°C, selected, Suntio et al. 1988)
0.032; 0.009–0.056 (shake flask-LSC; lit. range, Johnson-Logan et al. 1992)
1.83 (selected, Yalkowsky & Banerjee 1992)
0.056 (Montgomery 1993)
0.06 (20–25°C, selected, Augustijn-Beckers et al. 1994; Hornsby et al. 1996)

0.127 (calculated-group contribution fragmentation method, Kühne et al. 1995)
0.10 (Tomlin 1994; Milne 1995)
0.061, 0.002 (calculated-molar volume, mp and mobile order thermodynamics, Ruelle & Kesselring 1997)
log $[S_L/(mol/L)] = -0.880 - 1124/(T/K)$ (liquid, *cis*-isomer, Passivirta et al. 1999)
log $[S_L/(mol/L)] = -0.880 - 1118/(T/K)$ (liquid, *trans*-isomer, Passivirta et al. 1999)
0.451, 0.402 (*cis*-chlordane, supercooled liquid: LDV derivation of literature-derived value, FAV final-adjusted value, Shen & Wania 2005)
0.451, 0.615 (*trans*-chlordane, supercooled liquid: LDV derivation of literature-derived value, FAV final-adjusted value, Shen & Wania 2005)

Vapor Pressure (Pa at 25°C and reported temperature dependence equations):

0.0013 (Martin 1972, Spencer 1973, 1982)
0.0013 (SRI International 1980; Tucker et al. 1983)
0.00227, 1.6×10^{-5}, 1.3×10^{-5} (estimated-bp, Tucker et al. 1983)
2.9×10^{-3}, 3.86×10^{-3} (*cis*-, *trans*-chlordane, 20°C, supercooled liquid P_L, Bidleman et al. 1986)
0.0013 (Hartley & Kidd 1987)
0.0011 (20°C, selected, Suntio et al. 1988)
0.0613, 0.00133 (technical, refined, Worthing & Walker 1987)
0.00293, 0.00040 (*cis*-isomer, GC-RT correlation, supercooled liquid P_L, solid crystal P_S, Foreman & Bidleman 1987)
0.00387, 0.00052 (*trans*-isomer, GC-RT correlation, supercooled liquid P_L, solid crystal P_S, Foreman & Bidleman 1987)
0.0013 (Agency for Toxic Substances and Disease Registry 1988)
0.027, 0.31, 2.40, 14.0, 69.0 (25, 50, 70, 100, 125°C, chlordane mixture, gas saturation-GC, Rordorf 1989)
log $(P_L/Pa) = 11.968 - 4033.7/(T/K)$; measured range 70.4–115°C (chlordane mixture, liquid, gas saturation-GC, Rordorf 1989)
0.0080, 0.011, 0.98, 6.70, 36 (α-chlordane, 25, 50, 70, 100, 125°C, gas saturation-GC, Rordorf 1989)
log $(P_L/Pa) = 12.435 - 4332.5/(T/K)$; measured range 50.1–135°C (α-chlordane, liquid, gas saturation-GC, Rordorf 1989)
0.013, 0.16, 1.40, 9.30, 48 (β-chlordane, 25, 50, 70, 100, 125°C, gas saturation-GC, Rordorf 1989)
log $(P_S/Pa) = 12.318 - 4235.5/(T/K)$; measured range 50/1–135°C (β-chlordane, liquid, gas saturation-GC, Rordorf 1989)
log $(P_L/Pa) = 13.396 - 4803.6/(T/K)$; measured range 49.5–140°C (gas saturation-GC, Rordorf 1989)
4.5×10^{-3}, 5.1×10^{-3}, 4.8×10^{-3} (*cis*-chlordane, GC-RT correlation, supercooled liquid P_L, Hinckley et al. 1990)
6.3×10^{-3}, 6.9×10^{-3}, 6.7×10^{-3} (*trans*-chlordane, GC-RT correlation, supercooled liquid P_L, Hinckley et al. 1990)
log $(P_L/Pa) = 12.04 - 4284/(T/K)$ (*cis*-chlordane, supercooled liquid P_L, GC-RT correlation, Hinckley et al. 1990; quoted, Passivirta et al. 1999)
log $(P_L/Pa) = 11.95 - 4216/(T/K)$ (*trans*-chlordane, supercooled liquid P_L, GC-RT correlation, Hinckley et al. 1990)
0.0013 (refined grade, Worthing & Hance 1991; Tomlin 1994)
0.0610 (technical grade, Worthing & Hance 1991)
0.00269, 0.00813 (*cis*-chlordane, supercooled liquid P_L at 20°C, 30°C, calculated from Hinckley et al. 1990; Cotham & Bidleman 1992)
0.000133 (20°C, Montgomery 1993)
0.00133 (20–25°C, selected, Augustijn-Beckers et al. 1994; Hornsby et al. 1996)
4.59×10^{-4} (quoted as mean of *cis* and *trans* forms from Howard 1991, Mortimer & Connell 1995)
4.68×10^{-3}, 4.15×10^{-3}; 6.57×10^{-4} (*cis*-chlordane, supercooled liquid P_L: calculated, GC-RT correlation; converted to solid P_S with fugacity ratio F, Passivirta et al. 1999)
6.58×10^{-3}, 5.84×10^{-3}; 9.66×10^{-4} (*trans*-chlordane, supercooled liquid P_L: calculated, GC-RT correlation; converted to solid P_S with fugacity ratio F, Passivirta et al. 1999)
log $(P_S/Pa) = 14.99 - 5407/(T/K)$ (*cis*-chlordane, solid, Passivirta et al. 1999)
log $(P_S/Pa) = 14.91 - 5333/(T/K)$ (*trans*-chlordane, solid, Passivirta et al. 1999)
0.080, 0.0073 (*cis*-chlordane, supercooled liquid P_L: LDV literature derived value, FAV final adjusted value, Shen & Wania 2005)

0.013, 0.010 (*trans*-chlordane, supercooled liquid P_L: LDV literature derived value, FAV final adjusted value, Shen & Wania 2005)
log (P_L/Pa) = – 4238/(T/K) + 12.32 (*cis*-chlordane, supercooled liquid P_L: linear regression, Shen & Wania 2005)

Henry's Law Constant (Pa·m^3/mol at 25°C or as indicated and reported temperature dependence equations):
2.92–9.5 (Callahan et al. 1979)
4.92 (gas stripping-GC, Warner et al. 1980)
112 (batch stripping, average of *cis*- and *trans*- isomers, Atlas et al. 1982)
87.7, 134 (exptl,: α-chlordane, γ-chlordane, Atlas et al. 1982;)
9.12 (Mabey et al. 1982)
3.44 (estimated-group method of Hine & Mookerjee 1975, Tucker et al. 1983)
9.64 (calculated-P/C, Mackay et al. 1986)
0.248 (calculated-P/C, Jury et al. 1990)
4.86 (gas stripping-GC, Warner et al. 1987)
9.02 (20°C, calculated-P/C, Suntio et al. 1988; quoted, Cotham & Bidleman 1991; Majewski & Capel 1995)
9.66 (Ryan et al. 1988)
0.97 (Agency for Toxic Substances and Disease Registry 1988; quoted, Burmaster et al. 1991)
4.91 (technical chlordane, Howard 1991)
8.37 (23°C, γ-chlordane, wetted-wall column-GC/ECD, Fendinger et al. 1989)
5.66, 5.91 (22–24°C, γ-chlordane, fog chamber-GC/ECD, Fendinger et al. 1989)
0.87 (0°C, selected, Cotham & Bidleman 1991)
7.12 (calculated-bond contribution method, Meylan & Howard 1991)
9.02 (20°C), 140, 570 (23°C), 9.64 (25°C) (*trans*-chlordane, quoted, Iwata et al. 1993)
9.02 (20°C), 89, 420 (23°C), 9.64, 11.2 (25°C) (*cis*-chlordane, quoted, Iwata et al. 1993)
8.42 (γ-chlorane, wetted-wall column-concn ratio-GC/ECD, Fendinger et al. 1989)
5.45 (γ-chlorane, fog chamber-concn ratio-GC/ECD, Fendinger et al. 1989)
8.11 (calculated-bond contribution, Meylan et al. 1991)
log [H/(Pa m^3/mol)] = 12.92 – 3160/(T/K) (*cis*-chlordane, Passivirta et al. 1999)
log [H/(Pa m^3/mol)] = 12.84 – 3098/(T/K) (*trans*-chlordane, Passivirta et al. 1999)
6.0, 5.7 (*cis*-chlordane, LDV literature-derived value, FAV final adjusted value, Shen & Wania 2005)
6.0, 6.8 (*trans*-chlordane, LDV literature-derived value, FAV final adjusted value, Shen & Wania 2005)

Octanol/Water Partition Coefficient, log K_{OW}:
2.78 (shake flask-LSC, Sanborn et al. 1976)
6.00 (Veith et al. 1979, 1980; Veith & Kosian 1983)
5.16 (calculated, Kenaga 1980a, b)
3.32 (Rao & Davidson 1980)
5.89 (selected, Dao et al. 1983)
5.54 (CLOGP 1986; Thor 1989; Howard 1991)
2.78, 5.48 (Schnoor et al. 1987)
5.9, 6.1 (*cis*-, *trans*-chlordane, Kawano et al. 1988)
6.21 (estimated by QSAR & SPARC, Kollig 1993)
5.16; 2.78. 3.32; 5.08, 6.00 (quoted lit. exptl. values; Sangster 1993)
6.00 (Montgomery 1993; Devillers et al. 1996)
5.08 (RP-HPLC-RT correlation, Sicbaldi & Finizio 1993)
5.80 (LOGSTAR or CLOGP, Sabljic et al. 1995)
5.66, 5.62, 5.44, 6.10, 6.22 (α-, β-, γ-, *cis-*, *trans*-chlordane, shake flask/slow stirring-GC, Simpson et al. 1995)
5.08, 5.80, 4.75 (RP-HPLC-RT correlation, ClogP, calculated-S, Finizio et al. 1997)
6.10, 6.20 (*cis*-chlordane, LDV literature-derived value, FAV final-adjusted value, Shen & Wania 2005)
6.23, 6.27 (*trans*-chlordane, LDV literature-derived value, FAV final-adjusted value, Shen & Wania 2005)

Octanol/Air Partition Coefficient, log K_{OA} at 25°C and reported temperature dependence equation. Additional data at other temperatures designated * are compiled at the end of this section:
8.70 (*cis*-chlordane, calculated-K_{OW}/K_{AW}, Wania & Mackay 1996)
8.50 (*trans*-chlordane, calculated-K_{OW}/K_{AW}, Wania & Mackay 1996)

9.027*, 8.916 (*cis*-chlordane, gas saturation-GC/MS interpolated, measured range 5–25°C, Shoeib & Harner 2002)
log K_{OA} = –8.29 + 5217/(T/K), temp range 5–25°C (*cis*-chlordane, gas saturation-GC, Shoeib & Harner 2002)
8.967*, 8.872 (*trans*-chlordane, gas saturation-GC/MS, interpolated, measured range 5–25°C, Shoeib & Harner 2002)
log K_{OA} = –8.03 + 5036/(T/K), temp range 5–25°C (*trans*-chlordane, gas saturation-GC, Shoeib & Harner 2002)
8.3887*, 8.387 (oxychlordane, gas saturation-GC/MS, interpolated, measured range 5–25°C, Shoeib & Harner 2002)
log K_{OA} = –5.636 + 4179/(T/K), temp range: 5–25°C (oxychlordane, gas saturation-GC, Shoeib & Harner 2002)
8.91, 8.85 (*cis*-chlordane, LDV literature-derived value, FAV final-adjusted value, Shen & Wania 2005)
8.86, 8.85 (*trans*-chlordane, LDV literature-derived value, FAV final-adjusted value, Shen & Wania 2005)

Bioconcentration Factor, log BCF at 25°C or as indicated:

3.51–3.92; 3.60–3.78; 3.28–3.36; 4.10–4.27 (wet wt. basis 96-h test, eastern oysters; pink shrimp; grass shrimp; pin fish, Parrish et al. 1976)
4.69 (*Oedogonium cardiacum*, Sanborn et al. 1976)
3.66 (spot fish, 24-h flow system, *trans*-chlordane, Schimmel et al. 1976)
3.57–4.23 (96 h exposures of *trans*-chlordane to whole marine fish, Schimmel et al. 1976)
4.11–4.34 (186-d chronic exposures, *trans*-chlordane to sheephead minnow, Parrish et al. 1978)
3.85–4.46 (exposures *trans*-chlordane to 28-d old second generation sheephead minnow, Parrish et al. 1978)
4.58 (fathead minnows, 32-d exposure, Veith et al. 1979, 1980; Veith & Kosian 1983)
4.01 (green algae, Glooschenko et al. 1979)
4.06, 3.92 (fish: flowing water, static ecosystem, Kenaga 1980a, b; Kenaga & Goring 1980)
3.50 (calculated-S, Kenaga 1980a)
–0.523 (average beef fat diet, Kenaga 1980b)
2.08, 4.32 (estimated-S, K_{OW}, Bysshe 1982)
3.68, 3.64 (α-, γ-chlordane, clam fat, 60-d expt., Hartley & Johnson 1983)
4.06–4.58 (fish, Bysshe 1987)
5.04–5.88 (earthworms, Gish & Hughes 1982;)
3.57–4.20 mean 4.20; 3.36–4.34 mean 4.34 (α-chlordane, rainbow trout, 15°C, steady-state BCF on 7- to 96-d laboratory study in 2 tanks with different water concn, Oliver & Niimi 1985)
33.30–4.18 mean 4.18; 3.26–4.30 mean 4.30 (γ-chlordane, rainbow trout, 15°C, steady-state BCF on 7- to 96-d laboratory study in 2 tanks with different water concn, Oliver & Niimi 1985)
4.23, 4.26 (α-, γ-chlordane, rainbow trout, steady-state BCF-concentration ratio., Oliver & Niimi 1985)
4.45, 4.20 (α-, γ-chlordane, rainbow trout, kinetic state BCF-ratio of rate const., Oliver & Niimi 1985)
6.15, 4.88 (α-, γ-chlordane, rainbow trout, Lake Ontario field BCF., Oliver & Niimi 1985)
4.58; 4.33, 4.40 (measured for fathead minnow; calculated-K_{OW} for sheepshead minnows, Zaroogian et al. 1985)
4.58; 3.90, 3.92 (measured for fathead minnow; calculated-K_{OW} for pinfish, Zaroogian et al. 1985)
4.58; 4.33, 4.40 (measured for fathead minnow; calculated-K_{OW} for oyster, Zaroogian et al. 1985)
3.70 (oyster, Hawker & Connell 1986)
6.73, 6.99 (total chlordanes, zooplankton, thick-billed murre, Kawano et al. 1986)
3.78, 4.30 (juvenile and adult sheepshead minnow, 28–129 d exposure, Parrish et al. 1978)
6.0–7.0 (zooplankton and Chum salmon, Kawano et al. 1988)
5.57 (Markwell et al. 1989)
3.52, 2.60 (large mouth bass, clams, 106–127 d exposure, NRC 1974)
3.86 (eastern oyster, 10-d exposure, NRC 1974)
3.74 (white sucker and redhorse, Roberts et al. 1977)
2.03, 2.51, 3.0 (frogs, bluegills, goldfish, Verschueren 1983)
6.73, 7.89, 6.99 (total chlordane: zooplankton, Dall's porpoise, thick-billed murre, Kawano et al. 1986)
4.58 (estimated-S and K_{OW}, Isnard & Lambert 1988)
–2.13 (beef biotransfer factor log B_b, correlated-K_{OW} from Kenaga 1980, Travis & Arms 1988)
–3.43 (milk biotransfer factor log B_m, correlated-K_{OW} from Dorough & Hemken 1973, Travis & Arms 1988)
–1.81 (vegetation, correlated-K_{OW} from Dorough & Pass 1973; Tafuri et al. 1977; Travis & Arms 1988)
3.03 (*Hydrilla*, Hinman & Klaine 1992)
4.01, 3.50; 2.80 (estimated: fish-based, duckweed-based, Hinman & Klaine 1992)

3.117, 3.098 (*cis*-, *trans*-chlordane, goldfish, Park & Erstfeld 1997)
>4.58, >5.56 (fathead minnow, uptake 32-d: wet wt basis, lipid wt basis, Geyer et al. 2000)
4.38, 5.20 (*Daphnia:* wet wt basis, lipid wt basis, α-chlordane, Geyer et al. 2000)
4.45, 5.58 (fathead minnow: wet wt basis, lipid wt basis, α-chlordane, Geyer et al. 2000)
5.26, 6.31 (Chum salmon, 91% lipid: wet wt basis, lipid wt basis, α-chlordane, Geyer et al. 2000)
3.04, 3.74 (algae: wet wt basis, dry wt basis, γ-chlordane, Geyer et al. 2000)
3.04, 3.74 (*Daphnia*: wet wt basis, lipid wt basis, γ-chlordane, Geyer et al. 2000)
4.21, 5.35 (fathead minnow: wet wt basis, lipid wt basis, γ-chlordane, Geyer et al. 2000)
5.04, 6.18 (chum salmon, 9.2% lipid: wet wt basis, lipid wt basis, γ-chlordane, Geyer et al. 2000)
3.68; 3.67 (*Oncorhynchus mykiss*, wet wt. basis: quoted exptl.; calculated-QSAR model based on quantum chemical parameters, Wei et al. 2001)

Sorption Partition Coefficient, log K_{OC} at 25°C or as indicated:
4.33 (calculated-S as per Kenaga & Goring 1978, Kenaga 1980a, b)
1.58 (screening model calculations, Jury et al. 1987b)
4.64, 4.09 (calculated-K_{OW} as per Kenaga & Goring 1980, Chapman 1989)
5.50, 5.60 (α-chlordane: field sediment trap material, calculated-K_{OW}, Oliver & Charlton 1984)
5.40, 5.60 (γ-chlordane, field sediment trap material, calculated-K_{OW}, Oliver & Charlton 1984)
4.58 (soil, screening model calculations, Jury et al. 1987b, 1990)
4.39, 4.19 (calculated-K_{OW} and solubility, Howard 1991)
4.77, 4.94 (α-chlordane: quoted, calculated-MCI χ, Meylan et al. 1992)
5.45, 4.40–4.86 (Aldrich humic acid, soil, Johnson-Logan et al. 1992)
5.90 (estimated by QSAR and SPARC, Kollig 1993)
4.85–5.57 (Montgomery 1993)
4.30 (20–25°C, selected, Augustijn-Beckers et al. 1994; Hornsby et al. 1996)
5.15 (soil, calculated-MCI χ, Sabljic et al. 1995)
4.33, 4.42 (log K_P, *cis*-, *trans*-chlordane, Park & Erstfeld 1997)
5.15; 5.03 (soil, quoted exptl.; estimated-general model, Gramatica et al. 2000)

Environmental Fate Rate Constants, k, or Half-Lives, $t_{1/2}$:

Volatilization: the volatilization $t_{1/2}$ ~ 7.3 and 7.9 h for γ- and α- chlordane, respectively, from a model river 1 m deep flowing 1 m/s with a wind velocity of 3 m/s (Lyman et al. 1982, Howard 1991); and $t_{1/2}$ ~ 18–26, 3.6–5.2, 14.4–20.6 d from a model environmental pond (2 m deep), river (3 m deep) and lake (5 m deep), respectively, (Lyman et al. 1982; Howard 1991); $t_{1/2}$ ~ 43 h from a model river 1-m deep flowing 1 m/s based, on the Henry's law constant of technical chlordane (Lyman et al. 1982, Howard 1991);
measured rate constant $k = 0.3\ d^{-1}$ (Glotfelty et al. 1984; Glotfelty et al. 1989);
calculated rate constant $k = 1.0\ d^{-1}$ (Glotfelty et al. 1989).

Photolysis:

Oxidation: $t_{1/2}$ = 5.2–51.7 h in air, based on estimated photooxidation half-life in air (Atkinson 1987; quoted, Howard et al. 1991);
$k_{OH}(aq.) = 8 \times 10^8\ M^{-1}\ s^{-1}$ for the reaction (photo-Fenton with reference to lindane) with hydroxyl radical in aqueous solutions at pH 3.3 and at 24 ± 1°C (Buxton et al. 1988; quoted, Faust & Hoigné 1990; Haag & Yao 1992)
$k(aq.) < 0.04\text{-} > 300\ M^{-1}\ s^{-1}$ for direct reaction with ozone in water at pH 6.2–6.4 and 19 ± 2°C, with 2 min > $t_{1/2}$ > 10 d at t pH 7 (Yao & Haag 1991).
$k(aq.) = (6–170) \times 10^8\ M^{-1}\ s^{-1}$ for the reaction (photo-Fenton with reference to acetophenone) with hydroxyl radicals in aqueous solutions at pH 3.3 and at 24 ± 1°C (Haag & Yao 1992).

Hydrolysis: $t_{1/2}$ > 4 yr (Callahan et al. 1979);
first-order $t_{1/2}$ > 197000 yr, based on base rate constant $k = 4.3 \times 10^{-3}\ M^{-1}\ h^{-1}$ at pH 7.0 and 25°C (Ellington et al. 1987, 1988; quoted, Howard et al. 1991).
$t_{1/2} = 7.2 \times 10^7$ d at pH 7 and $t_{1/2}$ = 670 d at pH 12 in natural waters (Capel & Larson 1995)

Biodegradation: aqueous aerobic $t_{1/2}$ = 5712–33264 h, based on unacclimated aerobic river die-away test data (Eichelberger & Lichtenberg 1971; quoted, Howard et al. 1991) and reported soil grab sample data (Castro & Yoshida 1971; quoted, Howard et al. 1991);
$k = 0.0024\ d^{-1}$ with a biodegradation $t_{1/2}$ = 1214 d under field conditions (Rao & Davidson 1980);

aqueous anaerobic $t_{1/2}$ = 24–168 h, based on soil and freshwater mud grab sample data for aldrin, dieldrin, endrin and heptachlor epoxide (Maule et al. 1987; quoted, Howard et al. 1991);
$t_{1/2}$ = 100 d in soil (Jury et al. 1990)
$t_{1/2}$(aerobic) = 240 d, $t_{1/2}$(anaerobic) = 1 d in natural waters (Capel & Larson 1995)
Biotransformation:
Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants:
$k_1 = 340\ d^{-1}$ (α-, γ-chlordane, rainbow trout, Oliver & Niimi 1985)
$k_2 = 1.92\ d^{-1}$ (α-chlordane, rainbow trout, Oliver & Niimi 1985)
$k_2 = 0.021\ d^{-1}$ (γ-chlordane, rainbow trout, Oliver & Niimi 19850
$k_2 = 0.0974\ d^{-1}$ (γ-chlordane from rats, Dearth & Hites 1991)
$k_2 = 0.1170\ d^{-1}$ (α-chlordane from rats, Dearth & Hites 1991)

Half-Lives in the Environment:
Air: $t_{1/2}$ = 5.2–51.7 h, based on estimated photooxidation half-life in air (Atkinson 1987; quoted, Howard et al. 1991; Mortimer & Connell 1995);
atmospheric transformation lifetime was estimated to be >1 d (Kelly et al. 1994);
$t_{1/2}$ = in the Great Lake's atmosphere. 16 ± 5.7 yr at Eagle Harbor, 10 ± 2.3 yr at Sleeping Bear Dunes and 6.8 ± 0.8 yr at Sturgeon Point (Buehler et al. 2004).
Surface water: $t_{1/2}$ = 5712–33264 h, based on unacclimated aerobic river die-away test data (Eichelberger & Lichtenberg 1971; quoted, Howard et al. 1991; Mortimer & Connell 1995) and reported soil grab sample data (Castro & Yoshida 1971; quoted, Howard et al. 1991; Mortimer & Connell 1995)
measured rate constant $k < 0.04\text{-} > 300\ M^{-1}\ s^{-1}$ for direct reaction with ozone in water at pH 6.2–6.4 and 19 ± 2°C, with a half-life, 2 min > $t_{1/2}$ > 10 d at pH 7 (Yao & Haag 1991)
Biodegradation $t_{1/2}$(aerobic) = 240 d, $t_{1/2}$(anaerobic) = 1 d; hydrolysis $t_{1/2} = 7.2 \times 10^7$ d at pH 7 and $t_{1/2}$ = 670 d at pH 12 in natural waters (Capel & Larson 1995)
Ground water: $t_{1/2}$ = 11424–66528 h, based on estimated aqueous aerobic biodegradation half-life (Howard et al. 1991).
Sediment: $t_{1/2}$ = 20000 h (quoted mean value from Howard et al. 1991, Mortimer & Connell 1995).
Soil: $t_{1/2}$ ~ 6 yr persistence in soil (Nash & Woolson 1967);
estimated persistence of 5 yr in soil (Kearney et al. 1969; Edwards 1973; quoted, Morrill et al. 1982; Jury et al. 1987);
$t_{1/2}$ = 5712–33264 h, based on unacclimated aerobic river die-away test data (Eichelberger & Lichtenberg 1971; quoted, Howard et al. 1991) and reported soil grab sample data (Castro & Yoshida 1971; quoted, Howard et al. 1991);
rate constant $k = 0.0024\ d^{-1}$ with a biodegradation $t_{1/2}$ = 1214 d under field conditions (Rao & Davidson 1980);
field $t_{1/2}$ = 9 d in fallow soil (Glotfelty 1981; quoted, Nash 1983);
persistent with $t_{1/2}$ > 100 d (Willis & McDowell 1982);
microagroecosystem $t_{1/2}$ = 10–13 d in moist fallow soil (Nash 1983);
$t_{1/2}$ ~ 1 yr in soil (Hartley & Kidd 1987; quoted, Montgomery 1993);
$t_{1/2}$ = 3500 d from screening model calculations (Jury et al. 1987b);
$t_{1/2}$ > 50 d when subject to plant uptake via volatilization (Ryan et al. 1988);
degradation $t_{1/2}$ = 100 d in soil (Jury et al. 1990);
mean $t_{1/2}$ = 3.3 yr under field conditions (Howard 1991);
estimated field $t_{1/2}$ ~ 350 d (Augustijn-Beckers et al. 1994; Tomlin 1994; Hornsby et al. 1996);
$t_{1/2}$ = 1–20 yr in soil, $t_{1/2}$ = 5015 yr in the environment (Geyer et al. 2000)
$t_{1/2}$ = 240 and 7.2 yr for control and sludge-amended Luddington soils, respectively, for *cis*-chlordane and $t_{1/2}$ = 12.9 and 9.2 yr for control and sludge-amended Luddington soils, respectively, for *trans*-chlordane (Meijer et al. 2001).
Biota: $t_{1/2}$ = 1 d for daphinds and $t_{1/2}$ = 60 d for fish (Callahan et al. 1979; quoted, Wilcock et al. 1993);
elimination $t_{1/2}$ ~ 60 d for α-chlordane and $t_{1/2}$ = 33 d for γ-chlordane in rainbow trout (Oliver & Niimi 1985);
biochemical $t_{1/2}$ = 3500 d from screening model calculations (Jury et al. 1987b);
depuration $t_{1/2}$ = 7.1 d for γ-chlordane, and $t_{1/2}$ = 5.9 d for α-chlordane (rats, Dearth & Hites 1991);
$t_{1/2}$ = 12 d for elimination from *T. liliana* (Wilcock et al. 1993).

TABLE 18.1.1.13.1
Reported octanol-air partition coefficients of chlordane at various temperatures

cis-chlordane		*trans*-chlordane		oxychlordane	
Shoeib & Harner 2002		Shoeib & Harner 2002		Shoeib & Harner 2002	
generator column-GC/MS		generator column-GC/MS		generator column-GC/MS	
t/°C	log K_{OA}	t/°C	log K_{OA}	t/°C	log K_{OA}
5	10.2162	5	10.1292	5	9.4204
10	9.7963	10	9.7568	10	9.0757
15	9.4916	15	9.4375	15	8.9090
20	9.0896	20	9.0500	20	8.6184
25	9.0271	25	8.9671	25	8.3887
25	8.916	25	8.872	25	8.387
log K_{OA} = A + B/(T/K)		log K_{OA} = A + B/(T/K)		log K_{OA} = A + B/(T/K)	
A	–8.289	A	–8.027	A	–5.636
B	5127	B	5036	B	4179
enthalpy of phase change ΔH_{OA}/(kJ mol^{-1}) = 97.5		enthalpy of phase change ΔH_{OA}/(kJ mol^{-1}) = 96.4		enthalpy of phase change ΔH_{OA}/(kJ mol^{-1}) = 80.0	

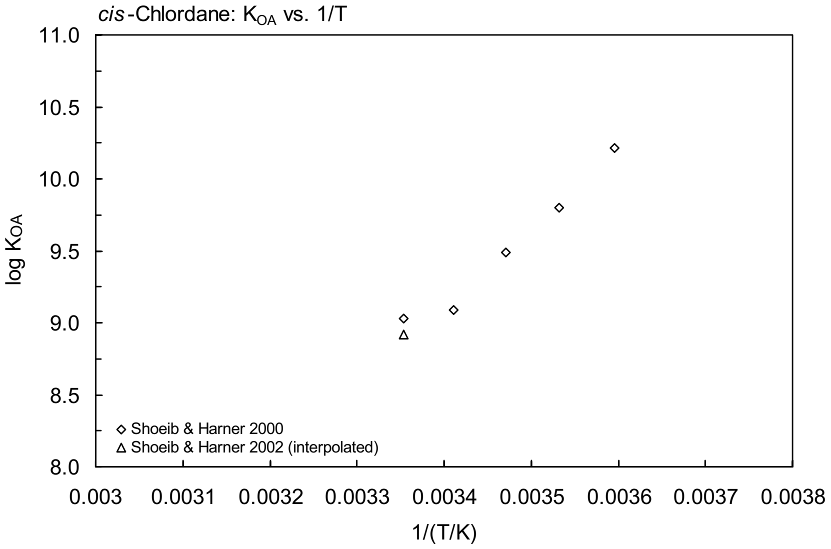


FIGURE 18.1.1.13.1A Logarithm of K_{OA} versus reciprocal temperature for *cis*-chlordane.

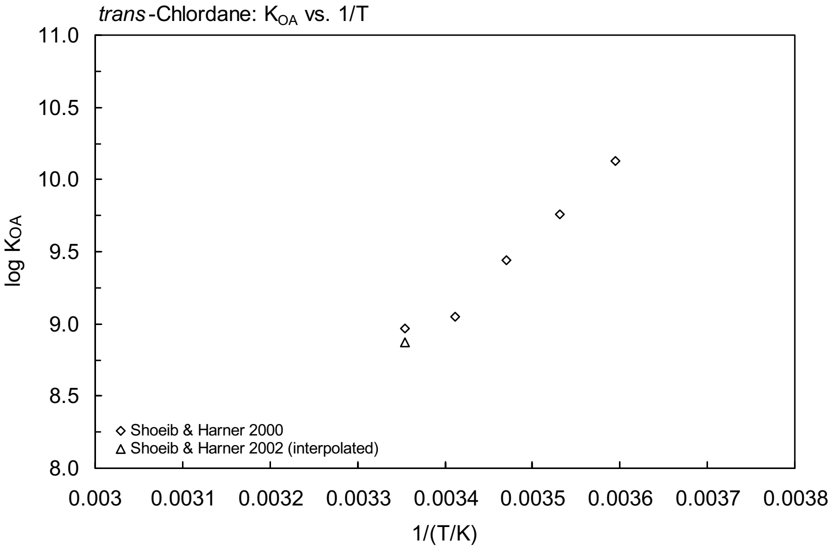


FIGURE 18.1.1.13.1B Logarithm of K_{OA} versus reciprocal temperature for *trans*-chlordane.

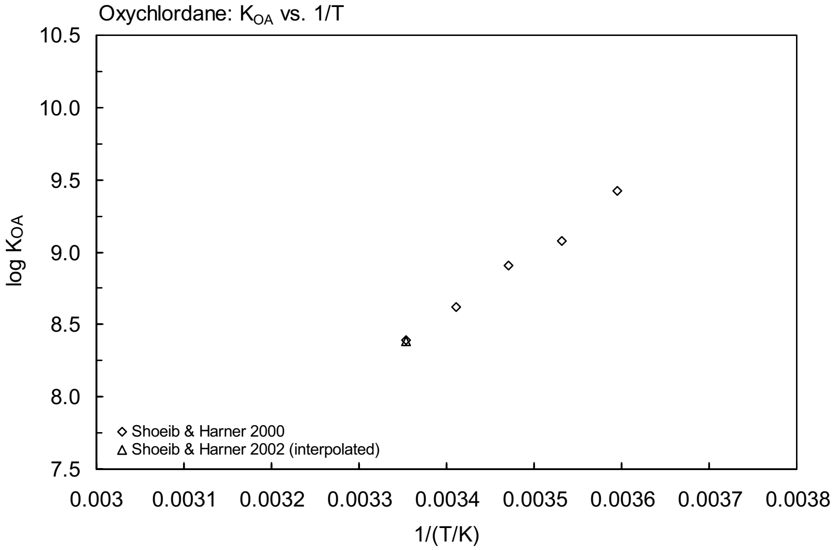
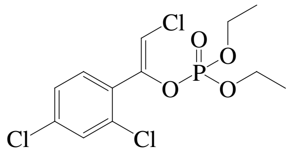


FIGURE 18.1.1.13.1C Logarithm of K_{OA} versus reciprocal temperature for oxychlordane.

18.1.1.14 Chlorfenvinphos



Common Name: Chlorfenvinphos
Synonym: Apachlor, Birlane, Clofenvenfos, GC 4092, Sapecron, SD 7859
Chemical Name: 2-chloro-1-(2,4-dichlorophenyl)vinyl diethyl phosphate; 2-chloro-1-(2,4-dichlorophenyl)ethenyl diethyl phosphate
Uses: soil application of insecticide to control root flies, root worms and other soil insects in vegetables; foliar application to control Colorado beetles on potatoes; scale insects and mite eggs on citrus fruit; stem borers and leafhoppers on rice, maize and sugar cane; and white flies on cotton; aside from control of mosquito larvae, it is also used as acaricide and animal ectoparasiticide.
CAS Registry No: 470-90-6 (*Z*)-isomer, 18708-87-7 (*E*)-isomer or *cis*-chlorfenvinphos, 18708-86-6 *trans*-chlorfenvinphos
Molecular Formula: $C_{12}H_{14}Cl_3O_4P$
Molecular Weight: 359.569
Melting Point (°C):
–19 (Lide 2003)
Boiling Point (°C):
167–170 (at 0.5 mmHg, Hartley & Kidd 1987; Tomlin 1994)
Density (g/cm^3 at 20°C):
1.36 (Hartley & Kidd 1987; Tomlin 1994)
Molar Volume (cm^3/mol):
321.4 (calculated-Le Bas method at normal boiling point)
Dissociation Constant, pK_a:
Enthalpy of Vaporization, ΔH_V (kJ/mol):
96.34 (Rordorf 1989)
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
Entropy of Fusion, ΔS_{fus} (J/mol K):
Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F: 1.0

Water Solubility (g/m^3 or mg/L at 25°C or as indicated):
145 (20°C, Melnikov 1971)
145 (Martin & Worthing 1977; Milne 1995)
145 (23°C, Khan 1980)
146 (20°C, Briggs 1981)
124 (20°C, shake flask-GC, Bowman & Sans 1983a, b)
145 (23°C, Hartley & Kidd 1987; Worthing & Walker 1987, 1991; Tomlin 1994)
130 (20°C, selected, Suntio et al. 1988)

Vapor Pressure (Pa at 25°C or as indicated and reported temperature dependence equations):
0.00053 (20°C, Khan 1980)
2.7×10^{-5} (Verschueren 1983)
0.0010 (Hartley & Kidd 1987; Tomlin 1994)
0.00010 (20°C, selected, Suntio et al. 1988)
8.20×10^{-4}, 1.70×10^{-2}, 0.22, 2.0, 14.0 (25, 50, 70, 100, 125°C, gas saturation-GC, Rordorf 1989)
$\log (P_L/Pa) = 13.794 - 5032.8/(T/K)$; measured range 36.9–129°C (liquid, gas saturation-GC, Rordorf 1989)
0.00053 (20°C, Worthing & Hance 1991)
8.91×10^{-4}; 1.35×10^{-3}, 0.0038 (gradient GC method; estimation using modified Watson method: Sugden's parachor, McGowan's parachor, Tsuzuki 2000)

Henry's Law Constant (Pa·m^3/mol at 25°C or as indicated and reported temperature dependence equations):

0.00028 (20°C, calculated-P/C, Suntio et al. 1988)
0.00029 (calculated-P/C, this work)
0.324 (20°C, selected from literature experimentally measured data, Staudinger & Roberts 2001)
log K_{AW} = 0.173 – 1187/(T/K) (van't Hoff eq. derived from literature data, Staudinger & Roberts 2001)

Octanol/Water Partition Coefficient, log K_{OW}:

3.23	(shake flask-UV, Lord et al. 1980)
3.10	(20°C, shake flask-GC, Briggs 1981)
3.81	(shake flask-GC, Bowman & Sans 1983)
3.84	(shake flask, Eadsforth & Moser 1983)
3.79	(HPLC-RT correlation method, Eadsforth & Moser 1983)
3.56	(RP-HPLC-RT correlation, Sicbaldi & Finizio 1993)
3.81	(recommended, Sangster 1993)
3.85, 4.22	(*Z*) isomer, (*E*) isomer, Tomlin 1994)
3.10	(recommended, Hansch et al. 1995)
3.56	(RP-HPLC-RT correlation, Finizio et al. 1997)

Bioconcentration Factor, log BCF:

1.57	(calculated-S, Kenaga 1980)
2.30	(earthworms, Lord et al. 1980; quoted, Connell & Markwell 1990)

Sorption Partition Coefficient, log K_{OC}:

2.45 (calculated-S, Kenaga 1980)
2.47 (soil, sorption isotherm, converted from reported log K_{OM} of 2.23, Briggs 1981)
2.77 (soil, calculated-MCI χ and fragment contribution, Meylan et al. 1992)
2.47 (soil, calculated-MCI $^1\chi$, Sabljic et al. 1995)
2.47; 2.42, 3.04 (soil, *cis*-chlorfenvinphos, quoted exptl.; estimated-class-specific model, estimated-general model, Gramatica et al. 2000)
2.47; 2.40, 3.11 (soil, *trans*-chlorfenvinphos, quoted exptl.; estimated-class-specific model, estimated-general model, Gramatica et al. 2000)

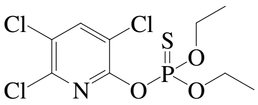
Environmental Fate Rate Constants, k, or Half-Lives, $t_{½}$:

Hydrolysis: at 38°C: $t_{½}$ > 700 h at pH 1.1 and $t_{½}$ > 400 h at pH 9.1; $t_{½}$ = 1.28 h at pH 13 and 20°C (Tomlin 1994).

Half-Lives in the Environment:

Soil: $t_{½}$ > 24 wk in sterile sandy loam and $t_{½}$ < 1.0 wk in nonsterile sandy loam; $t_{½}$ > 24 wk in sterile organic soil and $t_{½}$ = 1.0 wk in nonsterile organic soil (Miles et al. 1979).

18.1.1.15 Chlorpyrifos



Common Name: Chlorpyrifos

Synonym: Brodan, Chlorpyrifos-ethyl, Detmol UA, Dowco 179, Dursban, ENT 27311, Eradex, Killmaster, Lorsban, NA 2783, OMS 971, Pyrinex

Chemical Name: *O,O*-diethyl *O*-3,5,6-trichloro-2-pyridyl phosphorothioate; *O,O*-diethyl *O*-(3,5,6-trichloro-2-pyridinyl) phosphorothioate

Uses: insecticide used to control insects on a wide variety of crops including fruits, vegetables, ornamentals and trees.

CAS Registry No: 2921-88-2

Molecular Formula: $C_9H_{11}Cl_3NO_3PS$

Molecular Weight: 350.586

Melting Point (°C):

42	(Lide 2003)

Boiling Point (°C):

Density (g/cm^3 at 20°C):

Molar Volume (cm^3/mol):

298.8	(calculated-Le Bas method at normal boiling point)

Dissociation Constant, pK_a:

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

25.94	(DSC method, Plato & Glasgow 1969)

Entropy of Fusion, ΔS_{fus} (J/mol K):

Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F: 0.681 (mp at 42°C)

Water Solubility (g/m^3 or mg/L at 25°C or as indicated):

0.40, 0.47	(23, 25°C, Brust 1966)
2.0	(Spencer 1973; Windholz 1983; Hartley & Kidd 1987; Worthing & Walker 1987, Worthing & Hance 1991; Milne 1995)
1.12	(shake flask-GC, Felsot & Dahm 1979)
0.70. 0.73	(19, 20°C, shake flask-GC, Bowman & Sans 1979)
0.30	(23°C, Kenaga 1980a, b)
0.30	(Dow Chemical Data, Kenaga & Goring 1980)
2.00	(35°C, Khan 1980)
2.00	(20–25°C, Willis & McDowell 1982)
0.40	(Verschueren 1983)
0.73	(20°C, shake flask-GC, Bowman & Sans 1983a, b)
1.07, 0.42	(generator column, RP-HPLC-RT correlation, Swann et al. 1983)
0.30	(Kanazawa 1989)
0.40	(20–25°C, selected, Wauchope et al. 1992; Hornsby et al. 1996)
1.93	(Racke 1993)
0.73, 1.30	(20°C, 30°C, Montgomery 1993)
1.40	(Tomlin 1994)
1.18	(quoted lit., Armbrust 2000)
1.61, 1.94	(supercooled liquid S_L: literature-derived value LDV, final adjusted value FAV, Muir et al. 2004)

Vapor Pressure (Pa at 25°C at 25°C or as indicated):

0.00145	(20°C, Eichler 1965; Wolfdietrich 1965)
0.0025	(Brust 1966; Neely & Blau 1977)
0.0037	(Hamaker 1975)
0.00253	(Melnikov 1971)
0.0104	(30°C, NIEHS 1975)
0.0012	(20°C, Hartley & Graham-Bryce 1980)

0.00088 (20°C, GC-RT correlation without mp correlation, Kim et al. 1984; Kim 1985)
0.00052 (20°C, GC-RT with mp correction, Kim et al. 1984; Kim 1985)
0.0025 (Hartley & Kidd 1987; Worthing & Hance 1991; Montgomery 1993)
0.0015 (20°C, selected, Suntio et al. 1988)
0.0067 (supercooled liquid P_L, GC-RT correlation method, Hinckley et al. 1990)
0.0022; 0.0040 (liquid P_L, GC-RT correlation; quoted lit., Donovan 1996)
0.0023 (20–25°C, selected, Wauchope et al. 1992; Hornsby et al. 1996)
0.0022 (gradient GC method, Tsuzuki 2000)
2.18×10^{-3}; 1.86×10^{-3}, 0.00407 (gradient GC method; estimation using modified Watson method: Sugden's parachor, McGowan's parachor, Tsuzuki 2000)
0.0038, 0.0031 (supercooled liquid P_L: literature-derived value LDV, final adjusted value FAV, Muir et al. 2004)

Henry's Law Constant (Pa·m^3/mol at 25°C and reported temperature dependence equations):

1.0 (Mackay 1985)
1.75 (20°C, calculated-P/C, Suntio et al. 1988)
0.418 (calculated-P/C, Fendinger & Glotfelty 1990; Fendinger et al. 1990)
7.902 (calculated-P/C, Howard 1991)
4.06×10^{-3} (calculated-bond contribution method LWAPC, Meylan & Howard 1991)
0.421 (23°C, quoted, Schomburg et al. 1991)
0.421 (calculated-P/C, Montgomery 1993)
0.317, 0.492 (20°C, distilled water, salt water 33.3l, wetted wall column-GC, Rice et al. 1997b)
$\log K_{AW} = -1187.0/(T/K) + 0.173$; temp range 8.3–43.5°C, (distilled water, wetted-wall column-GC, Rice et al. 1997b)
$\log K_{AW} = -916.0/(T/K) - 0.674$; temp range 8.3–43.5°C, (salt water solution, 33.3l NaCl, wetted-wall column-GC, Rice et al. 1997b)
0.366, 0.366; 0.390 (20°C, microlayer, subsurface natural water of salinity 17l and TOC 0.4–1.0 ppm, from Pt. Lookout, Chesapeake Bay; estimated value adjusted to salinity, Rice et al. 1997b)
0.341, 0.390; 0.390 (20°C, microlayer, subsurface natural water of salinity 16l and TOC 0.5–0.6 ppm, from Solomons, Chesapeake Bay; estimated adjusted to salinity, Rice et al. 1997b)
0.317, 0.341; 0.366 (20°C, microlayer, subsurface natural water of salinity 12l, TOC 0.6 ppm, from Sandy Point, Chesapeake Bay; estimated value adjusted to salinity, Rice et al. 1997b)
0.366, 0.414; 487 (20°C, microlayer, subsurface water of salinity 32l, TOC 2.2–46 ppm, ocean water from Bering/Chukchi Sea; estimated value adjusted to salinity, Rice et al. 1997b)
0.340, 0.414, 0.869 (8.3, 20, 43.5°C, subsurface water from Bering Sea, TOC 2.14 ppm, wetted-wall column-GC, Rice et al. 1997b)
0.284, 0.356; 0.738 (8.3, 20, 43.5°C, surface microlayer water from Bering Sea, TOC 3.14 ppm, wetted-wall column-GC, Rice et al. 1997b)
0.337, 0.424, 0.782 (8.3, 20, 43.5°C, subsurface water from Chukchi Sea, TOC 3.3 ppm, wetted-wall column-GC, Rice et al. 1997b)
0.294, 0.369; 0.750 (8.3, 20, 43.5°C, surface microlayer water from Chukchi Sea, TOC 45.5 ppm, wetted-wall column-GC, Rice et al. 1997b)
0.224, 0.268, 0.674 (8.3, 20, 43.5°C, melted surface ice from the Arctic Ocean, TOC 48.8 ppm, wetted-wall column-GC, Rice et al. 1997b)
$\log K_{AW} = -872/(T/K) - 0.775$; temp range 8.3–43.5°C, (ocean water from the Chukchi Sea, wetted-wall column-GC, Rice et al. 1997b)
$\log K_{AW} = -633/(T/K) - 1.665$; temp range 8.3–43.5°C, (surface microlayer of ocean water from the Chukchi Sea, wetted-wall column-GC, Rice et al. 1997b)
0.74 (quoted lit., Armbrust 2000)
1.090 (calculated-P/C, this work)
0.472, 0.568 (literature-derived value LDV, final adjusted value FAV, Muir et al. 2004)

Octanol/Water Partition Coefficient, $\log K_{OW}$:

5.11 (20°C, shake flask-GC, Chiou et al. 1977; Freed et al. 1977, 1979)
4.99 (Kenaga 1980b; Kenaga & Goring 1980)
4.82 (Veith et al. 1979)

4.67, 4.77 (RP-HPLC correlation, McDuffie 1981)
4.96 (22°C, shake flask-GC, Bowman & Sans 1983b)
5.20 (shake flask-GC, Schimmel et al. 1983)
4.77 (HPLC-RT correlation, De Kock & Lord 1987)
5.14 (HPLC-RT correlation, Liu & Qian 1988)
5.267 (shake flask/slow-stirring method, De Bruijn et al. 1989)
4.70 (Worthing & Hance 1991; Tomlin 1994; Milne 1995)
3.31–5.27 (Montgomery 1993)
4.73 (RP-HPLC, Saito et al. 1993)
3.99 (RP-HPLC-RT correlation, Sicbaldi & Finizio 1993)
4.96 (recommended, Sangster 1993)
5.25 (shake flask-HPLC, Ankley et al. 1994)
5.27 (recommended, Hansch et al. 1995)
4.96 (RP-HPLC-RT correlation using short ODP column, Donovan & Pescatore 2002)
5.11 (literature-derived value LDV, Muir et al. 2004)

Octanol/Air Partition Coefficient, log K_{OA}:
8.75 (final adjusted value FAV, Muir et al. 2004)

Bioconcentration Factor, log BCF:
2.67 (rainbow trout, Neely & Blau 1977; quoted, McLeese et al. 1976)
2.67 (mosquito fish for 35-d exposure, Veith et al. 1979; Veith & Kosian 1983)
2.65, 2.51 (fish: flowing water, static water; Kenaga 1980b; Kenaga & Goring 1980)
3.09; 3.04 (calculated-S; calculated-K_{OC}, Kenaga 1980a)
–1.70 (average beef fat diet, Kenaga 1980b)
2.67 (mosquito fish for 30-d exposure, Veith et al. 1980)
2.65; 2.38 (quoted exptl., calculated-K_{OW}, Briggs 1981)
3.54 (estimated-regression from log K_{OW}, Lyman et al. 1982)
3.08 (estimated-regression from S, Lyman et al. 1982; quoted, Howard 1991)
3.50 (calculated-K_{OW}, Mackay 1982)
2.67 (mosquito fish, Veith & Kosian 1983)
–3.55 (beef biotransfer factor log B_b, correlated-K_{OW} from Kenaga 1980, Travis & Arms 1988)
–4.73 (milk biotransfer factor log B_m, correlated-K_{OW} from McKellar et al. 1976, Travis & Arms 1988)
2.67; 2.51 (rainbow trout; mosquito fish, wet wt. basis, De Bruijn & Hermens 1991)
4.32 (stickleback, lipid-based lab data, Deneer 1994)
2.68 (Pait et al. 1992)

Sorption Partition Coefficient, log K_{OC}:
4.13 (soil, quoted from Dow Chemical Data, Kenaga 1980a, b; Kenaga & Goring 1980)
3.93 (calculated-S as per Kenaga & Goring 1978, Kenaga 1980)
3.78 (average of 3 soils, HPLC-RT correlation, McCall et al. 1980)
3.96, 4.87 (estimated-S, calculated-S and mp, Karickhoff 1981)
2.92, 4.43, 4.72 (estimated-K_{OW}, Karickhoff 1981)
4.11 (soil, Thomas 1982; quoted, Nash 1988)
3.79, 4.0 (soil slurry method, RP-HPLC, Swann et al. 1983)
1.61 (av. value calculated from Freundlich coeffs. without Baldwin Lake site data, Corwin & Farmer 1984)
3.35 (calculated-MCI χ, Gerstl & Helling 1987)
3.78 (soil, screening model calculations, Jury et al. 1987b)
3.27 (average of 2 soils, Kanazawa 1989)
3.78 (soil, 20–25°C, selected, Wauchope et al. 1992)
3.77–4.13 (Montgomery 1993)
3.93 (average, Racke 1993)
4.37 (selected, Lohninger 1994)
3.70 (soil, calculated-MCI $^1\chi$, Sabljic et al. 1995)

3.46 (sediment, estimated, Paraiba et al. 1999)
3.78 (soil, 20–25°C, recommended, Hornsby et al. 1996)
4.00 (quoted lit., Armbrust 2000)
3.70; 3.83, 3.76 (soil, quoted obs.; estimated-class-specific model, estimated-general model using molecular descriptors, Gramatica et al. 2000)
3.62, 3.63 (soils: organic carbon OC ≥ 0.1%, OC ≥ 0.5%, average, Delle Site 2001)
3.46–4.23 (sediments of San Diego Creek and Bonita Creek, shake flask-GC, Bondarenko & Gan 2004)

Sorption Partition Coefficient, log K_{OM}:
3.42 (Felsot & Dahm 1979)
3.78 (average of 3 soils, McCall et al. 1980)
3.90 (exptl., Briggs 1981)
3.10–4.31 (Mingelgrin & Gerstl 1983)
4.24 (quoted, Karickhoff 1985; Neely & Blau 1985)
4.50 (best estimate at low sediment concn., Karickhoff 1985)
4.13, 3.74 (selected, estimated, Magee 1991)

Environmental Fate Rate Constants, k, or Half-Lives, $t_{1/2}$:

Volatilization: based on Henry's law constant, $t_{1/2}$ ~ 9.0 d for a model river 1 m deep, flowing 1 m/s with a wind velocity of 3 m/s (Howard 1991);
initial $k = 8.8 \times 10^{-2}\ h^{-1}$ and predicted $k = 1.3 \times 10^{-3}\ h^{-1}$ from soil with $t_{1/2}$ = 533 h (Thomas 1982);
$t_{1/2}$ = 0.3–3.2 d for disappearance from an inert surface at 25°C (Meikle et al. 1983).

Photolysis: $t_{1/2}$(exptl) = 22 d determined under midday summer sunlight in California (Meikle et al. 1983; quoted, Howard 1991)
$k_P = (2.19 \pm 0.17) \times 10^{-2}\ h^{-1}$, $(2.09 \pm 0.17) \times 10^{-2}\ h^{-1}$ at different initial solute concentrations in aqueous solution at pH 7.0 and 25°C irradiated with a 450-W Hanovia mercury arc lamp. Under various environmental conditions, the estimated $t_{1/2}$ = 31 d at a depth of 0.001 cm, $t_{1/2}$ = 43 d at a depth of 1-m pure water, $t_{1/2}$ = 2.7 yr at 1-m depth river water for midsummer conditions; $t_{1/2}$ = 345 d at a depth of 1-m pure water under midwinter surface conditions, all at pH 2 at 40°N latitude, with average light attenuation (Dilling et al. 1984; quoted, Howard 1991; Montgomery 1993)

Oxidation: photooxidation $t_{1/2}$ = 6.34 h for the vapor phase reaction with OH radical in air (Howard 1991).

Hydrolysis:
$t_{1/2}$ = 53 d at pH 7.4 and 20°C (NIEHS 1975; quoted, Freed et al. 1977, 1979);
$t_{1/2}$ = 120 d at pH 6.1 and $t_{1/2}$ = 53 d at pH 7.4 in water and soil at 20°C as per Ruzicka et al. 1967 using GC-RT correlation for hydrolysis rates determination (Freed et al. 1979; quoted, Montgomery 1993)
k(alkaline) = $0.1\ M^{-1}\ s^{-1}$, k(neutral) = $1 \times 10^{-7}\ s^{-1}$, 10^{-7}–10^{-9} M in aqueous buffer at 20°C (Harris 1982)
$k = (1.08 - 2.0) \times 10^{-3}\ h^{-1}$ corresponding to half-lives of 13–27 d at pH 7 buffer solution and 25°C (Dilling et al. 1984)
$t_{1/2}$ = 78 d relatively independent of pH 1 to 7 (Macalady & Wolfe 1983; quoted, Howard 1991)
$t_{1/2}$ = 1.5 d in water at pH 8 and 25°C (Worthing & Hance 1991; Tomlin 1994)

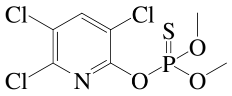
Hydrolytic k(acidic) < 0.008 d^{-1} in acidic soils with pH ≤ 7.0, corresponding to $t_{1/2}$ = 92–341 d and k(alkaline) = (0.006 – 0.063) d^{-1} in alkaline soils corresponding to $t_{1/2}$ = 11–200 d in abiotic hydrolysis in 37 different soils with pH 3.8–8.5. (Racke et al. 1996)
$k = 0.0009\ d^{-1}$ at pH 5, $k = 0.023\ d^{-1}$ at pH 7, $k = 0.044\ d^{-1}$ at pH 9; measured hydroxy radical rate constant for chlorpyrifos $1.3 \times 10^{13}\ M^{-1}\ h^{-1}$ (Armbrust 2000).

Biodegradation:
$k = 0.014\ d^{-1}$ in soil at 28°C (Miles et al. 1979; quoted, Klečka 1985)
k = 0.008–0.025 d^{-1} in soil at 25°C (Getzin 1981; quoted, Klečka 1985)
k = (–000945 to –0.00243) h^{-1} in nonsterile sediment and k = (–0.000562 to –0.00151) h^{-1} in sterile sediment by shake-tests at Range Point and also k = (–0.00109 to –0.00231) h^{-1} in nonsterile water and k = (–0.00144 to –0.00197) h^{-1} in sterile water by shake-tests at Range Point (Walker et al. 1988)
$t_{1/2}$ = 39–51 d in loamy and clay soils under anaerobic conditions, $t_{1/2}$ = 150–200 d in anaerobic pond sediments (Racke 1993)
k(aerobic) = $9.47 \times 10^{-4}\ h^{-1}$ for exposure analysis (Armbrust 2000).

Biotransformation:
Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants:
elimination $t_{½}$ = 3.3 d in channel catfish (Barron et al. 1991)
k_1 = 7000 ± 2000) L kg^{-1} d^{-1} (guppy, lipid-based modeling data, Deneer 1993)
k_2 = (0.40 ± 0.11) d^{-1} (guppy, lipid-based modeling data, Deneer 1993)
k_1 = (26 ± 8.0) × 10^3 L kg^{-1} d^{-1} (stickleback, lipid-based lab data, Deneer 1994).
k_2 = (1.2 ± 0.4) d^{-1} (stickleback, lipid-based lab data, Deneer 1994).

Half-Lives in the Environment:
Air: $t_{½}$ = 6.34 h for the vapor phase reaction with hydroxyl radicals in air (Atkinson 1987; quoted, Howard 1991); reaction rate k = 4.77 × 10^{-4} min^{-1} in air (Paraiba et al. 1999).
Surface water: based on Henry's law constant, volatilization $t_{½}$ ~ 9.0 d for a model river 1-meter deep, flowing 1 m/s with a wind velocity of 3 m/s (Lyman et al. 1982; quoted, Howard 1991);
half-lives of a 100 mL pesticide-seawater solution containing 10 g of sediment were: $t_{½}$< 2.0 d, indoor at 25°C with 12-h photo-period white fluorescent light, $t_{½}$ = 4.6 d, outdoor-light (stoppered, Pyrex flasks exposed to ambient sunlight with temperature 22–45°C), $t_{½}$ = 7.1 d, outdoor-dark (foil-covered flasks) and $t_{½}$ = 24 d in an estuary (Schimmel et al. 1983; quoted, Montgomery 1993)
$t_{½}$ = 120 d in water at pH 6.1, 20°C (quoted, Lartiges & Garrigues 1995);
reaction rate k = 3.80 × 10^{-4} min^{-1} in water (Paraiba et al. 1999).
Ground water:
Sediment: $t_{½}$ = 24 d in 10 g untreated sediment/100 mL of a pesticide-seawater solution and $t_{½}$ > 28 d in 10 g sterile sediment/100 mL of a pesticide-seawater solution (Schimmel et al. 1983)
$t_{½}$ = 150–200 d in anaerobic pond sediments (Racke 1993)
reaction rate k = 2.85 × 10^{-5} min^{-1} in sediment (Paraiba et al. 1999)
First-order degradation k = 0.034 d^{-1} with $t_{½}$ = 20.3 d under aerobic conditions, k = 0.003 d^{-1} with $t_{½}$ = 223 d under anaerobic conditions in sediment from San Diego Creek, Orange County, CA; first-order degradation k = 0.029 d^{-1} with $t_{½}$ = 23.7 d under aerobic conditions, k = 0.012 d^{-1} with $t_{½}$ = 57.6 d under anaerobic conditions in sediment from Bonita Creek, Orange County, CA (Bondarendo & Gan 2004)
Soil: $t_{½}$ = 17.0 wk in sterile sandy loam and $t_{½}$ < 1.0 wk in nonsterile sandy loam; $t_{½}$ > 24 wk in sterile organic soil and $t_{½}$ = 2.5 wk in nonsterile organic soil (Miles et al. 1979);
$t_{½}$ = 12 and 24 wk in a silt loam and clay loam, $t_{½}$ = 24 wk while in sterilized soils; however, temperature also had noticeable effects on decomposition as $t_{½}$ = 25, 13, and 6 wk for soil samples incubated at 15, 25, and 35°C, respectively (Getzin 1981a; quoted, Montgomery 1993);
hydrolysis $t_{½}$ = 8 d in Sultan silt loam (Getzin 1981b; quoted, Montgomery 1993);
$t_{½}$ = 80–100 d slowly degraded in soil (Hartley & Kidd 1987; quoted, Montgomery 1993);
$t_{½}$ = 63 d from screening model calculations (Jury 1987b);
persists in soil for 60–120 d (Worthing & Hance 1991);
Selected field $t_{½}$ = 30 d (Wauchope et al. 1992; quoted, Dowd et al. 1993; Richards & Baker 1993; Hornsby et al. 1996);
$t_{½}$ = 30 d (Pait et al. 1992);
Field dissipation $t_{½}$ = 39–51 d in loamy and clay soils under anaerobic conditions; and aerobic solid degradation $t_{½}$ = 5–141 d (Racke 1993)
$t_{½}$ = of 60–120 d (Tomlin 1994)
Dissipation $t_{½}$ ≤ 7 d when applied to dry soils or the soil surface ($t_{½}$ = 7–14 d); and $t_{½}$ = 30–60 d when incorporated into the soil profile (Racke et al. 1996)
First order rate constants for photolytic decline in sandy soil: k = 2.91 × 10^{-3} h^{-1} with $t_{½}$ = 240 h irradiated in moisture-maintained, k = 2.06 × 10^{-3} h^{-1} with $t_{½}$ = 340 h, irradiated in air-dried k = 1.67 × 10^{-3} h^{-1} with $t_{½}$ = 420 h in dark control moist and k = 0.99 × 10^{-3} h with $t_{½}$ = 700 h in dark control air-dried sandy soil from Sauk County, WI. The photolytic k = 8.43 × 10^{-4} h^{-1} with $t_{½}$ = 820 h in moist soil, k = 1.07 × 10^{-3} h^{-1} with $t_{½}$ = 650 h in dry soil. The contribution of moisture to irradiated metabolism k = 1.24 × 10^{-3} h^{-1} with $t_{½}$ = 560 h, but for dark control system for k = 6.78 × 10^{-4} h^{-1} with $t_{½}$ = 1020 h (Graebing & Chib 2004)
Biota: $t_{½}$ = 335 h clearance from fish (Neely 1980);
biochemical $t_{½}$ = 63 d from screening model calculations (Jury et al. 1987b);
elimination $t_{½}$ ~ 3.3 d in channel catfish (Barron et al. 1991)

18.1.1.16 Chlorpyrifos-methyl



Common Name: Chlorpyrifos-methyl
Synonym: Reldan
Chemical Name: *O,O*-dimethyl *O*-3,5,6-trichloro-2-pyridyl phosphorothioate
Uses: insecticide
CAS Registry No: 5598-13-0
Molecular Formula: $C_7H_7Cl_3NO_3PS$
Molecular Weight: 322.534
Melting Point (°C):

43	(Lide 2003)

Boiling Point (°C):
Density (g/cm^3):
Acid Dissociation Constant, pK$_a$:
Molar Volume (cm^3/mol):
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
Entropy of Fusion, ΔS_{fus} (J/mol K):
Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F: 0.666 (mp at 43°C)

Water Solubility (g/m^3 or mg/L at 25°C):

4.76	(20°C, shake flask-GC, Chiou et al. 1977)
0.40	(Spencer 1982)
4.0	(Kenaga 1980a, b, Kenaga & Goring 1980)
3.2	(20°C, shake flask, Bowman & Sans 1983b)
4.0	(24°C, Hartley & Kidd 1987; Tomlin 1994)
4.0	(selected, 20–25°C, Augustijn-Beckers et al. 1994; Hornsby et al. 1996)

Vapor Pressure (Pa at 25°C):

5.63×10^{-3}	(Spencer 1982, Hartley & Kidd 1987; Tomlin 1994)
5.60×10^{-3}	(selected, Augustijn-Beckers et al. 1994; Hornsby et al. 1996)

Henry's Law Constant (Pa·m^3/mol at 25°C):

Octanol/Water Partition Coefficient, log K_{OW}:

4.31	(shake flask-GC, Chiou et al. 1977)
4.17	(Kenaga 1980a; Kenaga & Goring 1980)
3.29, 4.30	(Rao & Davidson 1980)
4.30	(shake flask-concn ratio-GC; Bowman & Sans 1983b)
4.31	(recommended, Sangster 1993)
3.99	(HPLC-RT correlation, Sicbaldi & Finizio 1993)
4.24	(Tomlin 1994)
4.31	(recommended, Hansch et al. 1995)

Octanol/Air Partition Coefficient, log K_{OA}:

Bioconcentration Factor, log BCF or log K_B:

1.98	(fish, static water, Kenaga & Goring 1980)
2.45, 2.36	(calculated-solubility, K_{OW}, Kenaga 1980b)
1.98	(fish, microcosm conditions, Garten & Trabalka 1983)

Sorption Partition Coefficient, log K_{OC}:

3.52	(soil, Kenaga 1980a; Kenaga & Goring 1980)
3.30	(soil, calculated, Kanga 1980b)
3.76	(soil, Sabljic 1987)
3.48	(estimated, soil, Augustijn-Beckers et al. 1994; Hornsby et al. 1996)
3.52	(soil, calculated-MCI χ, Sabljic et al. 1995)

3.52; 3.36, 3.49 (soil, estimated-class-specific model, estimated-general model using molecular descriptors, Gramatica et al. 2000)

Environmental Fate Rate Constant and Half-Lives, $t_{½}$:

Volatilization:

Photolysis: under goes rapid photodecomposition in UV light (Spencer 1982).

Photooxidation:

Hydrolysis: relatively stable under neutral conditions, but hydrolyzed by acids (pH 4–6) and, more readily by alkalis (pH 8–10), $t_{½}$ = 3 d at pH 8 (Tomlin 1994)

Biodegradation:

Biotransformation:

Bioconcentration and Uptake and Elimination Rate Constants (k_1 and k_2):

Half-Lives in the Environment:

Air:

Surface water: estimated $t_{½}$ ~ 38 d in buffered water at pH 6 (Spencer 1982);
relatively stable under neutral conditions, but hydrolyzed by acids (pH 4–6) and, more readily by alkalis (pH 8–10), $t_{½}$ = 3 d at pH 8 (Tomlin 1994).

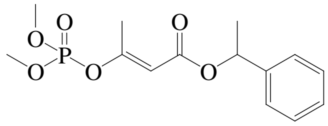
Ground water:

Sediment:

Soil: field $t_{½}$ = 7 d (Augustjin-Beckers et al. 1994; Hornsby et al. 1996);
$t_{½}$ = 1.5 and 33 d depending upon soil type and microbial activity (Tomlin 1994).

Biota:

18.1.1.17 Crotoxyphos



Common Name: Crotoxyphos
Synonym: Ciodrin, Ciovap, Cyodrin, Cypona EC, Decrotox, Duo-kill, Duravos, ENT 24717, Volfazol
Chemical Name: dimethyl(*E*)-1-methyl-2-(1-phenyl-ethoxycarbonyl)vinyl phosphate
Uses: insecticide
CAS Registry No: 7700-17-6
Molecular Formula: $C_{14}H_{19}O_6P$
Molecular Weight: 314.271
Melting Point (°C): liquid
Boiling Point (°C):
135 (at 0.03 mmHg, Montgomery 1993)
Density (g/cm^3 at 20°C):
1.2 (Spencer 1982)
1.19 (25°C, Montgomery 1993)
Molar Volume (cm^3/mol):
264.1 (calculated-density)
Dissociation Constant, pK_a:
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
Entropy of Fusion, ΔS_{fus} (J/mol K):
Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F: 1.0

Water Solubility (g/m^3 or mg/L at 25°C):
1000 (Günther et al. 1968)
1000 (Melnikov 1971; Spencer 1973, 1982;)
1000 (Martin & Worthing 1977; Worthing & Walker 1987; Montgomery 1993)

Vapor Pressure (Pa at 25°C or as indicated):
0.0019 (20°C, Khan 1980)
0.00187, 0.0052, 0.013 (20, 30, 40°C, Spencer 1982)
0.0019 (20°C, Montgomery 1993)

Henry's Law Constant (Pa·m^3/mol at 25°C or as indicated):
0.00063 (20–25°C, calculated-P/C, Montgomery 1993)
0.00060 (calculated-P/C, this work)

Octanol/Water Partition Coefficient, log K_{OW}:
3.00 (Callahan et la. 1979)
2.23 (Kenaga 1980)
3.30 (shake flask, Log P Database, Hansch & Leo 1987)
3.30 (selected, Sangster 1993)
3.30 (selected, Hansch et al. 1995)

Bioconcentration Factor, log BCF:
1.10 (calculated-S as per Kenaga 1980, this work)

Sorption Partition Coefficient, log K_{OC}:
2.23 (soil, Hamaker & Thompson 1972; Kenaga & Goring 1980)
2.00, 1.70 (soil, quoted exptl., calculated-MCI χ and fragment contribution, Meylan et al. 1992)
2.23 (Montgomery 1993)

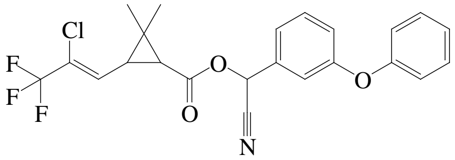
2.00 (soil, calculated-MCI $^1\chi$, Sabljic et al. 1995)
2.00; 2.07, 2.59 (soil, quoted obs.; estimated-class-specific model, estimated-general model using molecular descriptors, Gramatica et al. 2000)

Environmental Fate Rate Constants, k, or Half-Lives, $t_{½}$:

Half-Lives in the Environment:

Surface water: biodegradation $t_{½}$ = 7.5 d at pH 9 and $t_{½}$ = 22.5 d at pH 2 from river die-away tests (Konrad & Chester 1969; quoted, Scow 1982).

18.1.1.18 Cyhalothrin



Common Name: Cyhalothrin
Synonym: Grenade, cyhalothrine
Chemical Name: (*RS*)-α-cyano-3-phenoxybenzyl(*Z*)-(1*RS*,3*RS*)-(2-chloro-3,3,3-trifluoropropanyl)-2,2-dimethylcyclopropanecarboxylate
Uses: insecticide
CAS Registry No: 68085-85-8
Molecular Formula: $C_{23}H_{19}ClF_3NO_3$
Molecular Weight: 449.850
Melting Point (°C):
yellow to brown viscous oil (technical, Hartley & Kidd 1987; Tomlin 1994)
Boiling Point (°C):
187–190/0.2 mmHg (Hartley & Kidd 1987; Tomlin 1994)
Density (g/cm^3):
1.25 (25°C, Hartley & Kidd 1987; Tomlin 1994)
Acid Dissociation Constant, pK_a:
Molar Volume (cm^3/mol):
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
Entropy of Fusion, ΔS_{fus} (J/mol K):
Fugacity Ratio at 25°C, F: 1.0

Water Solubility (g/m^3 or mg/L at 25°C or as indicated):
< 1.0 (Worthing & Walker 1983)
0.003 (20°C, Hartley & Kidd 1987; Worthing & Walker 1987)
0.004 (20°C, Tomlin 1994)

Vapor Pressure (Pa at 25°C or as indicated):
$\sim 1.0 \times 10^{-6}$ (20°C, Hartley & Kidd 1987)
0.001×10^{-3} (20°C, Tomlin 1994)
1.90×10^{-5} (40°C, Knudsen effusion method, Goodman 1997)
$\log (P/Pa) = 13.47 - 5723/(T/K)$ (Antoine eq., measured range 45–85°C, Goodman 1997)
1.51×10^{-5} (P^S, GC-RT correlation, Tsuzuki 2001)

Henry's Law Constant (Pa·m^3/mol):

Octanol/Water Partition Coefficient, $\log K_{OW}$:
6.02 (HPLC-RT correlation, Hu & Leng 1992)
6.80 (20°C, Tomlin 1994)

Octanol/Air Partition Coefficient, $\log K_{OA}$:

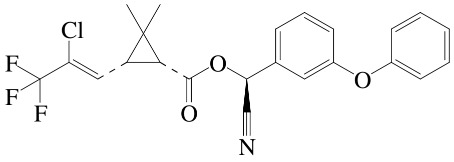
Bioconcentration Factor, log BCF or $\log K_B$:

Sorption Partition Coefficient, $\log K_{OC}$:

Environmental Fate Rate Constants, k, and Half-Lives. $t_{1/2}$:
Hydrolysis: slowly hydrolysed in sunlight at pH 7–9, more rapidly at pH >9 (Hartley & Kidd 1987; Tomlin 1994).

Half-Lives in the Environment:
Soil: $t_{1/2} \sim$ 4–12 wks (Hartley & Kidd 1987; Tomlin 1994)

18.1.1.19 Lambda-cyhalothrin



Common Name: lambda-cyhalothrin
Synonym: lambda-cyhalothrin
Chemical Name: equal quantities of (*S*)-α-cyano-3-phenoxybenzyl(*Z*)-(1*R*,3*R*)-3-(2-chloro-3,3,3-trifluoropropanyl)-2,2-dimethylcyclopropanecarboxylate and (*S*)-α-cyano-3-phenoxybenzyl(*Z*)-(1*S*,3*S*)-3-(2-chloro-3,3,3-trifluoropropanyl)-2,2-dimethylcyclopropanecarboxylate
Uses: insecticide
CAS Registry No: 91465-08-6
Molecular Formula: $C_{23}H_{19}ClF_3NO_3$
Molecular Weight: 449.850
Melting Point (°C):
49.2 (Hartley & Kidd 1987; Tomlin 1994; Lide 2003)
Boiling Point (°C):
Density (g/cm^3):
1.33 (25°C, Tomlin 1994)
Acid Dissociation Constant, pK_a:
Molar Volume (cm^3/mol):
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
Entropy of Fusion, ΔS_{fus} (J/mol K):
Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F: 0.579 (mp at 49.2°C)

Water Solubility (g/m^3 or mg/L at 25°C or as indicated):
0.005 (20°C, pH 6.5, Hartley & Kidd 1987)
0.005, 0.004 (pH 6.5 in purified water, pH 5.0 in buffered water Tomlin 1994)

Vapor Pressure (Pa at 25°C or as indicated and reported temperature dependence equations. Additional data at other temperatures designated *, are compiled at the end of this section):
2.0×10^{-7} (20°C, Hartley & Kidd 1987)
2.0×10^{-7}, 2.0×10^{-4} (20, 60°C, Tomlin 1994)
7.80×10^{-6}* (40°C, Wollerton & Husband 1988, quoted in Goodman 1997)
19×10^{-6}* (40°C, Knudsen effusion method, measured range 40–80°C, Goodman 1997)
1.88 (extrapolated-Antoine eq., Goodman 1997)
$\log (P/kPa) = 13.47 - 5723/(T/K)$; temp range 40–80°C (Antoine eq., Knudsen effusion, Goodman 1997)

Henry's Law Constant ($Pa{\cdot}m^3/mol$ at 25°C):

Octanol/Water Partition Coefficient, $\log K_{OW}$:
7.0 (20°C, Tomlin 1994)

Octanol/Air Partition Coefficient, $\log K_{OA}$:

Bioconcentration Factor, log BCF or $\log K_B$:

Sorption Partition Coefficient, $\log K_{OC}$:

Environmental Fate Rate Constants, k, and Half-Lives, $t_{½}$:

Half-Lives in the Environment:

Air:
Surface water:
Ground water:
Sediment: $t_{½}$ ~ 20 d in water-sediment mixture in sunlight (Tomlin 1994).
Soil: $t_{½}$ ~ 4–12 wk (Hartley & Kidd 1987; Tomlin 1994)
Biota:

TABLE 18.1.1.19.1
Reported vapor pressures of lambda-cyhalothrin at various temperatures and the coefficients for the vapor pressure equations

$\log P = A - B/(T/K)$ (1) $\ln P = A - B/(T/K)$ (1a)
$\log P = A - B/(C + t/°C)$ (2) $\ln P = A - B/(C + t/°C)$ (2a)
$\log P = A - B/(C + T/K)$ (3)
$\log P = A - B/(T/K) - C \cdot \log (T/K)$ (4)

Wollerton & Husband 1988		Goodman 1997	
quoted in Goodman 1997		Knudsen effusion	
t/°C	P/Pa	t/°C	P/Pa
40	7.8×10^{-6}	40	1.9×10^{-5}
50	4.0×10^{-5}	50	4.7×10^{-5}
60	1.9×10^{-4}	60	1.7×10^{-4}
70	8.2×10^{-4}	70	6.5×10^{-4}
80	3.2×10^{-3}	80	2.0×10^{-3}
		eq. 1	P/Pa
		A	13.47
		B	5723

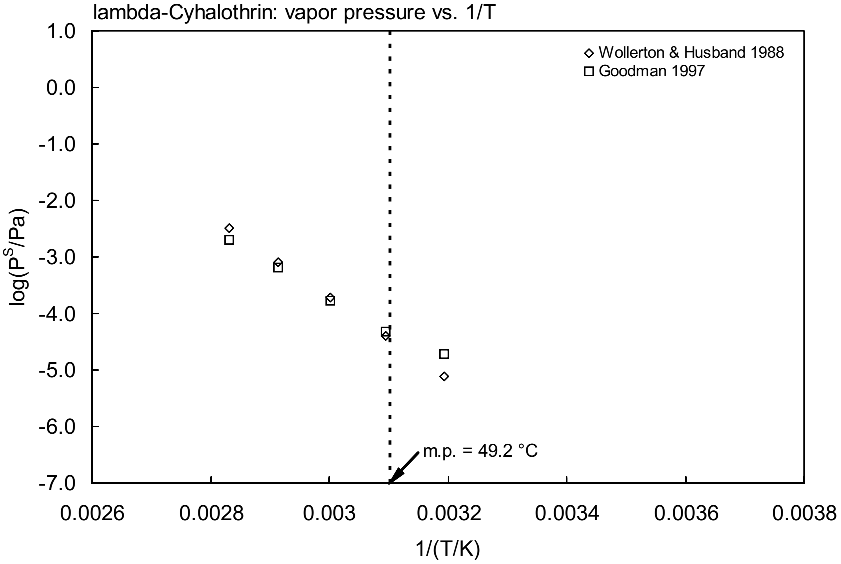
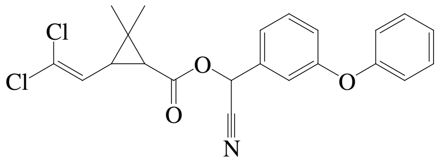


FIGURE 18.1.1.19.1 Logarithm of vapor pressure versus reciprocal temperature for lambda-cyhalothrin.

18.1.1.20 Cypermethrin



Common Name: Cypermethrin

Synonym: Agrothrin, Ambush C, Barricade, CCN 52, Cymbush, Cyperkill, Demon, FMC 30980, Folcord, Imperator, Kafil Super, Polytrin, Ripcord, Sherpa, Stocade, Toppel

Chemical Name: cyano(3-phenoxyphenyl)methyl 3-(2,2-dichloroethenyl)-2,2-dimethylcyclo-propanecarboxylate; (*RS*)-α-cyano-3-phenoxybenzyl(1*RS*,3*RS*;1*RS*,3*SR*)-3(2,2-dichlorovinyl)-2,2-dimethylcyclopropane-carboxylate

Uses: nonsystemic insecticide with contact and stomach action to control a wide range of insects in fruits, vegetables, vines, potatoes, cucurbits, capsicums, cereals, maize, soybeans, cotton, coffee, coca, rice, pecans, ornamentals and forestry, etc.; also used to control flies in animal houses and mosquitoes, cockroaches, houseflies and other pests in public health.

CAS Registry No: 52315-07-8

Molecular Formula: $C_{22}H_{19}Cl_2NO_3$

Molecular Weight: 416.297

Melting Point (°C):
70 (Lide 2003)

Boiling Point (°C):

Density (g/cm^3 at 20°C):
1.23 (Tomlin 1994)
1.25 (Milne 1995)

Molar Volume (cm^3/mol):
457.7 (calculated-Le Bas method at normal boiling point)
335.7 (calculated-density)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

Entropy of Fusion, ΔS_{fus} (J/mol K):

Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F: 0.362 (mp at 70°C)

Water Solubility (g/m^3 or mg/L at 25°C or as indicated):
0.041 (shake flask-GC, Coats & O'Donnell-Jefferey 1979)
0.005–0.01 (Stephenson 1982)
0.010 (20°C, Hartley & Kidd 1987)
0.01–0.2 (21°C, Worthing & Walker 1987)
0.004 (20–25°C, selected, Wauchope 1989; Wauchope et al. 1992; Hornsby et al. 1996)
0.004 (Montgomery 1993)
0.004 (at pH 7, Tomlin 1994)
0.009 (20°C, selected, Siebers & Mattusch 1996)

Vapor Pressure (Pa at 25°C or as indicated):
8.7×10^{-7} (Barlow 1978)
4.3×10^{-7} (gas saturation, Grayson et al. 1982)
$<1.3 \times 10^{-5}$ (Spencer 1982)
5.1×10^{-10} (70°C, Hartley & Kidd 1987)
2.4×10^{-6} (GC-RT correlation, supercooled liquid P_L, Hinckley et al. 1990)
1.9×10^{-7} (20–25°C, selected, Wauchope et al. 1992; Hornsby et al. 1996)
1.9×10^{-7} (20°C, extrapolated, Montgomery 1993)
2.3×10^{-7} (20°C, Tomlin 1994)
2.75×10^{-6}; 2.4×10^{-6}, 1.86×10^{-6}, 1.15×10^{-6} (liquid P_L, GC-RT correlation; quoted lit. values, Donovan 1996)
2.3×10^{-6} (20°C, selected, Siebers & Mattusch 1996)
3.23×10^{-6} (solid P^S, converted from P_L by GC-RT correlation, Tsuzuki 2001)

Henry's Law Constant (Pa·m^3/mol) at 25°C or as indicated:

0.0199 (20–25°C, calculated-P/C, Montgomery 1993)
0.0194 (20–25°C, calculated-P/C as per Wauchope et al. 1992, Majewski & Capel 1995)
0.080 (selected, Siebers & Mattusch 1996)
0.0195 (calculated-P/C, this work)

Octanol/Water Partition Coefficient, log K_{OW}:

4.47 (shake flask-GC, Coats & O'Donnell-Jefferey 1979)
5.90 (Schimmel et al. 1983)
5.2 ± 0.6 (*cis*-form, HPLC-RT correlation, Muir et al. 1985)
5.0 ± 0.6 (*trans*-form, HPLC-RT correlation, Muir et al. 1985)
6.60 (Montgomery 1993)
4.47, 6.0 (quoted, Sangster 1993)
6.60 (Tomlin 1994)
6.60 (Milne 1995)
6.05, 6.05 (α-, β-isomer, Hansch et al. 1995)
5.56, 6.35, 5.60 (RP-HPLC correlation, ClogP, calculated-S, Finizio et al. 1997)
5.62 (RP-HPLC-RT correlation using short ODP column, Donovan & Pescatore 2002)

Bioconcentration Factor, log BCF:

2.99 (activated sludge, Freitag et al. 1984)
3.52, 2.62, 2.99 (algae, golden ide, activated sludge, Freitag et al. 1985)
1.73–2.34 (*trans*-form on sediment, 24 h BCF for chironomid larvae in water, Muir et al. 1985)
1.63–2.39 (*trans*-form on sediment, 24 h BCF for chironomid larvae in sediment, Muir et al. 1985)
1.49–2.05 (*trans*-form on sediment, 24 h BCF for chironomid larvae in sediment/pore water, Muir et al. 1985)
1.53–2.38 (*cis*-form on sediment, 24 h BCF for chironomid larvae in water, Muir et al. 1985)
1.84–2.59 (*cis*-form on sediment, 24 h BCF for chironomid larvae in sediment, Muir et al. 1985)
1.68–2.02 (*cis*-form on sediment, 24 h BCF for chironomid larvae in sediment/pore water, Muir et al. 1985)
2.89 (*Oncorhynchus mykiss*, Muir et al. 1994; quoted, Devillers et al. 1996)
2.92 (*Oncorhynchus mykiss*, Muir et al. 1994; quoted, Devillers et al. 1996)

Sorption Partition Coefficient, log K_{OC}:

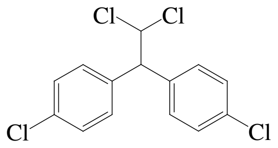
2.36 (*cis*-form, silt, K_P on 24% DOC, Muir et al. 1985)
2.57 (*cis*-form, clay, K_P on 56% DOC, Muir et al. 1985)
2.59 (*trans*-form, silt, K_P on 10% DOC, Muir et al. 1985)
5.00 (soil, 20–25°C, estimated, Wauchope et al. 1992; quoted, Lohninger 1994; Hornsby et al. 1996)
4.0–4.53 (Montgomery 1993)
5.54 (sediments, Maund et al. 2002)

Environmental Fate Rate Constants, k, or Half-Lives, $t_{1/2}$:

Half-Lives in the Environment:

Air:
Surface water: $t_{1/2}$ = 5 d in river water (Tomlin 1994).
Ground water:
Sediment:
Soil: estimated field $t_{1/2}$ = 30 d (Wauchope et al. 1992; Hornsby et al. 1996).
Biota:

18.1.1.21 DDD



Common Name: DDD
Synonym: dichloro diphenyl dichloroethane; *p,p′*-DDD; Dilene; ENT 4225; ME 1700; NCI-C00475; Rhothane; *p,p′*-TDE; TDE; tetrachlorodiphenylethane
Chemical Name: 1,1-dichloro-2,2-bis(4-chlorophenyl)ethane; 1,1′-(2,2-dichloroethylidene)bis[4-chlorobenzene
Uses: degradation product of DDT used as insecticide.
CAS Registry No: 72-54-8 (*p,p′*-DDD or DDD); 53-10-0 (*o,p′*-DDD)
Molecular Formula: $C_{14}H_{10}Cl_4$
Molecular Weight: 321.041
Melting Point (°C):
109.5 (Ballschmiter & Wittlinger 1991; Kühne et al. 1995; Lide 2003)
Boiling Point (°C):
Density (g/cm^3 at 20°C):
Molar Volume (cm^3/mol):
312.6 (calculated-LeBas method at normal boiling point)
246.4 (Ruelle & Kesselring 1997; Passivirta et al. 1999)
Dissociation Constant, pK_a:
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
30.96 (DSC method, Plato & Glasgow 1969)
27.313 (Ruelle & Kesselring 1997)
Entropy of Fusion, ΔS_{fus} (J/mol K):
81.17 (Plato & Glasgow 1969; Hinckley et al. 1990)
Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F: 0.148 (mp at 109.5°C)

Water Solubility (g/m^3 or mg/L at 25°C and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):
0.002 (shake flask-LSC, Metcalf et al. 1973)
0.005, 0.015, 0.09* (shake flask-GC with particle sizes: 0.01, 0.05, 5.0 micron, Biggar & Riggs 1974)
0.24 (*p, p′*-DDD shake flask-GC, *o, p′*-DDD with particle sizes: 0.05 micron, Biggar & Riggs 1974)
0.060, 0.10, 0.25, 0.315 (shake flask-GC, *o, p′*-DDD at 15, 25, 35, 45°C with particle sizes: 5.0 micron or less, Biggar & Riggs 1974)
0.020 (generator column-GC/ECD, Weil et al. 1974)
0.005 (Martin & Worthing 1977)
0.09, 0.10 (quoted, *p,p′*-, *o,p′*-DDD, Callahan et al. 1979)
0.004 (shake flask-nephelometry, Hollifield 1979)
0.10 (20°C, selected, *o,p′*-DDD, Suntio et al. 1988)
0.16 (Agency for Toxic Substances & Disease Registry 1988; quoted, Burmaster et al. 1991)
0.020 (20–25°C, selected, Hornsby et al. 1996)
0.050; 0.010, 0.0035 (quoted; predicted-molar volume, mp and mobile order thermodynamics, Ruelle & Kesselring 1997)
$\log [S_L/(\text{mol/L})] = 0.2910 - 1442/(T/K)$ (liquid, Passivirta et al. 1999)
0.90, 0.738 (*p,p′*-DDD, supercooled liquid: derivation of literature-derived value LDV, final-adjusted value FAV, Shen & Wania 2005)

Vapor Pressure (Pa at 25°C and reported temperature dependence equations):
2.52×10^{-4} (30°C, *o, p′*-DDD, gas saturation-vapor density-GC, Spencer & Cliath 1972; Spencer 1975)
1.36×10^{-4} (30°C, *p, p′*-DDD, gas saturation-GC, Spencer & Cliath 1972; Spencer 1975)
1.63×10^{-3}, 6.24×10^{-4} (P_{GC} by GC-RT correlation, different stationary phases, Bidleman 1984)
4.34×10^{-4} (supercooled liquid P_L, converted from literature P_S with ΔS_{fus} Bidleman 1984)

1.00×10^{-4} (20°C, selected, Suntio et al. 1988)
2.00×10^{-4} (20°C, *o,p′*-, selected, Suntio et al. 1988)
4.35×10^{-4}, 9.84×10^{-4} (supercooled P_L, converted from literature P_S with different ΔS_{fus} values, Hinckley et al. 1990)
1.63×10^{-3}, 1.10×10^{-3} (P_{GC} by GC-RT correlation with different reference standards, Hinckley et al. 1990)
$\log (P_L/Pa) = 12.49 - 4622/(T/K)$ (supercooled liquid, GC-RT correlation, Hinckley et al. 1990; quoted, Passivirta et al. 1999)
1.33×10^{-4} (20–25°C, estimated, Hornsby et al. 1996)
9.69×10^{-4}, 1.13×10^{-4}; 9.16×10^{-5} (*p,p′*-DDD, supercooled liquid P_L: calculated, GC-RT correlation ; converted to solid P_S with fugacity ratio F, Passivirta et al. 1999)
$\log (P_S/Pa) = 16.23 - 6062/(T/K)$ (solid, *p,p′*-DDD, Passivirta et al. 1999)
0.00097, 0.0023 (*p,p′*-DDD, supercooled liquid P_L: LDV literature derived value, FAV final adjusted value, Shen & Wania 2005)

Henry's Law Constant (Pa·m^3/mol at 25°C and reported temperature dependence equations):

2.18 (calculated-P/C, Yoshida et al. 1983)
0.27 (Agency for Toxic Substances & Disease Registry 1988; quoted, Burmaster et al. 1991)
0.64 (20°C, calculated-P/C, Suntio et al. 1988; quoted, Majewski & Capel 1995)
9.00 (calculated-P/C, Ballschmiter & Wittlinger 1991)
0.669 (*p,p′*-DDD, wetted wall column-GC, Altschuh et al. 1999)
$\log [H/(Pa\ m^3/mol)] = 12.20 - 3168/(T/K)$ (*p,p′*-DDD, Passivirta et al. 1999)
0.67, 0.50 (*p,p′*-DDD, LDV literature-derived value, FAV final adjusted value, Shen & Wania 2005)

Octanol/Water Partition Coefficient, log K_{OW}:

5.99 (O'Brien 1975)
6.02 (Ernst 1977)
6.02 (Veith & Morris 1978; Veith et al. 1979)
5.69 (Hansch & Leo 1979)
5.99, 6.08 (*p,p′*-, *o,p′*-DDD, Callahan et al. 1979)
6.00 (Kenaga & Goring 1980)
5.19 (RP-HPLC-RT correlation, Chin et al. 1986)
5.00 (RP-HPLC-RT correlation, De Kock & Lord 1987)
6.217 ± 0.031 (*p,p′*-DDD, shake flask/slow-stirring method, De Bruijn et al. 1989)
6.02 (recommended, Sangster 1993)
4.82 (RP-HPLC-RT correlation, Sicbaldi & Finizio 1993)
6.22 (recommended, Hansch et al. 1995)
4.87 (*o,p′*-, RP-HPLC-RT correlation, Finizio et al. 1997)
6.02 (*p,p′*-DDD, calculated, Passivirta et al. 1999)
6.22, 6.33 (*p,p′*-DDD, LDV literature-derived value, FAV final-adjusted value, Shen & Wania 2005)

Octanol/Air Partition Coefficients, log K_{OA} at 25°C and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section:

8.90 (*p,p′*-DDD, calculated-K_{OW}/K_{AW}, Wania & Mackay 1996)
9.45 (*p,p′*-DDD, calculated, Finizio et al. 1997)
10.11*, 10.27 (*p,p′*-DDD, gas saturation-GC/MS, calculated, measured range 5–35°C, Shoeib & Harner 2002)
$\log K_{OA} = -5.193 + 4610/(T/K)$, temp range: 5–35°C (*p,p′*-DDD, gas saturation-GC, Shoeib & Harner 2002)
10.10, 10.03 (*p,p′*-DDD, LDV literature derived value, FAV final adjusted value, Shen & Wania 2005)

Bioconcentration Factor, log BCF:

4.92, 3.92 (*Gambusia, Physa,* Metcalf et al. 1973)
3.96 (mussel, Ernst 1977)
4.72 (fathead minnow, Veith et al. 1979)
4.09 (calculated-S, Kenaga 1980)
4.11 (calculated-S or K_{OW}, Kenaga & Goring 1980)
3.30 (*Triaenodes tardus*, Belluck & Felsot 1981)

4.34, 4.42 (mussel, oyster; calculated-K_{OW}, Zaroogian et al. 1985)
4.68 (oyster, Zaroogian et al. 1985; quoted, Hawker & Connell 1986)
2.85–4.29 (benthic macroinvertebrates, Reich et al. 1986)
4.81 (calculated-S and K_{OW}, Isnard & Lambert 1988)
–1.90 (beef biotransfer factor log B_b, correlated-K_{OW} from Fries et al. 1969, Travis & Arms 1988)
–2.52 (milk biotransfer factor log B_m, correlated-K_{OW} from Fries et al. 1969, Travis & Arms 1988)
0.301 (earthworms, quoted, Menzie et al. 1992)
–0.456, –0.745, –0.602 (earthworms, field/lab. estimated, field leaf litter, calculated-modeled, Menzie et al. 1992)
4.68 (calculated-log K_{OW} as per Mackay 1982, this work)

Sorption Partition Coefficient, log K_{OC}:
4.91 (calculated-S, Kenaga 1980)
4.63 (calculated-S or K_{OW}, Kenaga & Goring 1980;)
5.86 (calculated-S, Mill et al. 1980; quoted, Adams 1987)
5.89 (estimated-QSAR & SPARC, Kollig 1993)
5.00 (20–25°C, estimated, Hornsby et al. 1996)

Environmental Fate Rate Constants, k, or Half-Lives, $t_{1/2}$:

Volatilization: aquatic half-life of a few days to about a month (summarized data, Callahan et al. 1979).

Photolysis: aquatic $t_{1/2} > 150$ d (summarized data, Callahan et al. 1979).

Oxidation: aquatic $t_{1/2} \sim 22$ yr (summarized data, Callahan et al. 1979);
photooxidation $t_{1/2} = 13.3$–133 h in air, based on estimated rate constant for reaction with hydroxyl radical in air (Atkinson 1987; quoted, Howard et al. 1991).

Hydrolysis:
$t_{1/2} \sim 570$ d at pH 9 and $t_{1/2} = 190$ yr at pH 5 (summarized data, Callahan et al. 1979);
$t_{1/2} = 28$ yr at pH 7 and 25°C, calculated from measured neutral and base catalyzed hydrolysis constants of $(2.8 \pm 0.9) \times 10^{-6}$ h^{-1} and 5.2 M^{-1} h^{-1} (Ellington et al. 1987, 1988, 1989; quoted, Howard et al. 1991);
rate constant $k = 2.5 \times 10^{-2}$ yr^{-1} at pH 7 and 25°C (Kollig 1993).

Biodegradation: aqueous aerobic $t_{1/2} = 2$–15.6 yr, based on observed rates of biodegradation of DDT in aerobic soils under field conditions (Lichtenstein & Schultz 1959; Stewart & Chisholm 1971; quoted, Howard et al. 1991); aqueous anaerobic $t_{1/2} = 70$–294 d, based on anaerobic flooded soil die-away study data for two flooded soils (Castro & Yoshida 1971; quoted, Howard et al. 1991).

Biotransformation:

Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants:
$k_1 = 52.9$ h^{-1}; $k_2 = 0.0058$ h^{-1} (mussel, Ernst 1977; quoted, Hawker & Connell 1986)

Half-Lives in the Environment:

Air: $t_{1/2} = 17.7$–177 h, based on estimated photooxidation half-life in air (Howard et al. 1991).

Surface water: $t_{1/2} = 2$–15.6 yr, based on observed rates of biodegradation of DDT in aerobic soils under field conditions (Lichtenstein & Schultz 1959; Stewart & Chisholm 1971; quoted, Howard et al. 1991)
dehydrochlorination rate constant $k = 5.0 \times 10^{-2}$ h^{-1} with $t_{1/2} = 13.9$ h for 1.0 ppm *p,p′*-DDD and $k = 0.76 \times 10^{-2}$ h^{-1} with $t_{1/2} = 96.3$ h for *o,p′*-DDD both at 21 ± 2°C and pH 12.8 (in 0.1 N NaOH solution) (Choi & Chen 1976)
estimated $t_{1/2} = 45$ d for surface waters in case of a first order reduction process may be assumed (Zoeteman et al. 1980)

Ground water: $t_{1/2} = 1680$–270,000 h, based on anaerobic flooded soil die-away study data for two flooded soils (Castro & Yoshida 1971; quoted, Howard et al. 1991) and observed rates of biodegradation of DDT in aerobic soils under field conditions (Lichtenstein & Schultz 1959; Stewart & Chisholm 1971; quoted, Howard et al. 1991).

Sediment:

Soil: $t_{1/2} = 2$–15.6 yr, based on observed rates of biodegradation of DDT in aerobic soils under field conditions (Lichtenstein & Schultz 1959; Stewart & Chisholm 1971; quoted, Howard et al. 1991);
estimated field $t_{1/2} \sim 1000$ d (20–25°C, Hornsby et al. 1996).

Biota: $t_{1/2} = 119$ h in mussel (Ernst 1977).

TABLE 18.1.1.21.1
Reported aqueous solubilities and octanol-air partition coefficients of DDD at various temperatures

Aqueous solubility						log K_{OA}	
p,p′-DDD				*o,p*-DDD		p,p′-DDD	
Biggar & Riggs 1974				Biggar & Riggs 1974		Shoeib & Harner 2002	
shake flask-GC				shake flask-GC		generator column-GC/MS	
t/°C	S/g·m^{-3}	S/g·m^{-3}	S/g·m^{-3}	t/°C	S/g·m^{-3}	t/°C	log K_{OA}
particle size	0.01μ	0.05μ	5.0μ	particle size	5.0μ		
15	–	–	0.050	15	0.060	5	11.287
25	0.005	0.015	0.090	25	0.100	15	11.238
35	–	–	0.150	35	0.280	20	10.286
45	–	–	0.240	45	0.315	25	10.110
						35	9.870
						log K_{OA} = A + B/(T/K)	
						A	–5.193
						B	4610
						enthalpy of phase change	
						ΔH_{OA}/(kJ mol^{-1}) = 80.1	

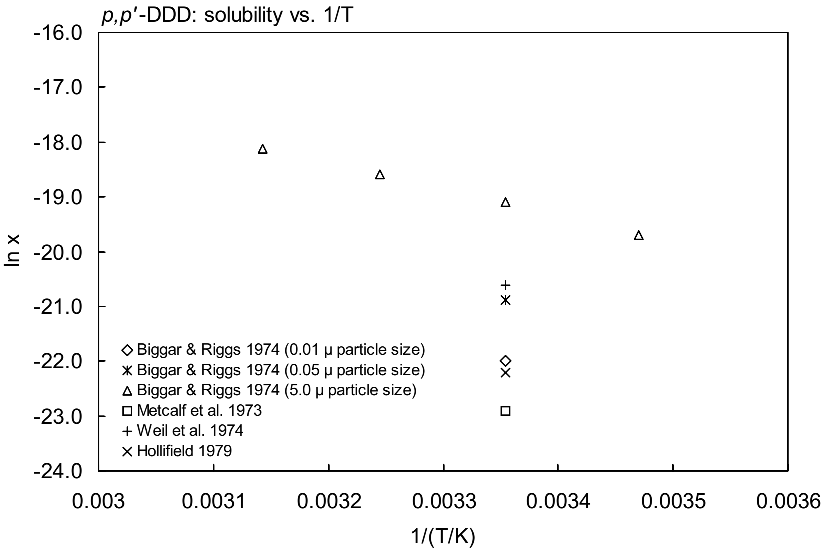


FIGURE 18.1.1.21.1A Logarithm of mole fraction solubility (ln *x*) versus reciprocal temperature for *p,p′*-DDD.

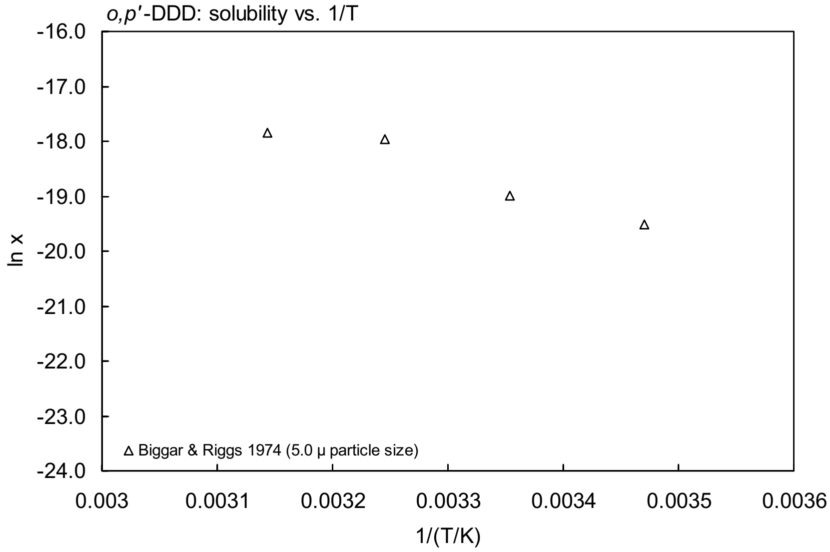


FIGURE 18.1.1.21.1B Logarithm of mole fraction solubility (ln *x*) versus reciprocal temperature for *o,p*′-DDD.

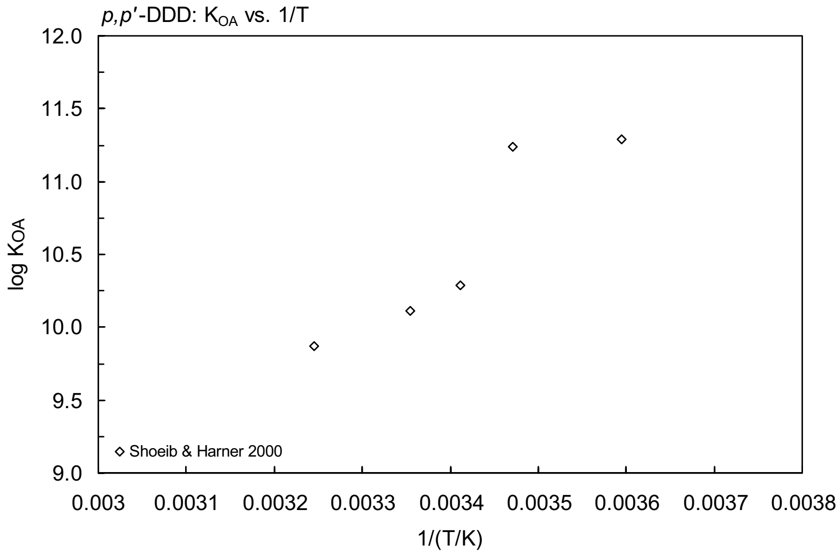
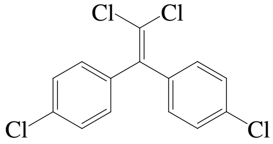


FIGURE 18.1.1.21.2 Logarithm of K_{OA} versus reciprocal temperature for *p,p*′-DDD.

18.1.1.22 DDE



Common Name: DDE (*p,p′*-DDE; *o,p′*-DDE)
Synonym: 4,4′-DDE, DDE; 2,4-DDE
Chemical Name: 1,1-dichloro-2,2-bis(*p*-chlorophenyl)-ethylene
CAS Registry No: 72-55-9 (*p,p′*-DDE); 3424-82-6 (*o,p*-DDE)
Molecular Formula: $C_{14}H_8Cl_4$
Molecular Weight: 319.0
Melting Point (°C):
  89 (Lide 2003)
Boiling Point (°C):
Density (g/cm³ at 20°C):
Molar Volume (cm³/mol):
  305.2 (calculated-Le Bas method at normal boiling point)
  243.1 (Ruelle & Kesselring 1997; Passivirta et al. 1999)
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
  30.543 (*o,p′*-DDE, DSC method, Plato & Glasgow 1969)
  24.267 (*p,p′*-DDE, DSC method, Plato & Glasgow 1969)
Entropy of fusion, ΔS_{fus} (J/mol K):
  67.0 (Hinckley et al. 1990; Passivirta et al. 1999)
Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F: 0.236 (mp at 89°C)

Water Solubility (g/m³ or mg/L at 25°C or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):
p,p′-DDE
  0.0013 (shake flask-LSC, Metcalf et al. 1973, 1975)
  0.12* (shake flask-GC for particles 5μ - or less, measured range 15–45°C, Biggar & Riggs 1974)
  0.014 (generator column-GC/ECD, Weil et al. 1974)
  0.040 (20°C, shake flask-GC, Chiou et al. 1977; Freed et al. 1977)
  0.065 (shake flask-nephelometry, Hollifield 1979)
  0.0079 (Kenaga & Goring 1980)
  0.0017 (30°C, semimicro gas-saturation method, Westcott et al. 1981)
  0.0011, 0.006 (generator column-GC, HPLC-RT correlation, Swann et al. 1983)
  $\log [S_L/(\text{mol/L})] = 0.173 - 1263/(T/K)$ (liquid, Passivirta et al. 1999)
  0.00012 ± 0.00010 (mean literature value-basic statistics for uncensored original data, Pontolillo & Eganhouse 2001)
  0.258, 0.252 (supercooled liquid: derivation of literature-derived value LDV, final-adjusted value FAV, Shen & Wania 2005)
o,p-DDE
  0.140 (shake flask-GC for particles 5 - or less, Biggar & Riggs 1974)
  0.0013 (Zepp et al. 1978)
  0.10 (selected, Suntio et al. 1988; Hornsby et al. 1996)

Vapor Pressure (Pa at 25°C or as indicated and reported temperature dependence equations):
p,p′-DDE
  8.65×10^{-4} (30°C, gas saturation-vapor density-GC, Spencer & Cliath 1972)
  9.87×10^{-4} (GC-RT correlation, Westcott & Bidleman 1981)
  1.73×10^{-4} (30°C, gas saturation-GC, Westcott et al. 1981)
  8.66×10^{-4} (selected, Yoshida et al. 1983)
  2.70×10^{-3}, 2.09×10^{-3} (P_{GC} by GC-RT correlation, different stationary phases, Bidleman 1984)
  2.55×10^{-3} (supercooled liquid P_L, converted from literature P_S with ΔS_{fus} Bidleman 1984)

1.73×10^{-3} (20°C, supercooled liquid value, Bidleman et al. 1986)
7.50×10^{-5} (10°C, estimated, McLachlin et al. 1990)
0.00225, 0.00334 (supercooled liquid values, GC-RT correlation, Hinckley et al. 1990)
2.33×10^{-3}, 3.34×10^{-3} (supercooled P_L, converted from literature P_S with different ΔS_{fus} values, Hinckley et al. 1990)
2.58×10^{-3}, 1.87×10^{-3} (P_{GC} by GC-RT correlation with different reference standards, Hinckley et al. 1990)
$\log (P_L/Pa) = 12.79 - 4554/(T/K)$ (supercooled liquid, GC-RT correlation, Hinckley et al. 1990)
5.13×10^{-4}, 1.82×10^{-3} (supercooled liquid values at 10°C, 20°C, Cotham & Bidleman 1992)
4.36×10^{-3} (supercooled liquid value, quoted, Majewski & Capel 1995)
2.27×10^{-3}, 2.78×10^{-3}; 5.45×10^{-4} (supercooled liquid P_L: calculated; GC-RT correlation; converted to solid P_S with fugacity ratio F, Passivirta et al. 1999)
$\log (P_S/Pa) = 16.29 - 5816/(T/K)$ (solid, Passivirta et al. 1999)
0.0033, 0.0034 (supercooled liquid P_L: LDV literature derived value, FAV final adjusted value, Shen & Wania 2005)

o,p-DDE
8.21×10^{-4} (30°C, gas saturation-vapor density-GC, Spencer & Cliath 1972)
8.27×10^{-4} (Callahan et al. 1979, Mabey et al. 1982)
8.67×10^{-4} (isomer unspecified, estimated, Hornsby et al. 1996)

Henry's Law Constant (Pa·m³/mol at 25°C or as indicated and reported temperature dependence equations):

27.4	(Levins 1981; quoted, Tucker et al. 1983)
0.78	(estimated-group method per Hine & Mookerjee 1975)
6.89	(calculated-P/C, Mabey et al. 1982)
124	(gas stripping-GC, Atlas et al. 1982)
19.59	(calculated-P/C, Yoshida et al. 1983)
7.95	(calculated-P/C, Suntio et al. 1988)
1.25	(10°C, calculated-P/C, McLachlin et al. 1990)
34.0	(calculated-P/C, Ballschmiter & Wittlinger 1991)
120, 370	(23°C), 7.95 (20°C) (quoted, Iwata et al. 1993)
7.95	(20–25°C, calculated-P/C, Majewski & Capel 1995)
4.214	(*p,p′*-DDE, wetted wall column-GC, Altschuh et al. 1999)

$\log (H/(Pa\ m^3/mol)) = 12.62 - 3291/(T/K)$ (*p,p′*-DDE, Passivirta et al. 1999)

4.2, 4.2	(*p,p*-DDE, LDV literature-derived value, FAV final adjusted value, Shen & Wania 2005)

Octanol/Water Partition Coefficient, log K_{OW}:

5.80	(*o,p*-DDE, O'Brien 1975)
4.28	(correlated, Metcalf et al. 1975)
5.69	(*p,p′*-DDE, O'Brien 1975)
5.83	(*p,p′*-DDE, HPLC-RT correlation, Veith et al. 1979a)
5.69	(HPLC-RT correlation, Veith et al. 1979b)
5.77	(Kenaga & Goring 1980)
5.89	(HPLC-RT correlation, McDuffie 1981)
5.63	(RP-HPLC-RT correlation, Swann et al. 1983)
5.89	(estimated-HPLC/MS correlation, Burkhard et al. 1985)
6.51	(HPLC-RT correlation, Webster et al. 1985)
6.29	(RP-HPLC correlation, Chin et al. 1986)
6.09	(RP-HPLC correlation, De Kock & Lord 1987)

6.956 ± 0.011 (*p,p′*-DDE, shake flask/slow stirring method, De Bruijn et al. 1989; received highest ranking from Pontolillo & Eganhouse 2001)

6.51	(recommended, Sangster 1993)
5.78	(RP-HPLC correlation, Sicbaldi & Finizio 1993)
6.96	(recommended, Hansch et al. 1995)
5.43	(*o,p′*-, RP-HPLC correlation, Finizio et al. 1997)
6.65	(mean literature value-basic statistics for uncensored original data, Pontolillo & Eganhouse 2001)
6.96, 6.93	(*p,p′*-DDE, LDV literature-derived value, FAV final-adjusted value, Shen & Wania 2005)

Octanol/Air Partition coefficient, log K_{OA} at 25°C and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section:

8.40 (*p,p′*-DDE, calculated-K_{OW}/K_{AW}, Wania & Mackay 1996)
9.45 (*p,p′*-DDE, calculated, Finizio et al. 1997)
9.53*, 9.676 (*p,p′*-DDE, gas saturation-GC/MS, calculated, measured range 5–35°C, Shoeib & Harner 2002)
$\log K_{OA} = -7.49 + 5116/(T/K)$; temp range: 5–35°C (*p,p′*-DDE, gas saturation-GC, Shoeib & Harner 2002)
9.69, 9.70 (LDV literature derived value, FAV final adjusted value, Shen & Wania 2005)

Bioconcentration Factor, log BCF:

4.44, 4.29 (*Gambusia, Physa,* Metcalf et al. 1973)
4.05, 4.56, 4.77, 4.08 (alga, snail, mosquito, fish, Metcalf et al. 1975)
4.71 (fathead minnows, 32-d exposure, Veith et al. 1979; Veith & Kosian 1983)
3.80 (calculated-S or K_{OW}, Kenaga & Goring 1980)
4.71, 4.37 (quoted exptl, calculated-K_{OW}, Mackay 1982)
5.95 (microorganism-water: calculated-K_{OW}, Mabey et al. 1982)
3.34–4.00 mean 4.00; 4.26–4.15 mean 4.15 (*p,p′*-DDE, rainbow trout, 15°C, steady-state BCF on 7- to 96-d laboratory study in 2 tanks with different water concn, Oliver & Niimi 1985)
4.91, 4.08; 7.25 (*p,p′*-DDE, rainbow trout: kinetic BCF, steady-state BCF, Lake Ontario field BCF, Oliver & Niimi 1985)
3.70–5.32 (*p,p′*-DDE, benthic macroinvertebrates, Reich et al. 1986)
3.70–5.32 (*o,p′*-DDE, benthic macroinvertebrates, Reich et al. 1986)
4.13 (azalea leaves, Bacci & Gaggi 1987)
6.01 (*p,p*-DDE, Connell et al. 1988)
7.48 (Azalea leaves, Bacci et al. 1990)
1.025; –0.824; –0.602 (earthworms: quoted; field/lab. estimated; calculated-modeled, Menzie et al. 1992)
4.95, 6.05 (rainbow trout: wet wt basis, lipid wt basis, *p,p′*-DDE, Geyer et al. 2000)
>4.78, >5.76(fathead minnow, 32-d uptake: wet wt basis, lipid wt basis, *p,p′*-DDE, Geyer et al. 2000)

Bioaccumulation Factor, log BAF:

8.35 (rainbow trout, Thomann 1989)

Sorption Partition Coefficient, log K_{OC}:

4.48 (calculated-S or K_{OW}, Kenaga & Goring 1980;)
6.64 (sediment, calculated-K_{OW}, Mabey et al. 1982)
4.70, 5.17 (quoted, calculated-MCI χ, Sabljic 1984)
6.00, 5.30 (*p,p′*-DDE, field data of sediment trap material, calculated-K_{OW}, Oliver & Charlton 1984)
3.70 (soil, estimated, Hornsby et al. 1996)
4.82 (av. lit. value, Gerstl 1990)
4.82 (*p,p′*-DDE, soil, calculated- MCI χ, Sabljic et al. 1995)
4.85 (*p,p′*-DDE, soil, estimated-general model, Gramatica et al. 2000)

Environmental Fate Rate Constants, k, or Half-Lives, $t_{½}$:

Volatilization:
Photolysis: midday $t_{½}$ = 5 h in hydrocarbon media (Zepp et al. 1976)
$t_{½}$ = 1.5 d under sunlight in water (Mansour & Feicht 1994).
Oxidation:
Hydrolysis: the first-order rate constant $k = 1.4 \times 10^{-9}$ M^{-1} s^{-1} and the hydrolytic $t_{½}$ > 120 yr in water at 27°C (Wolfe et al. 1977);
hydrolytic $t_{½}$ = 120 yr at pH 7 and 25°C of 120 yr and a rate constant $k = 6.6 \times 10^{-7}$ h^{-1} (Callahan et al. 1979, Mabey et al. 1982).
Biodegradation:
Biotransformation:
Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants:
k_1 = 170.0 d^{-1}; k_2 = 0.021 d^{-1} (*p,p′*-DDE, rainbow trout, Oliver & Niimi 1985)

$k_2 = 0.950\ yr^{-1}$ (*Larus argentatus*, Norstrom et al. 1986)
$k_1 = 20800\ d^{-1}$; $k_2 = 0.020\ d^{-1}$ (*Oligochaetes*, Connell et al. 1988)
$k_2 = 0.0004\ h^{-1}$ (azalea leaves, Paterson et al. 1991)
$k_2 = 0.0030\ h^{-1}$ (midge *C. riparius*, water only system, Lydy et al. 1992)
$k_2 = 0.0046\ h^{-1}$ (midge *C. riparius*, screened, Lydy et al. 1992)
$k_2 = 0.0080\ h^{-1}$ (midge *C. riparius*, 3% organic carbon, Lydy et al. 1992)
$k_2 = 0.0046\ h^{-1}$ (midge *C. riparius*, 15% organic carbon, Lydy et al. 1992)

Half-Lives in the Environment:

Air: atmospheric transformation lifetime was estimated to be < 1 d (Kelly et al. 1994).
Surface water: midday $t_{1/2} = 5$ h in hydrocarbon media (Zepp et al. 1976)
hydrolytic $t_{1/2} > 120$ yr in water at 27°C (Wolfe et al. 1977);
estimated $t_{1/2} = 690$ d in surface waters in case of first order reduction process, and estimated $t_{1/2} > 300$ d in lakes in the Netherlands (Zoeteman et al. 1980);
photolysis $t_{1/2} = 1.5$ d under sunlight in water (Mansour & Feicht 1994).
Ground water:
Sediment:
Soil: field $t_{1/2} = 1000$ d (estimated, Hornsby et al. 1996);
$t_{1/2} > 20$ yr, very persistent (Geyer et al. 2000)
$t_{1/2} = 40.9$ and 17.2 yr for control and sludge-amended Luddington soils, respectively (Meijer et al. 2001).
Biota: elimination $t_{1/2} = 340$ d (*p,p′*-DDE, rainbow trout, Oliver & Niimi 1985);
$t_{1/2} = 264$ d in herring gulls compared to literature average $t_{1/2} = 300$ d for birds (Norstrom et al. 1986);
elimination $t_{1/2} = 2230$ h (Azalea leaves, Bacci & Gaggi 1987);
$t_{1/2} = 231$ h in the midge (*Chironomus riparius*) under varying sediment conditions (water only system with no sediment), $t_{1/2} = 150$ h (midge screened from the sediment), $t_{1/2} = 87$ h (midge screened from 3% organic carbon sediment), $t_{1/2} = 99$ h (midge screened from 3% organic carbon sediment) (Lydy et al. 1992).

TABLE 18.1.1.22.1
Reported aqueous solubilities of DDE at various temperatures

***p,p′*-DDE**				***o,p′*-DDE**			
Biggar & Riggs 1974				**Biggar & Riggs 1974**			
shake flask-GC				**shake flask-GC**			
t/°C	**$S/g \cdot m^{-3}$**	**$S/g \cdot m^{-3}$**	**$S/g \cdot m^{-3}$**	**t/°C**	**$S/g \cdot m^{-3}$**	**$S/g \cdot m^{-3}$**	**$S/g \cdot m^{-3}$**
particle size	0.01μ	0.05μ	5.0μ	particle size	0.01μ	0.05μ	5.0μ
15			0.055	15			
25	0.010	0.040	0.120	25	0.015	0.040	0.140
35			0.235	35			
45			0.450	45			

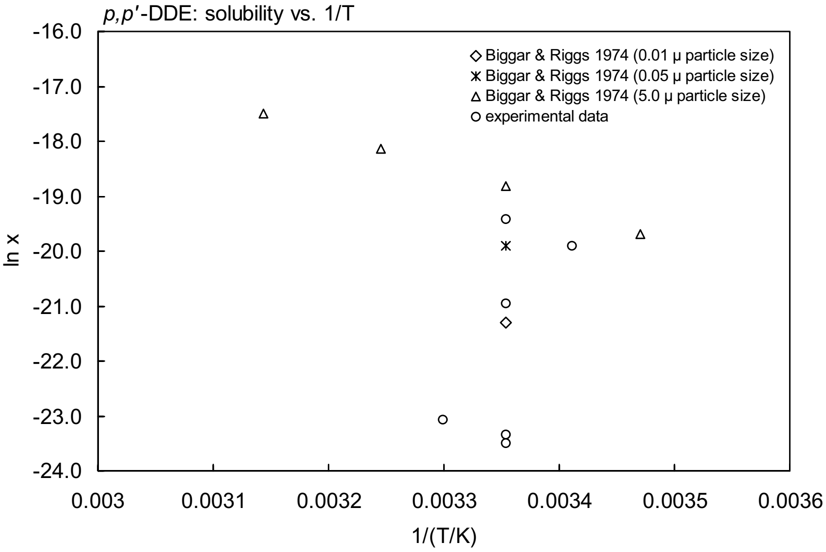


FIGURE 18.1.1.22.1A Logarithm of mole fraction solubility (ln *x*) versus reciprocal temperature for *p,p′*-DDE.

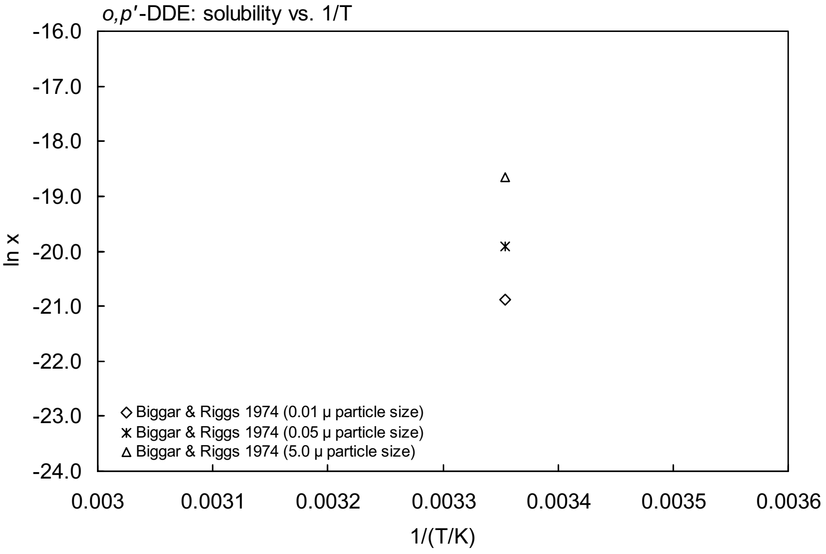


FIGURE 18.1.1.22.1B Logarithm of mole fraction solubility (ln *x*) versus reciprocal temperature for *o,p′*-DDE.

TABLE 18.1.1.22.2
Reported octanol-air partition coefficient of *p,p′*-DDE at various temperatures

Shoeib & Harner 2002	
generator column-GC/MS	
t/°C	log K_{OA}
5	10.905
15	10.361
20	9.906
25	9.530
35	9.196

log K_{OA} = A + B/(T/K)

A	–7.492
B	5116

enthalpy of phase change
$\Delta H_{OA}/(\text{kJ mol}^{-1}) = 98.0$

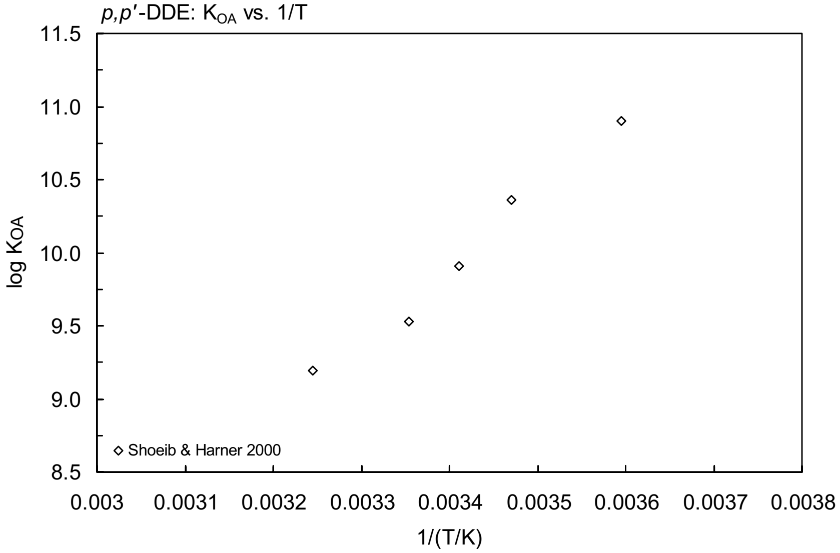
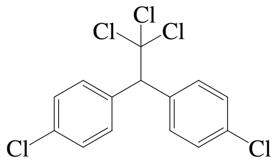


FIGURE 18.1.1.22.2 Logarithm of K_{OA} versus reciprocal temperature for *p,p′*-DDE.

18.1.1.23 DDT



Common Name: DDT

Synonym: Agritan, Anofex, Arkotine, Azotox, Bosan supra, Bovidermol, Cesarex, chlorophenoethane, Chlorophenothanum, Chlorophenotoxum, Citox, Clofenotan, Dedelo, Deoval, Devol, Detox, Detoxan, Dibovan, Dichophane, dichlorodiphenyltrichloroethane, Didigam, Didimac, Dodat, Dykol, ENT 1506, Estonate, Genitox, Gesafid, Gesapon, Gesarex, Gesarol, Guesarol, Gyron, Havero-extra, Ivoran, Ixodex, Kopsol, Mutoxin, Neocid, Parachlorocidum, PEBI, Pentachlorin, Pentech, p,p′-DDT, 4,4′-DDT, Rukseam, Santobane, Zeidane, Zerdane

Chemical Name: 1,1,1-trichloro-2,2-bis-(4-chlorophenyl)-ethane; 1,1′-(2,2,2-trichloroethylidene)-bis(4-chlorobenzene)

Uses: persistent nonsystemic insecticide with contact and stomach action to control mosquitoes for the eradication of malaria but is now prohibited and displaced with less persistent insecticides on crop application.

CAS Registry No: 50-29-3 (*p,p′*-DDT, DDT), 789-02-6 (*o,p′*-DDT)

Molecular Formula: $C_{14}H_9Cl_5$

Molecular Weight: 354.486

Melting Point (°C):
108.5 (Lide 2003)

Boiling Point (°C):
260 (Lide 2003)

Density (g/cm^3 at 20°C):
1.55 (Hadaway et al. 1970; Kenaga 1972)

Molar Volume (cm^3/mol):
250 (calculated-density, Chiou 1985)
333.5 (calculated-Le Bas method at normal boiling point)

Dissociation Constant, pK_a:

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
27.196 (*o,p′*-DDT, DSC method, Plato & Glasgow 1969)
26.36 (*p,p′*-DDT, DSC method, Plato & Glasgow 1969)
26.284 (Ruelle & Kesselring 1997)

Entropy of Fusion, ΔS_{fus} (J/mol K):
69.036 (Plato & Glasgow 1969)
70.29 (Hinckley et al. 1990)
72.8 (*p,p′*-DDT, Passivirta et al. 1999)

Fugacity Ratio at 25°C, F:
0.147 (assuming ΔS_{fus} = 56 J/mol K., Mackay et al. 1986)
0.130 (20°C, assuming ΔS_{fus} = 56 J/mol K, Suntio et al. 1988)

Water Solubility (g/m^3 or mg/L at 25°C or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):
0.0002–0.001(15°C, shake flask-bioassay, Richards & Cutkomp 1946)
0.0374 (shake flask-radiometric method, measured range 2–37.5°C, Babers 1955)
≤ 0.0012 (shake flask-radiometric method, Bowman et al. 1960)
0.035 (shake flask-colorimetric, Lipke & Kearns 1960)
0.0012 (Stephen & Stephen 1963)
0.0016 (99% pure DDT isomers plus DDE at rm. temp., shake flask-GC, Robeck et al. 1965)
0.0034 (Biggar et al. 1966)
0.0017 (ultracentrifugation-GC, Biggar et al. 1967)
0.0012–0.0374 (Günther et al. 1968)
0.0017*, 0.006*, 0.025* (shake flask-GC, *p,p′*-DDT, particle size: 0.01, 0.05, 5.0μ, Biggar & Riggs 1974)

0.004, 0.012, 0.085* (shake flask-GC, *o,p′*-DDT, particle size: 0.01, 0.05, 5.0μ size or less, Biggar & Riggs 1974)
0.0055 (generator column-GC/ECD, Weil et al. 1974)
0.0017 (Martin & Worthing 1977)
0.0010 (shake flask-GC, Paris et al. 1977)
0.004 (shake flask-nephelometry, Hollifield 1979)
0.0012 (Hartley & Graham-Bryce 1980)
0.040 (shake flask-HPLC, Ellgehausen et al. 1981)
0.0645 (shake flask-GC, Chiou et al. 1982)
0.0023 (generator column-GC, Swann et al. 1983)
0.020 (RP-HPLC-RT correlation, Swann et al. 1983)
0.0031–0.0034 (Verschueren 1983)
0.0045 (shake flask-GC or LSC, Gerstl & Mingelgrin 1984)
0.030 (RP-HPLC-RT correlation, Chin et al. 1986)
0.0054 (24°C, shake flask-GC/ECD, Chiou et al. 1986)
0.0055 (shake flask-GC, Chiou et al. 1991)
0.001–0.0055 (Montgomery 1993)
0.0055 (20–25°C, selected, Augustijn-Beckers et al. 1994; Hornsby et al. 1996)
log $[S_L/(mol/L)] = –0.195 – 1454/(T/K)$ (liquid, Passivirta et al. 1999)
0.00023 ± 0.00010 (mean literature value-basic statistics for uncensored original data, Pontolillo & Eganhouse 2001)
0.0956, 0.149 (*p,p′*-DDT, supercooled liquid S_L: derivation of literature-derived value LDV, final-adjusted value FAV, Shen & Wania 2005)

Vapor Pressure (Pa at 25°C or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):
2.0×10^{-5}* (*p,p′*-DDT, 20°C, effusion manometer, measured range 0–100°C, Balson 1947)
log (P/mmHg) = 14.191 – 6160/(T/K), temp range 66–100°C (Antoine eq., effusion, Balson 1947)
log (P/mmHg) = 13.778 – 6010/(T/K); temp range 50–90°C (Antoine eq., effusion, Dickinson 1947)
0.001973*, 0.002027* (*p,p′*-DDT, 50.1°C, gas saturation-spec., measured range 50.1–90.2°C, Dickinson 1956)
3.30×10^{-5} (interpolated exptl. data of Balson 1947, Spencer & Cliath 1970; Ballschmiter & Wittlinger 1991)
3.33×10^{-5} (20°C, partition coefficient, Atkins & Eggleton 1971)
2.53×10^{-5} (20°C, Melnikov 1971; Spencer 1973, 1982; Callahan et al. 1979, Mabey et al. 1982)
2.03×10^{-5}* (20°C, *p,p′*-DDT, 30°C, gas saturation-GC, measured range 20–40°C, Spencer & Cliath 1972)
log (P/mmHg) = 14.24 – 6176/(T/K); temp range 20–40°C (*p,p′*-DDT, 30°C, gas saturation-GC, Antoine eq., Spencer & Cliath 1972; Spencer 1975)
7.37×10^{-4} (*o,p′*-DDT, 30°C, gas saturation-GC, Spencer & Cliath 1972; Spencer 1975)
2.50×10^{-5} (20°C, Hartley & Graham-Bryce 1980; Worthing & Hance 1991)
5.73×10^{-5}* (*p, p′*-DDT, gas saturation-HPLC/liquid scintillation spectrometry, measured range 20–80°C, Rothman 1980)
2.00×10^{-5} (20–25°C, Weber et al. 1980)
1.50×10^{-4} (20°C, GC, Seiber et al. 1981)
6.0×10^{-4}, 1.12×10^{-3} (*o,p′*-DDT 25, 30°C, capillary GC-RT correlation, Westcott & Bidleman 1981)
1.17×10^{-3} (*o,p′*-DDT, 30°C, semi-micro gas-saturation-GC, Westcott et al. 1981)
4.30×10^{-5} (estimated-relative volatilization rate, Dobbs & Cull 1982)
2.67×10^{-3}, 2.67×10^{-5} (20°C, calculated values, Grain 1982)
$2.01 \times 10^{-5} – 2.8 \times 10^{-5}$ (gas saturation, Jaber et al. 1982)
1.96×10^{-5} (20°C, evaporation rate at 20–60°C, Gückel et al. 1982)
4.31×10^{-5} (20°C, relative loss rate, Dobbs & Cull 1982)
1.61×10^{-3}, 1.28×10^{-3} (*o,p′*-DDT, P_{GC} by GC-RT correlation, different stationary phases, Bidleman 1984)
1.33×10^{-3} (*o,p′*-DDT, supercooled liquid P_L, converted from literature P_S with ΔS_{fus} Bidleman 1984)
8.30×10^{-4}, 4.70×10^{-4} (*p,p′*-DDT, P_{GC} by GC-RT correlation, different stationary phases, Bidleman 1984)
3.16×10^{-4} (*p,p′*-DDT, supercooled liquid P_L, converted from literature P_S with ΔS_{fus} Bidleman 1984)
2.48×10^{-5} (20°C, GC-RT correlation, Kim 1985)
1.73×10^{-4} (20°C, supercooled liquid value, Bidleman et al. 1986)
2.50×10^{-5} (Hartley & Kidd 1987; Tomlin 1994)
1.33×10^{-3}, 1.83×10^{-3} (*o,p′*-DDT, supercooled liquid P_L, converted from literature P_S with different ΔS_{fus} values, Hinckley et al. 1990)

1.614×10^{-3}, 1.035×10^{-3} (*o,p′*-DDT, P_{GC} by GC-RT correlation with different reference standards, Hinckley et al. 1990)
log (P_L/Pa) = 12.77 – 4626/(T/K) (*o,p′*-DDT, supercooled liquid, GC-RT correlation, Hinckley et al. 1990)
3.16×10^{-4}, 5.12×10^{-4} (*p,p′*-DDT, supercooled liquid P_L, converted from literature P_S with different ΔS_{fus} values, Hinckley et al. 1990)
8.30×10^{-4} (*p,p′*-DDT, P_{GC} by GC-RT correlation with eicosane as reference standard, Hinckley et al. 1990)
log (P_L/Pa) = 13.02 – 4865/(T/K) (*p,p′*-DDT, GC-RT correlation, supercooled liquid, Hinckley et al. 1990)
6.92×10^{-5}, 2.69×10^{-4}, 9.33×10^{-4} (supercooled liquid values at 10°C, 20°C, 30°C, calculated from Hinckley et al. 1990; Cotham & Bidleman 1992)
2.27×10^{-8} (20°C, Montgomery 1993)
2.53×10^{-5} (20–25°C, selected, Augustijn-Beckers et al. 1994; Hornsby et al. 1996)
1.715×10^{-5}* (*p, p′*-DDT 20°C, gas saturation-GC/ECD, measured range 0–40°C, Wania et al. 1994)
log (P/Pa) = 16.62 – 6276/(T/K), temp range 0–40°C (Antoine eq., gas saturation, Wania et al. 1994)
1.05×10^{-4} (supercooled liquid P_L, GC-RT correlation; Donovan 1996)
5.01×10^{-4} (supercooled liquid P_L, Wania & Mackay 1996)
4.39×10^{-4}, 4.27×10^{-4}; 3.78×10^{-5} (supercooled liquid P_L, calculated; GC-RT correlation; solid P_S converted from P_L with fugacity ratio F, Passivirta et al. 1999)
log (P_S/Pa) = 16.62 – 6276/(T/K) (solid, quoted from Wania et al. 1994, Passivirta et al. 1999)
log (P_L/Pa) = 12.82 – 4823/(T/K) (supercooled liquid, Passivirta et al. 1999)
log (P_L/Pa) = (12.38 ± 0.48) – (4665 ± 166)/(T/K); ΔS_{fus} = 70.9 J mol^{-1} K^{-1} (*p,p′*-DDT, supercooled liquid, summary of literature exptl. data, Bidleman et al. 2003)
0.00056, 0.00048 (*p,p′*-DDT, supercooled liquid P_L: LDV literature derived value, FAV final adjusted value, Shen & Wania 2005)
log (P_L/Pa) = –4666/(T/K) + 12.40 (supercooled liquid, linear regression of literature data, Shen & Wania 2005)

Henry's Law Constant (Pa·m^3/mol at 25°C or as indicated and reported temperature dependence equations):
1.30 (measured, Atkins & Eggleton 1971)
3.94 (calculated-P/C, Mackay & Leinonen 1975)
6.02 (20–25°C, calculated, Thibodeaux 1979)
7.48 (20°C, volatilization rate, Burkhard & Guth 1981)
7.29 (calculated-P/C, Levins 1981)
5.30 (calculated-P/C, Mackay & Shiu 1981)
1.60 (calculated-P/C, Mabey et al. 1982)
3.85 (calculated-P/C, Thomas 1982)
0.466 (estimated-group method per Hine & Mookerjee 1975, Tucker et al. 1983)
4.96 (calculated-P/C, Jury et al. 1984, 1987a; Jury & Ghodrati 1989)
1.63 (calculated-P/C, Caron et al. 1984)
1.31 (calculated-P/C, Mackay et al. 1986)
4.96, 8.18 (calculated-P/C, Taylor & Glotfelty 1988)
2.36 (20°C, calculated-P/C, Suntio et al. 1988)
1.28, 1.33 (22–24°C, fog chamber-concn. ratio-GC/ECD, Fendinger et al. 1989)
0.862 (23°C, wetted-wall column-GC/ECD, Fendinger et al. 1989, 1990)
0.16 (0°C, selected, Cotham & Bidleman 1991)
2.90 (calculated-P/C, Calamari et al. 1991)
6.0 calculated-P/C, Ballschmiter & Wittlinger 1991)
1.55 (calculated-bond contribution method, Meylan & Howard 1991)
1.31, 0.86 (25°C, 24°C, Iwata et al. 1993)
1.31 (23°C, quoted, Montgomery 1993)
0.843 (*p,p′*-DDT, wetted wall column-GC, Altschuh et al. 1999)
log (H/(Pa m^3/mol)) = 13.02 – 3369/(T/K) (Passivirta et al. 1999)
1.1, 1.1 (*p,p′*-DDT, LDV literature-derived value, FAV final adjusted value, Shen & Wania 2005)

Octanol/Water Partition Coefficient, log K_{OW}:
3.98 (shake flask, Kapoor et al. 1973; Lu & Metcalf 1975)
6.19 (calculated, O'Brien 1975)

6.36 (shake flask-GC, Chiou et al. 1982)
4.89 (Wolfe et al. 1977; Callahan et al. 1979)
5.98 (Kenaga & Goring 1978, 1980; Kenaga 1980b)
6.19 (shake flask-GC, Freed et al. 1979)
3.98–6.19 (Hansch & Leo 1979)
6.36 (shake flask, Karickhoff et al. 1979)
5.75 (HPLC-RT correlation, Veith et al. 1979b, 1980; Veith & Kosian 1983)
6.69 (Belluck & Felsot 1981)
5.94 (shake flask-GC/LC, Ellgehausen et al. 1981)
5.55 (HPLC-k′ correlation, McDuffie 1981)
6.38 (HPLC-RT correlation, Hammers et al. 1982)
5.10 ± 0.1 (radioactive analysis method, Platford et al. 1982)
5.60 (shake flask-GC, Platford 1982, 1983)
5.90 (average of shake flask values, Eadsforth & Moser 1983)
6.12 (average of HPLC-RT correlation, Eadsforth & Moser 1983)
6.20 (Elgar 1983)
5.44 (shake flask-GC or LSC, Gerstl & Mingelgrin 1984)
6.40 (HPLC-RV correlation, Garst 1984)
5.44 (estimated-HPLC/MS; Burkhard et al. 1985)
6.22 (HPLC-RT correlation, Brooke 1986)
6.06 (RP-HPLC-RT correlation, Chin et al. 1986)
6.21 (HPLC-RT correlation, Eadsforth 1986)
6.19 (RP-HPLC correlation, De Kock & Lord 1987)
6.51 (HPLC-RT correlation, Liu & Leng 1988)
6.914 ± 0.030 (*p,p′*-, shake flask/slow-stirring method, De Bruijn et al. 1989; received highest ranking from Pontolillo & Eganhouse 2001)
6.307 ± 0.045; 6.914 ± 0.030 (shake flask-UV/GC/HPLC, BRE value, RITOX value, inter-laboratory studies, Brooke et al. 1990; received highest ranking from Pontolillo & Eganhouse 2001)
4.89–6.91 (Montgomery 1993)
5.50 (RP-HPLC correlation, Sicbaldi & Finizio 1993)
6.36 (recommended, Sangster 1993)
8.3064 (*o,p′*-DDT, calculated-UNIFAC group-interaction, Chen et al. 1993)
6.91 (recommended, Hansch et al. 1995)
5.65 (*o,p′*-DDT, RP-HPLC-RT correlation, Finizio et al. 1997)
5.50 (*p,p′*-DDT, RP-HPLC-RT correlation, Finizio et al. 1997)
6.50 (*p,p′*-DDT, quoted lit., calculated, Passivirta et al. 1999)
6.65 (mean literature value-basic statistics for uncensored original data, Pontolillo & Eganhouse 2001)
6.28, 6.39 (*p,p′*-DDT, LDV literature-derived value, FAV final-adjusted value, Xiao et al. 2004)

Octanol/Air Partition Coefficient, log K_{OA} at 25°C and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section:

10.09, 9.22 (*p,p′*-DDT, generator column-GC/ECD, calculated-K_{OW}/K_{AW}, Harner & Mackay 1995)
8.70 (calculated-K_{OW}/K_{AW}, Wania & Mackay 1996)
9.93 (*p,p′*-DDT, calculated, Finizio et al. 1997)
9.66* (*o,p′*-DDT, gas saturation-GC/MS, measured range 5–35°C, Shoeib & Harner 2002)
$\log K_{OA} = -11.291 + 6266/(T/K)$, temp range 5–35°C (*o,p′*-DDT, gas saturation-GC, Shoeib & Harner 2002)
9.879*, 9.816 (*p,p′*-DDT, gas saturation-GC/MS, calculated, measured range 5–45°C, Shoeib & Harner 2002)
$\log K_{OA} = -5.63 + 4603/(T/K)$, temp range 5–35°C (*p,p′*-DDT, gas saturation-GC, Shoeib & Harner 2002)
9.81, 9.73 (*p,p′*-DDT, LDV literature derived value, FAV final adjusted value, Shen & Wania 2005)

Bioconcentration Factor, log BCF:

5.31–6.23 (earthworms, Wheatley & Hardman 1968)
2.42 (*Cylindrotheca closterium*, Keil & Priester 1969)
4.40; 4.90; 4.40 (*Syracosphaera carterae*; *Amphidirium cartaria*; *Tholassiosira fluviatilus*, Cox 1970)
4.00 (pinfish, Hansen & Wilson 1970)
4.58 (Atlantic croaker, Hansen & Wilson 1970)

3.94 (soft clam, Butler 1971)
4.20–4.36 (*Daphnia magna* over concn. gradient 8 µg/L to 1.1 mg/L, Crosby & Tucker 1971)
5.00 (*Daphnia magna* at water level 80 ng/L, Johnson et al. 1971)
4.27 (*Daphnia magna,* wet wt. basis, Crosby & Tucker 1971)
4.45 (*Daphnia magna,* wet wt. basis, Johnson et al. 1971;)
4.08–4.60 (fishes, Menzie 1972)
4.93, 4.54 (*Gambusia, Physa,* Metcalf et al. 1973)
4.68 (oyster, Parrish 1974)
4.79 (*Ankistrodesmus*, Neudorf & Khan 1975)
3.52–3.63, 3.11–3.43 (bacteria, algae, Wolfe et al. 1977)
3.14 (trout muscle, Branson 1978)
4.47 (fathead minnow, 32-d exposure, Veith et al. 1979b, 1980)
4.72 (bluegill sunfish-kinetic value, Bishop & Maki 1980)
4.79, 4.93 (fish: flowing water, static water; Kenaga 1980a,b; Kenaga & Goring 1980)
4.35; 4.43 (calculated-S, calculated-K_{OC}, Kenaga 1980a)
–0.045 (average beef fat diet, Kenaga 1980b)
4.15 (pulex, Kenaga & Goring 1980)
4.11 (algae, estimated, Baughman & Paris 1981)
2.95–3.03; 3.02–3.13 (*Rhodotorulus solani*, *Alfafa tissue*, Baughman & Paris 1981)
2.10 (*Triaenodes tardus*, Belluck & Felsot 1981)
5.38 (calculated-K_{OW}, Briggs 1981)
5.11 (selected, Schnoor & McAvoy 1981, Schnoor 1992)
4.36, 4.15, 4.43 (estimated-S, calculated-K_{OW}, calculated-K_{OC}, Bysshe 1982)
4.47, 4.43 (fish: quoted, correlated, Mackay 1982)
4.37 (mussels, quoted average, Geyer et al. 1982)
6.90 (microorganism-water, Mabey et al. 1982)
2.30, 4.08 (trout, pinfish, Verschueren 1983)
4.71 (15°C, rainbow trout, Davies & Dobbs 1984)
5.00 (25°C, fathead minnow-steady state, Davies & Dobbs 1984)
4.15 (activated sludge, Freitag et al. 1984)
3.97, 3.46, 4.15 (algae, fish, activated sludge, Klein et al. 1984)
3.97, 3.28, 4.15 (algae, golden ide, activated sludge, Freitag et al. 1985)
4.97 (*Oncorhynchus mykiss*, Muir et al. 1985)
3.91, 3.08 (rainbow trout: kinetic, steady-state, Oliver & Niimi 1985)
4.47, 4.56 (oyster, calculated-K_{OW} & models, Zaroogian et al. 1985)
3.24–5.00 (*p,p′*-DDT, benthic macroinvertebrates, Reich et al. 1986)
3.44–5.71 (*o,p′*-DDT, benthic macroinvertebrates, Reich et al. 1986)
4.08 (*Selenastrum capricornutum*, Mailhot 1987)
6.50 (zooplankton, chum salmon; Kawano et al. 1988)
–1.55 (beef biotransfer factor log B_b, correlated-K_{OW} from Radeleff et al. 1952 & Kenaga 1980, Travis & Arms 1988)
–2.62 (milk biotransfer factor log B_m, correlated-K_{OW} from Fries et al. 1969; Saha 1969 & Whiting et al. 1973, Travis & Arms 1988)
–1.80 (vegetation, correlated-K_{OW} from Beall & Nash 1972 & Voerman & Besemer 1975, Travis & Arms 1988)
5.28, 7.64 (dry leaf, wet leaf, Bacci et al. 1990)
4.47, 4.30 (quoted, calculated, Banerjee & Baughman 1991)
4.72 (selected, Chessells et al. 1992)
–0.155, –1.0 (earthworms, quoted, field/lab., Menzie et al. 1992)
–1.0, –0.602 (earthworms, field leaf litter, calculated-model, Menzie et al. 1992)
4.81, 4.86, 4.95, 4.99 (*Oncorhynchus mykiss*, Muir et al. 1994)
4.05, 2.85, 3.70 (algae *Selenastrum capricornutum*, water flea *Daphnia magna*, catfish *Ictalurus melas*, wet wt. basis, Wang et al. 1996)
3.97, 4.81 (algae *Chlorella*: wet wt basis, dry wt basis, *p,p′*-DDT, Geyer et al. 2000)

4.45, 6.45 (*Daphnia*: wet wt basis, lipid wt basis, *p,p′*-DDT, Geyer et al. 2000)
5.14, 7.06 (oyster, flow-through 6 months: wet wt basis, lipid wt basis, *p,p′*-DDT, Geyer et al. 2000)
4.97, 6.67 (rainbow trout: wet wt basis, lipid wt basis, *p,p′*-DDT, Geyer et al. 2000)
>4.57, >5.55 (fathead minnow, 10.5% lipid, 28-d: wet wt basis, lipid wt basis, *o,p′*-DDT, Geyer et al. 2000)

Bioaccumulation Factor BAF:
1.27 (bioaccumulation factor log BAF, adipose tissue in male Albino rats, Berdanier & de Dennis 1977)
4.20; 3.539; 3.35 (log BF-bioaccumulation factor of algae; catfish; daphnids, Ellgehausen et al. 1980)
5.10 (fish, reported as log BAF_w, LeBlanc 1995)

Sorption Partition Coefficient, log K_{OC}:
5.38 (soil, Hamaker & Thompson 1972; Kenaga 1980; Kenaga & Goring 1980; Karickhoff 1981)
3.93 (sediment, Wolfe et al. 1977)
5.38 (calculated-K_{OW}, Kenaga 1980)
5.16 (soil, calculated-S as per Kenaga & Goring 1978, Kenaga 1980)
5.38 (Kenaga & Goring 1980; quoted, Hodson & Williams 1988)
5.18 (average 3 soils, HPLC-RT correlation, McCall et al. 1980)
5.39 (average soils/sediments, Rao & Davidson 1980)
5.20, 5.18, 5.18; 5.18 (commerce soil, Tracy soil, Catlin soil; average soil, McCall et al. 1980)
5.00 (selected, sediment/water, Schnoor & McAvoy 1981; Schnoor 1992)
5.62; 6.81, 5.80 (estimated-S; estimated-S and mp, calculated-K_{OW}, Karickhoff 1981)
6.59 (calculated-K_{OW}, Mabey et al. 1982)
5.38 (soil, Thomas 1982; quoted, Nash 1988)
5.20 (Pavlou & Weston 1983, 1984)
5.18, 4.64 (soil slurry method, HPLC-RT correlation, Swann et al. 1983)
5.38 (soil, Jury et al. 1984; quoted, Mackay & Stiver 1991)
5.38, 5.33 (soil: quoted, calculated-MCI χ, Sabljic 1984)
5.61 (Caron et al. 1984)
5.39 (soil, estimated, Karickhoff 1985)
6.00 (best estimate at low sediment concn., Karickhoff 1985)
5.11–5.45 (Aldrich humic acid, Landrum et al. 1984)
4.28–4.66 (natural water, Landrum et al. 1984)
5.61 ± 0.11 (Chiou et al. 1987; quoted, Chin et al. 1991)
6.03 (predicted-K_{OW}, Chiou et al. 1987)
5.39 (selected, Elzerman & Coates 1987)
3.94 (calculated-MCI χ, Gerstl & Helling 1987)
5.38 (soil, screening model calculations, Jury et al. 1987a,b; Jury & Ghodrati 1989)
5.38, 5.34 (quoted, calculated- MCI χ, Bahnick & Doucette 1988)
5.63 (RP-HPLC-k′ correlation, cyanopropyl column, Hodson & Williams 1988)
4.09 (calculated-K_{OW} as per Kenaga & Goring 1980, Chapman 1989)
5.15–6.26 (Montgomery 1993)
6.59 (estimated-QSAR and SPARC, Kollig 1993)
6.30 (20–25°C, estimated, Augustijn-Beckers et al. 1994; Hornsby et al. 1996)
5.31 (soil, calculated-MCI χ, Sabljic et al. 1995)
5.63; 5.34 (HPLC-screening method; calculated-PCKOC fragment method, Müller & Kördel 1996)
5.17 (*p,p′*-DDT, soil, estimated-general model, Gramatica et al. 2000)
6.08 (*p,p′*-DDT, average values for sediments OC ≥ 0.5%, Delle Site 2001)
5.63, 5.54 (*p,p′*-DDT, soils: organic carbon OC ≥ 0.1%, OC ≥ 0.5%, average, Delle Site 2001)
5.20 (soil humic acid, shake flask-HPLC/UV, Cho et al. 2002)

Sorption Partition Coefficient, log K_{OM}:
5.14 (exptl., Briggs 1981)
4.24 (calculated-Parachor, Briggs 1981)
4.88 – 5.41 (Mingelgrin & Gerstl 1983)
5.69, 5.59, 5.69 (average soil, sediment, soil and sediment, Gerstl & Mingelgrin 1984)

Environmental Fate Rate Constants, k, or Half-Lives, $t_{½}$:

Volatilization: $t_{½}$ = 3.7 d for water depth of 1 m (Mackay & Wolkoff 1973);
$t_{½}$ = 73.9 h (Mackay & Leinonen 1975, Branson 1978);
initial rate constant k = 6.9×10^{-4} h^{-1} and predicted rate constant k = 1.2×10^{-3} h^{-1} from soil with $t_{½}$ = 578 h; $t_{½}$(calc) = 45 h from water (Thomas 1982);
half-flux values times, 0.3 d from field study, 0.3–12 d from microagroecosystem, >80–1000 d from laboratory data (Nash 1983).

Photolysis: midsummer direct photolysis k = 8.5×10^{-8} s^{-1} with $t_{½}$ > 227000 h in water, $t_{½}$ = 280000 h in hydrocarbon media; midday $t_{½}$ > 460000 h (52.5 yr) average over all seasons in water at latitude 40°N, daily average direct photolysis $t_{½}$ > 150 yr (12-h days) in water in the Central U.S. (Zepp et al. 1976)
using fungus and either 254 or 300 nm UV light, more than 97% initial added amounts were metabolized in 3 wk of incubation (Katayama & Matsumura 1991).

Oxidation: $t_{½}$ = 22 yr, estimated first-order half-life in aquatic environment (Callahan et al. 1979)
k < 3600 M^{-1} h^{-1} for singlet oxygen, k = 3600 M^{-1} h^{-1} for RO_2 (Mabey et al., 1982)
photooxidation $t_{½}$ = 17.7–177 h in air, based on estimated rate constant for the reaction with hydroxyl radicals in air (Howard et al. 1991).
photooxidation $t_{½}$ = 168–8400 h in water, based on measured rate of photooxidation in two natural waters under sunlight for 7 d and 56 d (Howard et al. 1991)

Hydrolysis: k(alkaline) = 9.90×10^{-3} M^{-1} s^{-1} at 27°C corresponds to $t_{½}$ = 81 d at pH 9, k(neutral) = 1.9×10^{-9} s^{-1} corresponds to $t_{½}$ = 12 yr in 5% acetonitrile-water at pH 5 and 27°C (Wolfe et al. 1977b)
k(alkaline) = 9.90×10^{-3} M^{-1} s^{-1} at pH 9, k(neutral) = 1.9×10^{-9} s^{-1} for 1×10^{-8} M in water at 27°C (Harris 1982)
k = 1.57×10^{-4} h^{-1} at pH 7 (Neely & Blau 1985)
k = 6.0×10^{-2} yr^{-1} at pH 7.0 and 25°C (Kollig 1993).

Biodegradation: $t_{½}$(aq. aerobic) = 2–15.6 yr based on observed rates of biodegradation in aerobic soils under field conditions (Lichtenstein & Schultz 1959; Stewart & Chisholm 1971; quoted, Howard et al. 1991)
$t_{½}$(aq. anaerobic) = 16–100 d, based on anaerobic flooded soil die-away data for two flooded soils (Castro & Yoshida 1971; quoted, Howard et al. 1991)
$t_{½}$ = 3837 d (Hamaker 1972; quoted, Jury et al. 1983, 1984, 1987a, b, Jury & Ghodrati 1989)
k = 0.00013 d^{-1} from soil incubation studies, and k = 0.0035 d^{-1} from flooded soil incubation studies in anaerobic system both by die-away test (Rao & Davidson 1980; quoted, Scow 1982)
$t_{½}$(aq. aerobic) = 2–15.6 yr, based on aerobic degradation in soil; $t_{½}$(aq. anaerobic) = 16–100 d, based on anaerobic flooded soil die-away study data (Howard et al. 1991)

Biotransformation:

Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants:
k_2 = 0.002, 0.0007 h^{-1} (algae, daphnids, Ellgehausen et al. 1980)
k_2 = 0.052 d^{-1} (catfish, Ellgehausen et al. 1980)
k_1 = 170 d^{-1}; k_2 = 0.0021 d^{-1} (rainbow trout, Oliver & Niimi 1985)
k_1 = 818 d^{-1}; k_2 = 0.009 d^{-1} (rainbow trout, Muir et al. 1985)
k_2 = 8.60 yr^{-1}; k_2 = 4.50 yr^{-1} (*P. hoyi*, Evans et al. 1991)
k_1 = 20609 d^{-1}; k_2 = 1.845 d^{-1} (algae *Selenastrum capricornutum*, Wang et al. 1996)
k_1 = 135.6 d^{-1}; k_2 = 0.191 d^{-1} (water flea *Daphnia magna*, Wang et al. 1996)
k_1 = 9.761 d^{-1}; k_2 = 0.002 d^{-1} (catfish *Ictalurus melas*, Wang et al. 1996)

Half-Lives in the Environment:

Air: $t_{½}$ = 17.7–177 h, based on estimated rate constant for the reaction with hydroxyl radical in air (Howard et al. 1991; Mortimer & Connell 1995);
half-lives for ΣDDT in the Great Lake's atmosphere. $t_{½}$ = 17.0 ± 6.8 yr at Eagle Harbor, $t_{½}$ = 8.2 ± 1.4 yr at Sleeping Bear Dunes and $t_{½}$ = 7.1 ± 1.0 yr at Sturgeon Point (Buehler et al. 2004).

Surface water: dehydrochlorination rate constant k = 1.75×10^{-2} h^{-1} for 1 ppm *p,p′*-DDT and k = 1.65×10^{-2} h^{-1} for 1 ppm *o,p′*-DDT both at 21 ± 2°C and pH 12.8, in 0.1 N NaOH solution (Choi & Chen 1976);
degradation $t_{½}$ = 8 yr in water at 27°C (Wolfe et al. 1977);
midsummer direct photolysis $t_{½}$ > 227000 h in water, $t_{½}$ = 280000 h in hydrocarbon media; midday $t_{½}$ > 460000 h (52.5 yr) average over all seasons in water at latitude 40°N, daily average direct photolysis $t_{½}$ > 150 yr (12-h days) in water in the Central U.S. (Zepp et al. 1976)

$t_{½}$ = 73.9 h for a pond 1 m deep (Branson 1978);
$t_{½}$ = 168–8400 h, based on measured rate of photooxidation in two natural waters under sunlight for 7 d and 56 d (Callahan et al. 1979; quoted, Howard et al. 1991; Mortimer & Connell 1995);
estimated $t_{½}$ = 110 and 56 d for o,p- and p,p-DDT, respectively, in surface waters in case of first order reduction process may be assumed in the Netherlands (Zoeteman et al. 1980)
degradation $t_{½}$ ~ 10 yr average from the loss rates in Lake Michigan (Bierman & Swain 1982).

Ground water: $t_{½}$ = 16 d to 31.3 yr, based on anaerobic flooded soil die-away data for two flooded soils (Castro & Yoshida 1971; quoted, Howard et al. 1991) and observed rates of biodegradation in aerobic soils under field conditions (Lichtenstein & Schultz 1959; Stewart & Chisholm 1971; quoted, Howard et al. 1991).

Sediment: $t_{½}$ = 3 to 5 yr (Bierman & Swain 1982); $t_{½}$ = 21 yr (conversion of *p,p′*-DDT to *p,p′*-DDE in sediment, Oliver et al. 1989); $t_{½}$ = 78800 h (quoted mean value from Howard et al. 1991, Mortimer & Connell 1995).

Soil: $t_{½}$ = 2–15.6 yr, based on observed rates of biodegradation in aerobic soils under field conditions (Lichtenstein & Schultz 1959; Stewart & Chisholm 1971; quoted, Howard et al. 1991);
average $t_{½}$ ~ 12 yr in 3 different soils for ~50 ppm in soil (Nash & Woolson 1967);
estimated persistence of 4 yr in soil (Kearney et al. 1969; Edwards 1973; quoted, Morrill et al. 1982; Jury et al. 1987a);
field $t_{½}$ = 173 d when incorporated into soil (Willis et al. 1971; quoted, Nash 1983);
microagroecosystem $t_{½}$ > 50 d with open cotton canopy (quoted, Nash 1983);
persistence of more than 36 months (Wauchope 1978);
$t_{½}$ > 50 d and subject to plant uptake via volatilization (Callahan et al. 1979; quoted, Ryan et al. 1988);
estimated first-order $t_{½}$ = 14.6 yr from biodegradation rate constant k = 0.00013 d^{-1} from soil incubation studies and $t_{½}$ = 198 d from rate constant k = 0.0035 d^{-1} from flooded soil incubation studies in anaerobic system both by die-away test (Rao & Davidson 1980; quoted, Scow 1982);
very persistent in soils with $t_{½}$ > 100 d (Willis & McDowell 1982);
microagroecosystem $t_{½}$ > 50 d in moist fallow soil (Nash 1983);
$t_{½}$ = 3837 d from screening model calculations (Jury et al. 1984, 1987a, b; Jury & Ghorati 1989);
$t_{½}$ = 173 d from field study, $t_{½}$ > 50 d from microagroecosystem, $t_{½}$ = 116 d from laboratory data (Nash 1985);
$t_{½}$ = 3800 d (Jury et al. 1987; quoted, Montgomery 1993);
reaction $t_{½}$ = 3837 d and overall $t_{½}$ = in soil 9.4 yr (Mackay & Stiver 1991);
estimated field $t_{½}$ = 2000 d (Augustijn-Beckers et al. 1994; Hornsby et al. 1996);
$t_{½}$ = 14.0 and 12.0 yr for control and sludge-amended Luddington soils, respectively, for *o,p′*-DDT, and $t_{½}$ = 11.8 and 10.5 yr for control and sludge-amended Luddington soils, respectively, for *p,p′*-DDT (Meijer et al. 2001).

Biota: field $t_{½}$ = 15 d in fruit leaves (Decker et al. 1950; quoted, Nash 1983);
microagroecosystem $t_{½}$ = 29 d in cotton leaves (Nash & Harris 1977; quoted, Nash 1983);
$t_{½}$ = 915 h from fish compared with calculated value of $t_{½}$ = 517 h from regression (Neely 1980);
$t_{½}$ = 0.70 h in algae, $t_{½}$ = 3.65 d in catfish and $t_{½}$ = 315 h in daphnids (Ellgehausen et al. 1980);
$t_{½}$ = 340 d in rainbow trout (Oliver & Niimi 1985);
biochemical $t_{½}$ = 3837 d (Jury et al. 1987a, b; Jury & Ghodrati 1989);
biological $t_{½}$ = 77 d for trout, $t_{½}$ = 31 d for salmon, $t_{½}$ = 4 d for catfish (Niimi 1987).

TABLE 18.1.1.23.1
Reported aqueous solubilities of DDT at various temperatures

p,p′-DDT				*o,p′*-DDT			
Biggar & Riggs 1974				Biggar & Riggs 1974			
shake flask-GC				shake flask-GC			
t/°C	S/g·m^{-3}	S/g·m^{-3}	S/g·m^{-3}	t/°C	S/g·m^{-3}	t/°C	S/g·m^{-3}
particle size	0.01µ	0.05µ	5.0µ	particle size	0.01µ	0.05µ	5.0µ
15	0.001	0.0025	0.017	15			0.050
25	0.0017	0.006	0.025	25	0.004	0.012	0.085
35	0.0026	0.013	0.037	35			0.135
45	0.0039	0.0275	0.045	45			0.200

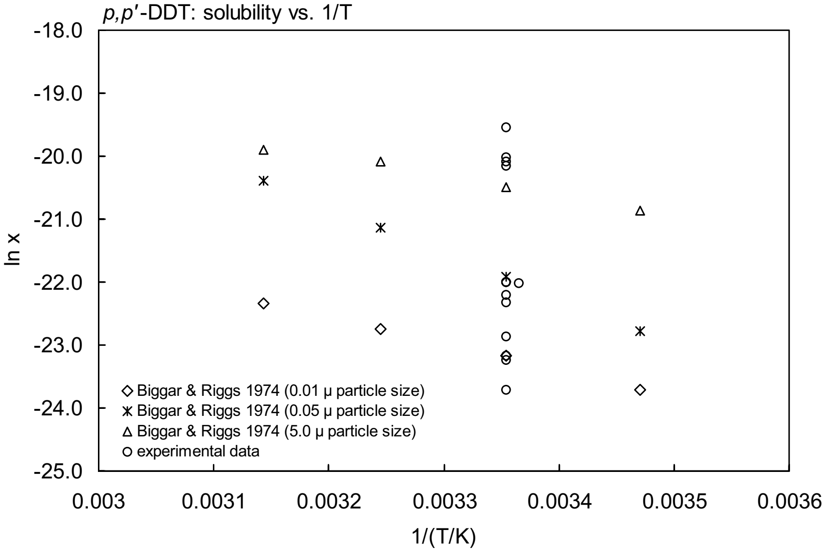


FIGURE 18.1.1.23.1A Logarithm of mole fraction solubility (ln *x*) versus reciprocal temperature for *p,p′*-DDT.

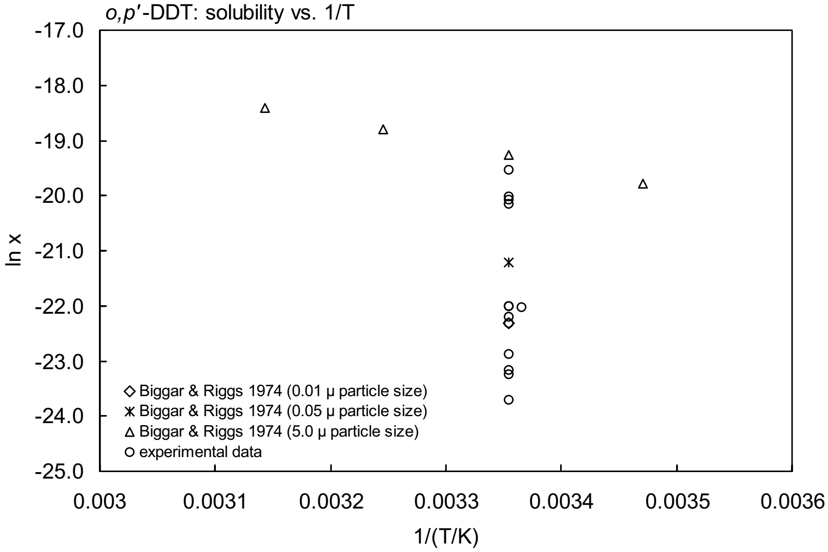


FIGURE 18.1.1.23.1B Logarithm of mole fraction solubility (ln *x*) versus reciprocal temperature for *o,p′*-DDT.

TABLE 18.1.1.23.2
Reported vapor pressures of DDT at various temperatures and the coefficients for the vapor pressure equations

$\log P = A - B/(T/K)$	(1)	$\ln P = A - B/(T/K)$	(1a)
$\log P = A - B/(C + t/°C)$	(2)	$\ln P = A - B/(C + t/°C)$	(2a)
$\log P = A - B/(C + T/K)$	(3)		
$\log P = A - B/(T/K) - C \cdot \log (T/K)$	(4)		

1.

Balson 1947		Dickinson 1956		Spencer & Cliath 1972		Rothman 1980	
effusion manometer		gas saturation-spec.		gas saturation-GC		radiotracer transpiration	
t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa
p,p′-DDT		*p,p′*-DDT		*p,p′*-DDT		*p,p′*-DDT	
0	5.87×10^{-7}	71.0	0.01947	20	2.03×10^{-5}	20	2.93×10^{-5}
10	3.60×10^{-6}	71.0	0.02586	30	9.68×10^{-5}	25	5.73×10^{-5}
20	2.00×10^{-5}	71.0	0.02733	40	4.43×10^{-4}	30	1.24×10^{-4}
30	9.60×10^{-5}	70.7	0.02706			40	5.33×10^{-4}
40	4.27×10^{-4}	70.7	0.02640	eq. 1	P/mmHg	50	2.0×10^{-3}
50	1.77×10^{-3}	70.7	0.02680	A	14.24	60	6.40×10^{-3}
60	4.00×10^{-3}	71.3	0.02973	B	6176	70	0.020
70	0.0231	71.3	0.02893			80	0.060
80	0.0301	50.1	0.001973	*o,p′*-DDT			
90	0.224	50.1	0.002027	30	7.37×10^{-4}	ΔH_{sub} = 100.6 kJ/mol	
100	0.640	60.1	0.007106				
		60.1	0.006999				
		60.1	0.007199				
eq. 1	P/mmHg	80.4	0.08053				
A	14.191	80.4	0.07666				
B	6160	80.4	0.07879				
temp range: 66–100°C		80.4	0.07599				
		88.8	0.2039				
		88.8	0.1933				
		90.2	0.2200				
		90.2	0.2346				
		eq. 1	P/mmHg				
		A	13.778				
		B	6010				

TABLE 18.1.1.23.2 (*Continued*)

2.

Westcott et al. 1981		Westcott & Bidleman 1981		Wania et al. 1994	
gas saturation-GC		capillary GC-RT correlation		gas saturation-GC/ECD	
t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa
o,p′-DDT		*o,p′*-DDT		*p,p′*-DDT	
30	1.17×10^{-3}	25	6.0×10^{-4}	0	5.003×10^{-7}
		30	1.12×10^{-3}	10	2.531×10^{-6}
				20	1.715×10^{-5}
		p,p′-DDT		30	8.180×10^{-5}
		30	1.87×10^{-3}	40	3.846×10^{-4}
				eq. 1	P/Pa
				A	16.62
				B	6276
				for temp range 0–40°C	
				enthalpy of sublimation: ΔH_{sub} = 120.2 kJ/mol	

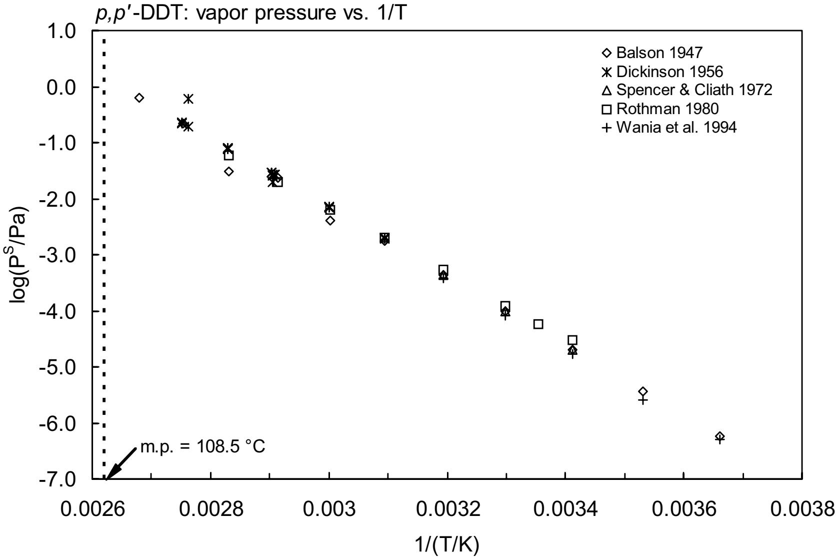


FIGURE 18.1.1.23.2 Logarithm of vapor pressure versus reciprocal temperature for *p,p′*-DDT.

TABLE 18.1.1.23.3
Reported octanol-air partition coefficients of DDT at various temperatures

p,p′-DDT				*o,p′*-DDT	
Harner & Mackay 1995		**Shoeib & Harner 2002**		**Shoeib & Harner 2002**	
generator column-GC/MS		**generator column-GC**		**generator column-GC**	
t/°C	**log K_{OA}**	**t/°C**	**log K_{OA}**	**t/°C**	**log K_{OA}**
15		15	10.307	5	10.905
25	10.09	25	9.879	15	10.455
35		35	9.295	20	9.881
45		45	8.824	25	9.660
		25	9.816	35	9.1959
log K_{OA} = A + B/(T/K)		log K_{OA} = A + B/(T/K)		log K_{OA} = A + B/(T/K)	
A	–3.20	A	–5.63	A	–11.291
B	3954	B	4603	B	6266
enthalpy of phase change $\Delta H_{OA}/(kJ\ mol^{-1}) = 75.7$		$\Delta H_{OA}/(kJ\ mol^{-1}) = 88.1$		$\Delta H_{OA}/(kJ\ mol^{-1}) = 87.9$	

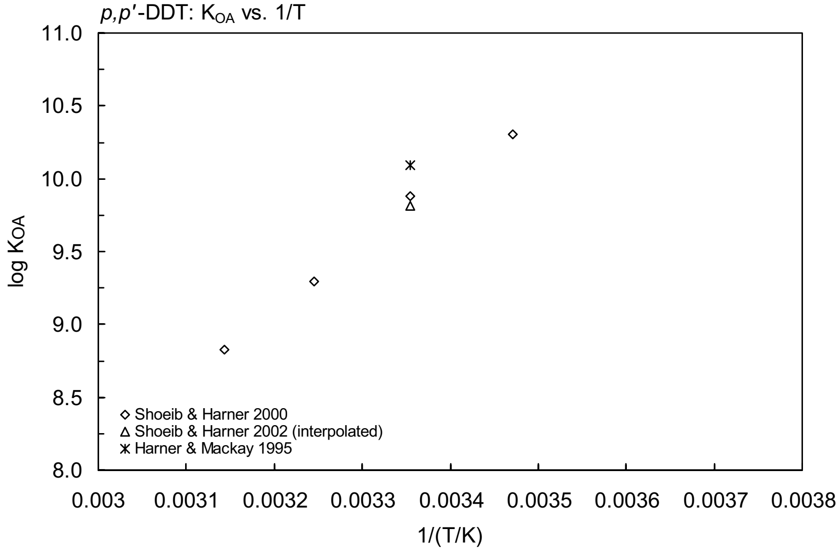


FIGURE 18.1.1.23.3A Logarithm of K_{OA} versus reciprocal temperature for *p,p′*-DDT.

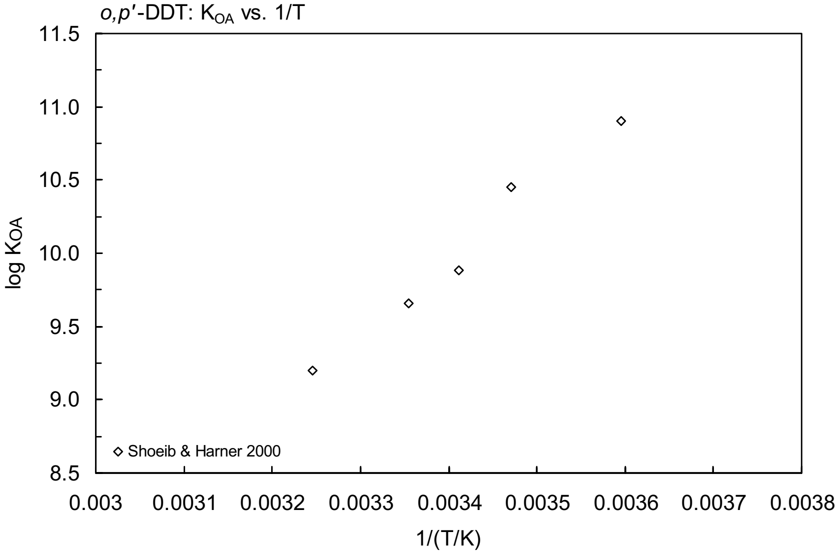
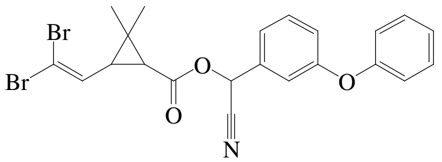


FIGURE 18.1.1.23.3B Logarithm of K_{OA} versus reciprocal temperature for *o,p′*-DDT.

18.1.1.24 Deltamethrin



Common Name: Deltamethrin
Synonym: Decis, K-Othrin, Butoss, RU 22074, Cislin, Crackdown
Chemical Name: *S*-α-cyano-3-phenoxybenzyl (1*R*,3*R*)-3-(2,2-dibromovinyl)-2,2-dimethyl cyclopropan-1-carboxylate
CAS Registry No: 52918-63-5
Uses: insecticide (pyrethroid)
Molecular Formula: $C_{22}H_{19}Br_2NO_3$
Molecular Weight: 505.199
Melting Point (°C):

98–101	(Hartley & Kidd 1987)
98–102	(Tomlin 1994)

Boiling Point (°C):
Density (g/cm^3 at 20°C):

0.55	(25°C, bulk density, Tomlin 1994)

Molar Volume (cm^3/mol):
Dissociation Constant, pK_a:
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
Entropy of Fusion, ΔS_{fus} (J/mol K):
Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F:

Water Solubility (g/m^3 or mg/L at 25°C):

<0.002	(20°C, Hartley & Kidd 1987)
<0.0002	(Tomlin 1994)

Vapor Pressure (Pa at 25°C):

2.0×10^{-6}	(Hartley & Kidd 1987)
$<1.33 \times 10^{-5}$	(Tomlin 1994)

Henry's Law Constant (Pa·m^3/mol):

12.6	(gas stripping-LSC, Muir et al. 1985a)

Octanol/Water Partition Coefficient, log K_{OW}:

5.20	(HPLC-RT correlation, Muir et al. 1985b)
6.20	(shake flask, Log P Database, Hansch & Leo 1987)
6.21	(HPLC-RT correlation, Hu & Leng 1992)
6.20	(recommended, Sangster 1993)
4.60	(Tomlin 1994)
6.20	(recommended, Hansch et al. 1995)
5.74	(RP-HPLC-RT correlation using short ODP column, Donovan & Pescatore 2002)

Octanol/Air Partition Coefficient, log K_{OA}:

Bioconcentration Factor, log BCF or log K_B:

1.53–3.0	(fathead minnows, Muir et al. 1985a)
2.06–2.48	(chironomid larvae, Muir et al. 1985b)
2.62, 2.70	(*Oncorhynchus mykiss*, flow-through condition, quoted, Devillers et al. 1996)

Sorption Partition Coefficient, log K_{OC}:

3.66–4.21 (Tomlin 1994)

Environmental Fate Rate Constants, k, or Half-Lives, $t_{½}$:

Volatilization:

Photolysis: $t_{½}$ = 9 d in soil (Tomlin 1994).

Oxidation:

Hydrolysis: more stable in acidic than in alkaline media with $t_{½}$ = 2.5 d at pH 9 and 25°C (Tomlin 1994).

Biodegradation: microbial degradation half-life are, $t_{½}$(aerobic) = 21–25 d, $t_{½}$(anaerobic) = 31–36 d in laboratory; $t_{½}$ < 23 d in field (Tomlin 1994)

Biotransformation:

Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants:

Half-Lives in the Environment:

Air:

Surface water: $t_{½}$ = 2–4 d in water of small outdoor ponds (Muir et al. 1985);
more stable in acidic than in alkaline media with $t_{½}$ = 2.5 d at pH 9 and 25°C (Tomlin 1994).

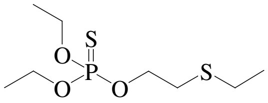
Ground water:

Sediment:

Soil: undergoes microbial degradation within 1–2 wk (Hartley & Kidd 1987)
microbial degradation half-life are, $t_{½}$(aerobic) = 21–25 d, $t_{½}$(anaerobic) = 31–36 d in laboratory; $t_{½}$ < 23 d in field; photolysis $t_{½}$ = 9 d (Tomlin 1994).

Biota:

18.1.1.25 Demeton



Common Name: Demeton
Synonym: Bayer 8169, Demeton-O, E-1059, mercaptophos, Systox-O
Chemical Name: *O,O*-diethyl-*O*-(2-ethylthioethyl)phosphorothioate mixture with *O,O*-diethyl-*S*-(2-ethylthioethyl)-phosphorothioate
Uses: insecticide to control sucking insects and mites in a wide range of crops, including fruit, nuts, vegetables, ornamentals, and field crops; also used as acaricide.
CAS Registry No: 8065-48-3, 298-03-3 demeton-O, systox-O
126-75-0 demoton-S, systox-S
Molecular Formula: $C_8H_{19}O_3PS_2$
Molecular Weight: 258.339
Melting Point (°C):
pale yellow oil (Hartley & Kidd 1987)
Boiling Point (°C):

123	(Khan 1980)
92–93	(at 0.15 mmHg, Hartley & Kidd 1987)

Density (g/cm^3 at 20°C):

1.119	(25°C, Spencer 1982)
1.119–1.132	(Hartley & Kidd 1987)

Molar Volume (cm^3/mol):

264.8	(calculated-Le Bas method at normal boiling point)

Dissociation Constant, pK_a:
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
Entropy of Fusion, ΔS_{fus} (J/mol K):
Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F: 1.0

Water Solubility (g/m^3 or mg/L at 25°C or as indicated):

60	(20°C, Kenaga 1980a)
60	(22°C, Khan 1980; Worthing & Walker 1983)
100	(20–25°C, Willis & McDowell 1982)
60	(rm. temp., Spencer 1982; Hartley & Kidd 1987)
60	(20–25°C, selected, Augustijn-Beckers et al. 1994; Hornsby et al. 1996)

Vapor Pressure (Pa at 25°C or as indicated):

0.0973, 0.0987	(30°C, demeton-O, demeton-S, Eichler 1965)
0.00331, 0.0347	(20°C, demeton-O, demeton-S, Melnikov 1971)
0.00373, 0.0347	(20°C, demeton-O, demeton-S, Hartley & Graham-Bryce 1980)
0.0331	(Khan 1980)
0.033	(20°C, Spencer 1982)
0.0167, 0.00707	(20°C, demeton-O, demeton-S, GC-RT correlation, Kim 1985)
0.034	(20°C, Hartley & Kidd 1987)
0.030	(20°C, selected, Suntio et al. 1988)
0.1333	(20–25°C, selected, Augustijn-Beckers et al. 1994; Hornsby et al. 1996)

Henry's Law Constant (Pa·m^3/mol at 25°C or as indicated):

0.130	(20°C, calculated-P/C, Suntio et al. 1988)

Octanol/Water Partition Coefficient, log K_{OW}:

Octanol/Air Partition Coefficient, log K_{OA}:

Bioconcentration Factor, log BCF:

1.79	(calculated-S, Kenaga 1980)

Sorption Partition Coefficient, log K_{OC}:

2.66	(soil, calculated-S, Kenaga 1980)
1.85	(20–25°C, estimated, Augustijn-Beckers et al. 1994; Hornsby et al. 1996)

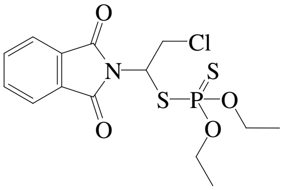
Environmental Fate Rate Constants, k, or Half-Lives, $t_{½}$:

Oxidation: calculated rate constant $k = 128 \times 10^{-12}$ cm^3 $molecule^{-1}$ s^{-1} for the vapor phase reaction with hydroxyl radical in air (Winer & Atkinson 1990).

Half-Lives in the Environment:

Soil: selected field $t_{½}$ = 15 d (Augustijn-Beckers et al. 1994; Hornsby et al. 1996).

18.1.1.26 Dialifor



Common Name: Dialifor
Synonym: dialiphos, Torak
Chemical Name: *S*-(2-chloro-(1,3-dihydro-1,3-dioxo-2*H*-isoindol-2-y)ethyl) *O*,*O*-diethyl phosphorodithioate
CAS Registry No: 10311-84-9
Uses: insecticide/acaricide
Molecular Formula: $C_{14}H_{17}ClNO_4PS_2$
Molecular Weight: 393.846
Melting Point (°C):
68 (Lide 2003)
Boiling Point (°C):
Density (g/cm^3 at 20°C):
Molar Volume (cm^3/mol):
Dissociation Constant, pK$_a$:
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
Entropy of Fusion, ΔS_{fus} (J/mol K):
Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F: 0.379 (mp at 68°C)

Water Solubility (g/m^3 or mg/L at 25°C):
0.18 (Chiou et al. 1977; Kenaga 1980b)
< 1.0 (Hartley & Kidd 1987)
0.18 (room temp., Montgomery 1993)

Vapor Pressure (Pa at 25°C):
0.133 (35°C, Hartley & Kidd 1987)
1.08×10^{-7} (20°C, Montgomery 1993)

Henry's Law Constant (Pa·m^3/mol at 25°C):
0.142 (20°C, calculated-P/C, Montgomery 1993)

Octanol/Water Partition Coefficient, log K_{OW}:
4.69 (shake flask-GC, Chiou et al. 1977; quoted, Rao & Davidson 1980; Sangster 1993)
4.69 (Montgomery 1993)

Octanol/Air Partition Coefficient, log K_{OA}:

Bioconcentration Factor, log BCF or log K_B:
3.21 (calculated, Kenaga 1980b)

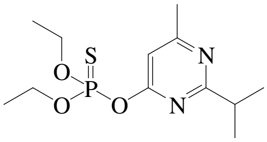
Sorption Partition Coefficient, log K_{OC}:
4.04 (soil, calculated, Kenaga 1980b)
4.05 (Montgomery 1993)

Environmental Fate Rate Constants, k, or Half-Lives, $t_{1/2}$:
Hydrolysis: $t_{1/2}$ = 14 h at 20°C and pH 7.4, $t_{1/2}$ = 1.8 h at 37.5°C and pH 7.4 (Montgomery 1993).

Half-Lives in the Environment:

Air:
Surface water: hydrolysis $t_{1/2}$ = 14 h at 20°C and pH 7.4, $t_{1/2}$ = 1.8 h at 37.5°C and pH 7.4 (Montgomery 1993).
Ground water:
Sediment:
Soil:
Biota: rapidly eliminated in animal (Hartley & Kidd 1987).

18.1.1.27 Diazinon



Common Name: Diazinon

Synonym: Alfa-Tox, AG-500, Basudin, Bazinon, Bazuden, Ciazinon, Dacutox, Dassitox, Dazzel, Desapon, Dianon, Diater, Diaterr-fos, Diazitol, Diazide, Diazol, Dicid, Dimpylate, Dipofene, Dizinon, Dyzol, ENT 19507, Flytrol, G 301, Gardentox, Geigy 24480, Kayazinon, Kayazol, NA 2763, Nedicisol, Neocidol, Nipsan, Nucidol, Sarolex, Spectracide

Chemical Name: *O,O*-diethyl *O*-2-isopropyl-6-methylpyrimidin-4-yl phosphorothioate; *O,O*-diethyl-*O*-(2-isopropyl-6-methyl 4-pyrimidinyl) phosphorothioate; *O,O*-diethyl 2-isopropyl-4-methylpyrimidinyl-6-thiophosphate

Uses: nonsystemic insecticide to control flies, aphids and spider mites in soil, fruit, vegetables and ornamentals; also used as acaricide.

CAS Registry No: 333-41-5

Molecular Formula: $C_{12}H_{21}N_2O_3PS$

Molecular Weight: 304.345

Melting Point (°C):
colorless oil (Hartley & Kidd 1987; Tomlin 1994)

Boiling Point (°C):
125 (at 1 mmHg, Hartley & Kidd 1987; Tomlin 1994; Milne 1995)
83–84 (at 0.0002 mmHg, Montgomery 1993; Tomlin 1994)

Density (g/cm^3 at 20°C):
1.11 (Worthing & Hance 1991)
1.116–1.118 (Montgomery 1993; Tomlin 1994; Milne 1995)

Molar Volume (cm^3/mol):
320.2 (calculated-Le Bas method at normal boiling point)

Dissociation Constant, pK_a:
< 2.5 (Albert 1963; Perrin 1989; Somasundaram et al. 1991; Montgomery 1993)

Enthalpy of Vaporization, ΔH_V (kJ/mol):
87.5 (Rordorf 1989)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

Entropy of Fusion, ΔS_{fus} (J/mol K):

Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F: 1.0

Water Solubility (g/m^3 or mg/L at 25°C):
40 (Spencer 1973, 1982; Martin & Worthing 1977; Worthing 1979, Worthing & Walker 1987)
40 (Wauchope 1978; Briggs 1981; Burkhard & Guth 1981; Kanazawa 1989)
68.8 (22°C, shake flask-GC, Bowman & Sans 1979, 1983a, b)
40 (Hartley & Graham-Bryce 1980)
40 (22°C, Khan 1980)
40.5 (20–25°C, shake flask-GC, Kanazawa 1981)
40 (20°C, Windholz 1983)
40 (20°C, Hartley & Kidd 1987; Worthing & Hance 1991; Tomlin 1994; Milne 1995)
60 (20–25°C, selected, Wauchope et al. 1992; Hornsby et al. 1996)
53.5, 43.7 (20°C, 30°C, Montgomery 1993)
52.36, 103.8 (supercooled liquid S_L: literature-derived value LDV, final adjusted value FAV, Muir et al. 2004)

Vapor Pressure (Pa at 25°C or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):
0.0187 (Margot & Stammbach 1964)
0.0111 (20°C, Wolfdietrich 1965)
0.0112 (20°C, Melnikov 1971)

0.0161 (gas saturation, Heiber & Szelagiewicz 1976)
0.020 (gas saturation method, measured range 32–73°C, Marti 1976)
log (P/mmHg) = 11.46 – 4569.55/(T/K), temp range 32–73°C (Marti 1976)
0.0187 (Worthing 1979)
0.019 (20°C, Hartley & Graham-Bryce 1980)
0.0187 (Khan 1980)
0.00971 (20°C, volatilization rate, Burkhard & Guth 1981)
0.00236–0.00469 (20°C, GC, Seiber et al. 1981)
0.0109* (gas saturation-GC, measured range 25.3–45. 0°C, Kim et al. 1984)
log (P/mmHg) = 9.3871 – 4014.67/(T/K); temp range 25.3–45°C (gas saturation, Kim et al. 1984)
0.0064 (20°C, extrapolated-Clausius-Clapeyron eq. with vapor pressures at several temp, Kim et al. 1984)
0.0024 (20°C, GC-RT correlation, Kim et al. 1984; Kim 1985)
9.7×10^{-5} (20°C, Hartley & Kidd 1987; Worthing & Hance 1991)
0.014* (gas saturation-GC, measured range 25–125°C, Rordorf 1989)
log (P_L/Pa) = 13.482 – 4571.2/(T/K); measured range 32.4–140°C (liquid, gas saturation-GC, Rordorf 1989)
0.020 (GC-RT correlation, supercooled liquid value, Hinckley et al. 1990)
0.008 (20–25°C, selected, Wauchope et al. 1992; Hornsby et al. 1996)
0.0113 (20°C, Montgomery 1993)
0.012 (20°C, Tomlin 1994)
0.0123 (liquid P_L, GC-RT correlation, Donovan 1996)
0.011 (gradient GC method; Tsuzuki 2000)
0.011; 0.0339, 0.0513 (gradient GC method; estimation using modified Watson method: Sugden's parachor, McGowan's parachor, Tsuzuki 2000)
0.014, 0.0073 (supercooled liquid P_L: literature-derived value LDV, final adjusted value FAV, Muir et al. 2004)

Henry's Law Constant (Pa m^3/mol at 25°C or as indicated. Additional data at other temperatures designated * are compiled at the end of this section):

0.074 (20°C, volatilization rate, Burkhard & Guth 1981)
0.0114 (calculated, Adachi et al. 1984)
0.124 (calculated-P/C, Jury et al. 1984, 1987a; Jury & Ghodrati 1989)
0.0114 (23°C, wetted-wall column-GC/ECD, Fendinger & Glotfelty 1988)
0.0669 (20°C, calculated-P/C, Suntio et al. 1988)
0.1438 (calculated-P/C, Taylor & Glotfelty 1988)
0.0138, 0.0101 (22–24°C, fog chamber-GC/ECD: drain water, cyclone water, Fendinger et al. 1989)
0.007 (calculated-bond contribution method LWAPC, Meylan & Howard 1991)
0.0114 (20°C, calculated-P/C, Montgomery 1993)
0.0406 (calculated-P/C, this work)
0.0338* (20°C, gas stripping-GC/MS, measured range 283–301 K, Feigenbrugel et al. 2004)
$H'/(M\ atm^{-1}) = (7.2 \pm 0.5) \times 10^{-15} \exp[(11900 \pm 700)/(T/K)]$; temp range 283–310 K (Arrhenius eq., gas stripping-GC/MS, Feigenbrugel et al. 2004)
0.0108, 0.0216 (literature-derived value LDV, final adjusted value FAV, Muir et al. 2004)

Octanol/Water Partition Coefficient, log K_{OW}:

3.02 (Rao & Davidson 1980)
3.11 (shake flask-UV, Lord et al. 1980)
3.11 (20°C, shake flask-UV, Briggs 1981)
3.14 (shake flask-GC, Kanazawa 1980, 1981)
3.81 (shake flask-GC, Bowman & Sans 1983b)
1.92 (Veith & Kosian 1983)
3.02 (shake flask, Log P Database, Hansch & Leo 1987)
3.02–3.81 (Montgomery 1993)
3.70 (RP-HPLC-RT correlation, Saito et al. 1993)
3.58 (RP-HPLC-RT correlation, Sicbaldi & Finizio 1993)
3.30 (Tomlin 1994)

3.81 (recommended, Hansch et al. 1995)
3.58 (RP-HPLC-RT correlation, Finizio et al. 1997)
4.23 (RP-HPLC-RT correlation, Nakamura et al. 2001)
3.81 (literature-derived value LDV, Muir et al. 2004)

Octanol/Air Partition Coefficient, log K_{OA}:
8.87 (final adjusted value FAV, Muir et al. 2004)

Bioconcentration Factor, log BCF:
2.39 (motsugo, Kanazawa 1975)
1.54 (fish in flowing water, Alison & Hermanutz 1977)
2.18, 1.56 (topmouth gudugeon, silver crucian carp, Kanazawa 1978, 1981)
1.81; 1.24 (carp; guppy, Kanazawa 1978)
0.69, 1.23, 0.77 (crayfish, red snail, pond snail, Kanazawa 1978)
1.83; 0.954 (fish; invertebrates, Kanazawa 1978)
1.89 (calculated-S, Kenaga 1980)
2.75 (earthworms, Lord et al. 1980)
2.08, 1.80 (carp, rainbow trout, Seguchi & Asaka 1981)
1.41, 0.477 (loach, shrimp, Seguchi & Asaka 1981)
1.81; 1.24; 2.18 (carp; guppy; topmouth gudgeon, Veith & Kosian 1983)
2.32 (topmouth gudgeon, Kanazawa 1983)
2.30 (sheepshead minnow, Zaroogian et al. 1985)
1.46 (Isnard & Lambert 1988)
–0.59 (vegetation, correlated-K_{OW}, Nash 1974)
2.39 (willow shiner, Tsuda et al. 1989; Tsuda et al. 1992)
1.81, 2.08 (carp, De Bruijn & Hermens 1991)
1.38, 1.81, 1.81 (loach, motsugo, rainbow trout, De Bruijn & Hermens 1991)
2.16–2.33 (sheepshead minnow, De Bruijn & Hermens 1991)
1.56, 2.18 (silver crucian carp, topmouth gudgeon, De Bruijn & Hermens 1991)
2.18, 1.79 (pale chub, ayu sweetfish, calculated-field data, Tsuda et al. 1992)
3.20 (eel, Sancho et al. 1993)
2.02 (killifish *Oryzias latipes*, after 24–72 h exposure, Tsuda et al. 1995)
1.34, 1.45 (*Oryzias latipes*, Tsuda et al. 1995; quoted, Devillers et al. 1996)

Sorption Partition Coefficient, log K_{OC}:
2.76 (calculated-S as per Kenaga & Goring 1978, Kenaga)
2.93 (Rao & Davidson 1980)
2.28, 2.40 (average of 3 soils, 1 sediment, Sharom et al. 1980)
2.36 (soil, sorption isotherm, converted from reported log K_{OM} of 2.12, Briggs 1981)
2.36 (estimated, Lyman et al. 1982; quoted, Howard 1991; Lohninger 1994)
2.93 (screening model calculations, Jury et al. 1987b; Jury & Ghodrati 1989)
2.40 (average of 2 soils, Kanazawa 1989)
2.12, 3.27 (reported, estimated as log K_{OM}, Magee 1991)
2.75, 3.13 (soil, quoted exptl., calculated-χ and fragment contribution, Meylan et al. 1992)
3.00 (soil, 20–25°C, estimated, Wauchope et al. 1992; Hornsby et al. 1996)
2.76 (soil, average value, Dowd et al. 1993)
3.00–3.27 (Montgomery 1993)
2.75 (soil, calculated-MCI $^1\chi$, Sabljic et al. 1995)
2.75, 3.05 (soil, estimated-class-specific model, estimated-general model, Gramatica et al. 2000)
2.74, 2.64, 2.90 (soils: organic carbon $OC \geq 0.1\%$, $OC \geq 0.5\%$, $0.1 \leq OC < 0.5\%$, average, Delle Site 2001)
3.12–3.16 (sediments from San Diego Creek and Bonita Creek, shake flask-GC, Bondarenko & Gan 2004)

Environmental Fate Rate Constants, k, or Half-Lives, $t_{1/2}$:
Volatilization: mostly dissipated through volatilization with $t_{1/2}$ = 19 d from soil (Glotfelty et al. 1990).

Photolysis: calculated $t_{1/2}$ = 15 d for photolysis in an aqueous buffer solution at pH 7 and 25°C under UV light for 24 h (Burkhard & Guth 1979; quoted, Montgomery 1993);

$t_{1/2}$ = 41 d without addition of humic substances; $t_{1/2}$ = 9 d and $t_{1/2}$ = 5 d with concn of humic acid 20 mg/L and 50 mg/L, respectively, under light intensity $\lambda \geq 290$ nm (Mansour & Feicht 1994)

Photodegradation ($\lambda > 290$ nm) half-lives in various diazinon aqueous solutions: $t_{1/2}$ ~ 1 d river water exposed to sunlight, $t_{1/2}$ ~ 5 d lake water exposed to sunlight and $t_{1/2}$ ~ 5.5 d with humic acid exposed to sunlight (Mansour et al. 1997)

photolytic $k = 2.39 \times 10^{-3}$ h^{-1} with $t_{1/2}$ = 290 h in moist sandy soil, $k = 6.62 \times 10^{-5}$ h^{-1} with $t_{1/2}$ = 10500 h in dry sandy soil; $k = 2.55 \times 10^{-3}$ h^{-1} in moist sandy loam (Graebing & Chib 2004)

Oxidation: photooxidation $t_{1/2}$ = 4.1 h in air, estimated from the vapor-phase reaction with 5×10^5 hydroxyl radicals/m^3 in air at 25°C (Martin & Worthing 1977; quoted, Howard 1991).

$k_{OH} = 9.7 \times 10^{-11}$ cm^3 molecule^{-1} s^{-1} at 298 K in gas phase with atmospheric lifetime of 4.1 h but reduced to .19 h at 283 K; log k_{OH}(aq.) = 8.2×10^9 M^{-1} s^{-1} in aqueous phase (Feigenbrugel et al. 2004)

Hydrolysis:

k(acid) = 2.1×10^{-2} M^{-1} s^{-1} for acid catalyzed hydrolysis, k(neutral) = 4.3×10^{-8} M^{-1} s^{-1} for neutral hydrolysis and k(alkaline) = 5.3×10^{-3} M^{-1} s^{-1} for base catalyzed hydrolysis with 10^{-5} M in aqueous buffer (Faust & Gomaa 1972; quoted, Freed 1976; Harris 1982)

$t_{1/2}$ = 11.77 h at pH 3.1, $t_{1/2}$ = 185 d at pH 7.4 and $t_{1/2}$ = 6.0 d at pH 10.4 in water at 20°C (Worthing & Hance 1991; Tomlin 1994)

$t_{1/2}$ = 11.77 h at pH 3.1, $t_{1/2}$ = 185 d at pH 7.4, $t_{1/2}$ = 136 d at pH 9.0, and $t_{1/2}$ = 6 d at pH 10.4 at 20°C (Montgomery 1993).

Biodegradation:

half-lives $t_{1/2}$ = 4.91 d at pH 3.1 and $t_{1/2}$ = 185 d at pH 7.4 from river die-away tests (Gomaa et al. 1969; quoted, Scow 1982)

$t_{1/2}$ = 12.5 wk in sterile soils and $t_{1/2}$ < 1 wk in nonsterile soils; $t_{1/2}$ = 6.5 wk in sterile sandy loam and $t_{1/2}$ = 2 wk in nonsterile sandy loam (Miles et al. 1979; quoted, Howard 1991)

$t_{1/2}$ = 32 d in 0–10 cm depth of soil by 100 d leaching screening test (Rao & Davidson 1980; quoted, Jury et al. 1983, 1984, 1987a, b; Jury & Ghodrati 1989)

k = 0.023 d^{-1} with estimated first-order $t_{1/2}$ = 30 d in soil incubation studies by soil die-away test (Rao & Davidson 1980; quoted, Scow 1982)

k(av.) = 0.0193 d^{-1} in silty clay with $t_{1/2}$ = 36 d; and k(av.) = 0.0245 d^{-1} in sandy clay with $t_{1/2}$ = 28 d (Sattar 1990)

Biotransformation:

Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants:

k_2 = 0.070 h^{-1} (willow shiner, Tsuda et al. 1989)

k_2 = 0.023 h^{-1} (eel's liver, Sancho et al. 1993)

k_2 = 0.019 h^{-1} (eel's muscle, Sancho et al. 1993)

k_2 = 0.21 h^{-1} (killifish *Oryzias latipes*, Tsuda et al. 1995)

Half-Lives in the Environment:

Air: photooxidation $t_{1/2}$ = 4.1 h, estimated from the vapor-phase reaction with 5×10^5 hydroxyl radicals/m^3 in air at 25°C (Martin & Worthing 1977; quoted, Howard 1991).

Surface water: photolysis $t_{1/2}$ = 41 d without humic substances; $t_{1/2}$ = 13 d and 5 d with concn of humic acid 20 mg/L and 50 mg/L, respectively, under light intensity $\lambda \geq 290$ nm (Mansour & Feicht 1994);

$t_{1/2}$ = 144 d at 6°C, $t_{1/2}$ = 69 d at 22°C in darkness for Milli-Q water; $t_{1/2}$ = 181 d at 6°C, $t_{1/2}$ = 80 d at 22°C in darkness, $t_{1/2}$ = 43 d under sunlight conditions for river water at pH 7.3; $t_{1/2}$ = 132 d at 6°C, $t_{1/2}$ = 52 d at 22°C in darkness for filtered river water at pH 7.3; $t_{1/2}$ = 125 d at 6°C, $t_{1/2}$ = 50 d at 22°C in darkness, $t_{1/2}$ = 47 d under sunlight conditions for seawater, pH 8.1 (Lartiges & Garrigues 1995).

Ground water:

Sediment: first-order degradation k = 0.048 d^{-1} with $t_{1/2}$ = 14.4 d under aerobic conditions, k = 0.022 d^{-1} with $t_{1/2}$ = 31.7 d under anaerobic conditions in sediment from San Diego Creek, Orange County, CA; first-order degradation k = 0.033 d^{-1} with $t_{1/2}$ = 21.1 d under aerobic conditions, k = 0.029 d^{-1} with $t_{1/2}$ = 23.7 d under anaerobic conditions in sediment from Bonita Creek, Orange County, CA (Bondarendo & Gan 2004)

Soil: $t_{1/2}$ = 43.8 d in sterile soil at pH 4.7 (Sethunathan & MacRae 1969; quoted, Montgomery 1993);

estimated persistence of 12 wk in soil (Kearney et al. 1969; Edwards 1973; quoted, Morrill et al. 1982; Jury et al. 1987a);

persistence of 3 months (Wauchope 1978);

$t_{1/2}$ = 12.5 wk in sterile sandy loam and $t_{1/2}$ < 1.0 wk in nonsterile sandy loam; $t_{1/2}$ = 6.5 wk in sterile organic soil and $t_{1/2}$ = 2.0 wk in nonsterile organic soil (Miles et al. 1979);

estimated first-order $t_{1/2}$ = 30 d in soil from biodegradation rate constant k = 0.023 d^{-1} for soil incubation studies by soil die-away test (Rao & Davidson 1980; quoted, Scow 1982);

moderate persistent in soil with $t_{1/2}$ = 20–100 d (Willis & McDowell 1982);

$t_{1/2}$ = 32 d from screening model calculations (Jury et al. 1987a, b; Jury & Ghodrati 1989);

dissipation $t_{1/2}$ = 19 d in soil (Glotfelty et al. 1990);

av. degradation rate constant k = 0.0193 d^{-1} in silty clay with $t_{1/2}$ = 36 d and average degradation rate constant k = 0.0245 d^{-1} in sandy clay with $t_{1/2}$ = 28 d (Sattar 1990)

selected field $t_{1/2}$ = 40 d (Wauchope et al. 1992; Dowd et al. 1993; Hornsby et al. 1996);

soil $t_{1/2}$ = 65 d (Pait et al. 1992)

$t_{1/2}$ = 40 d (selected, Halfon et al. 1996)

On sandy soil: first-order rate constants for photolytic decline, k = 5.45×10^{-3} h^{-1} with $t_{1/2}$ = 130 h irradiated in moisture-maintained soil, k = 0.84×10^{-3} h^{-1} with $t_{1/2}$ = 830 h irradiated in air-dried soil, k = 3.06×10^{-3} h^{-1} with $t_{1/2}$ = 230 h in dark control moist soil and k = 0.77×10^{-3} h^{-1} with $t_{1/2}$ = 900 h in dark control air-dried sandy soil from Sauk County, WI. The photolytic k = 2.39×10^{-3} h^{-1} with $t_{1/2}$ = 290 h in moist soil, k = 6.62×10^{-5} h^{-1} with $t_{1/2}$ = 10500 h in dry soil. The contribution of moisture to irradiated metabolism k = 4.61×10^{-3} h^{-1} with $t_{1/2}$ = 150 h, but for dark control system for k = 2.29×10^{-5} h^{-1} with $t_{1/2}$ = 300 h (Graebing & Chib 2004)

On sandy loam soil: first-order rate constants for photolytic decline, k = 4.07×10^{-3} h^{-1} irradiated in moisture-maintained soil, k = 1.07×10^{-3} h^{-1} irradiated in air-dried soil, k = 1.52×10^{-3} h^{-1} in dark control moist soil and no degradation in dark control air-dried sandy loam soil from Madia, CA. $t_{1/2}$ = 120 h for the first 96 h irradiation; over all $t_{1/2}$(calc) = 200 h from 96–168 h but in dark control system $t_{1/2}$ = 460 h in moist sandy loam soil; irradiated metabolism $t_{1/2}$ = 650 h in dry sandy loam soils. Rate constants due to photolysis k = 2.55×10^{-3} h, and due to moisture k = 3.0×10^{-3} h in moist sandy loam soil (Graebing & Chib 2004)

Biota: biochemical $t_{1/2}$ = 32 d from screening model calculations (Jury et al. 1987a, b; Jury & Ghodrati 1989);

excretion $t_{1/2}$ = 9.9 h by willow shiner (Tsuda et al. 1989)

$t_{1/2}$ = 25 h in eel's liver and $t_{1/2}$ = 26 h in eel's muscle (Sancho et al. 1993)

TABLE 18.1.1.27.1
Reported vapor pressures and Henry's law constants of diazinon at various temperatures

Vapor pressure				Henry's law constant	
Kim et al. 1984, Kim 1985		Rordorf 1989		Feigenbrugel et al. 2004	
gas saturation-GC		gas saturation-GC		gas stripping-GC/MS	
t/°C	P/Pa	t/°C	P/Pa	t/°C	H/(Pa m^3/mol)
25.3	0.0113	25	0.014	283.05	8.515×10^{-3}
34.9	0.0299	50	0.22	283.15	9.128×10^{-3}
45.0	0.0770	75	2.20	283.15	8.515×10^{-3}
20.0	0.0064	100	17.0	283.55	8.465×10^{-3}
25.0	0.0109	125	100	287.55	0.0138
				291.55	0.0166
log P = A – B/(T/K)		log P = A – B/(T/K)		293.05	0.0281
	P/mmHg		P/Pa	293.05	0.0390
A	9.3871	A	13.482	293.15	0.0349
B	4014.67	B	4571.2	293.15	0.0375
				293.25	0.0298
				293.25	0.0281
				295.35	0.0441
				297.55	0.0675
				299.45	0.0921
				301.45	0.101325
				ln H = A – B/(T/K)	
					H′/(M/atm)
				A	–32.5647
				B	11900

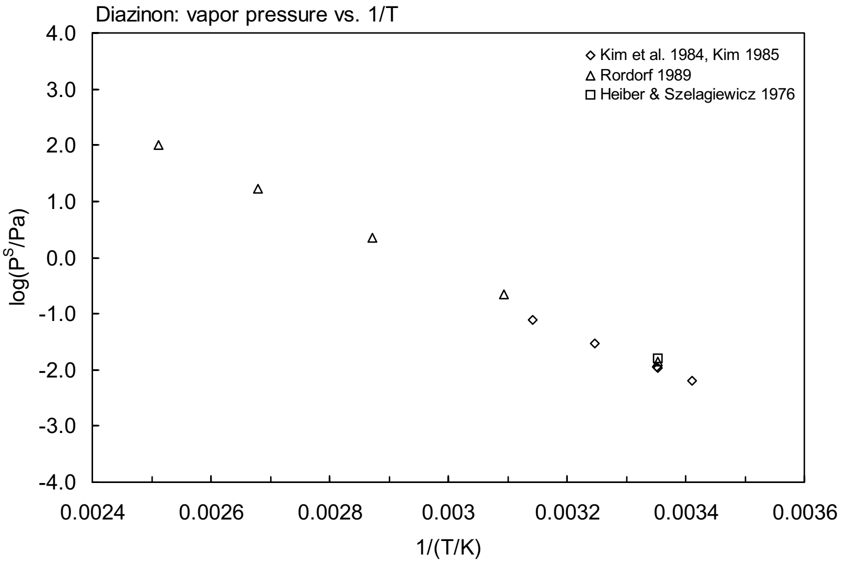


FIGURE 18.1.1.27.1 Logarithm of vapor pressure versus reciprocal temperature for diazinon.

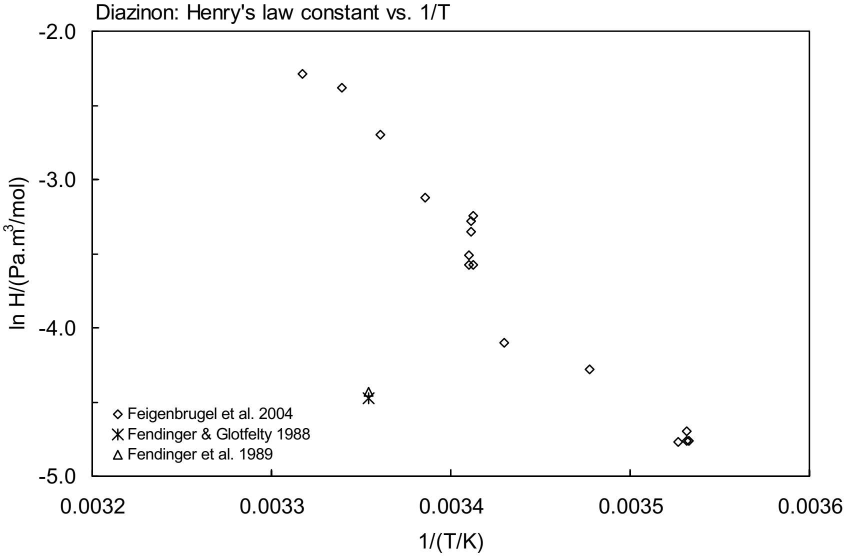
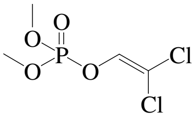


FIGURE 18.1.1.27.2 Logarithm of Henry's law constant versus reciprocal temperature for diazinon.

18.1.1.28 Dichlorvos



Common Name: Dichlorvos

Synonym: Apavap, Astrobot, Atgard, Bay 19149, Benfos, Bibesol, Brevinyl, Canogard, Cekusan, Chlorvinphos, Cyanophos, Cypona, DDVF, DDVP, Dedevap, Deriban, Derribante, Devikol, Dichlorman, Dichlorophos, Divipan, Duo-kill, Duravos, ENT 20738, Equigard, Equigel, Estrosel, Estrosol, Fecama, Fly-die, Fly fighter, Herkal, Herkol, Krecalvin, Lindan, Mafu, Mafu strip, Marvex, Mopari, NA 2783, Nerkol, Nogos, No-pest, Nuva, Nuvan, Oko, OMS 14, Phosvit, SD-1750, Szklarniak, Tap 9VP, Task, Tenac, Tetravos, UDVF, Unifos, Vapona, Vaponite, Vapora II, Verdican, Verdipor, Vinylofos, Vinylophos

Chemical Name: 2,2-dichlorovinyl-*O,O*-dimethyl phosphate; 2,2-dichloroethenyl-*O,O*-dimethyl phosphate

Uses: insecticide and fumigant to control flies, mosquitoes, and moths; also used as acaricide.

CAS Registry No: 62-73-7

Molecular Formula: $C_4H_7Cl_2O_4P$

Molecular Weight: 220.976

Melting Point (°C):
colorless to amber liquid (Hartley & Kidd 1987)

Boiling Point (°C):
35, 74, 117 (at 0.05, 1.0, 10 mmHg, Hartley & Kidd 1987; Worthing & Hance 1991)
234.1 (Tomlin 1994)

Density (g/cm^3 at 20°C):
1.415 (25°C, Spencer 1982; Hartley & Kidd 1987; Montgomery 1993; Milne 1995)
1.420 (25°C, Worthing & Hance 1991)
1.425 (Tomlin 1994)
1.440 (Montgomery 1993)

Molar Volume (cm^3/mol):
167.5 (calculated-Le Bas method at normal boiling point)

Dissociation Constant, pK_a:

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

Entropy of Fusion, ΔS_{fus} (J/mol K):

Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F: 1.0

Water Solubility (g/m^3 or mg/L at 25°C or as indicated):
10000 (Günther et al. 1968; Melnikov 1971; Kenaga 1980a; Khan 1980; Spencer 1982)
10000 (Martin & Worthing 1977; Worthing 1979; Worthing & Walker 1987)
10000 (20°C, Hartley & Kidd 1987; Worthing & Hance 1991; Milne 1995)
16000 (Kawamoto & Urano 1989)
16000 (20°C, Montgomery 1993)
10000 (20–25°C, estimated, Augustijn-Beckers et al. 1994; Hornsby et al. 1996)
8000 (Tomlin 1994)

Vapor Pressure (Pa at 25°C or as indicated. Additional data at other temperatures designated * are compiled at the end of this section):
1.60 (20°C, Eichler 1965; Wolfdietrich 1965)
1.60 (20°C, Melnikov 1971; Hartley & Graham-Bryce 1980; Spencer 1982; Montgomery 1993)
1.60* (20°C, evaporation rate-gravimetric method, measured range 293–333 K, Gückel et al. 1973)
1.60 (Khan 1980; Brouwer et al. 1994)
log (P/mmHg) = 9.9081 – 3464/(T/K); temp range not specified (quoted from literature, Gückel et al. 1982)
0.947* (20°C, evaporate rate-gravimetric method, measured range 20–60°C, Gückel et al. 1982)
7.026 (gas saturation-GC, Kim et al. 1984)
4.011 (20, 25°C, extrapolated-Clausius-Clapeyron eq., Kim et al. 1984)

0.67 (20°C, GC-RT correlation, Kim et al. 1984; Kim 1985)
1.60, 3.90 (20°C, 30°C, Hartley & Kidd 1987)
7.0 (20°C, selected, Suntio et al. 1988)
0.29 (20°C, Worthing & Hance 1991)
0.267 (20–25°C, estimated, Augustijn-Beckers et al. 1994; Hornsby et al. 1996)
2.10 (Tomlin 1994)
7.94 (gradient GC method; Tsuzuki 2000)
6.92; 8.51, 5.62 (gradient GC method; estimation using modified Watson method: Sugden's parachor, McGowan's parachor, Tsuzuki 2000)

Henry's Law Constant (Pa·m^3/mol at 25°C or as indicated. Additional data at other temperatures designated * are compiled at the end of this section):

0.190 (20°C, calculated-P/C, Suntio et al. 1988)
0.097 (calculated-P/C, Howard 1991)
506.5 (Montgomery 1993)
0.194 (calculated-P/C, this work)
0.0253* (gas stripping-GC/MS, measured range 10–25°C, Gautier et al. 2003)
$\ln [H'/(M\ atm^{-1})] = -28.904 + 11100/(T/K)$; temp range 283.5–298.15 K (Arrhenius eq., gas stripping-GC/MS, Gautier et al. 2003)

Octanol/Water Partition Coefficient, log K_{OW}:

1.40 (Leo et al. 1971; Hansch & Leo 1979)
2.29 (Rao & Davidson 1980)
1.47 (shake flask-GC, Bowman & Sans 1983)
1.16 (HPLC-RT correlation, Kawamoto & Urano 1989)
1.40–2.29 (Montgomery 1993)
1.73 (RP-HPLC-RT correlation, Sicbaldi & Finizio 1993)
1.43 (recommended, Sangster 1993)
1.90 (Tomlin 1994)
1.42 (selected, Hansch et al. 1995)
1.73 (RP-HPLC-RT correlation, Finizio et al. 1997)

Bioconcentration Factor, log BCF:

0.477 (calculated-S, Kenaga 1980a; quoted, Howard 1991)
–0.097 (whole body willow shiner after 24–168 h exposure, Tsuda et al. 1992; quoted, Devillers et al. 1996)
< –0.30 (whole body carp, Tsuda et al. 1993)

Sorption Partition Coefficient, log K_{OC}:

1.45 (soil, calculated-S, Kenaga 1980a; quoted, Howard 1991)
1.67 (correlated, Kawamoto & Urano 1989)
1.70 (calculated, Montgomery 1993)
1.48 (20–25°C, estimated, Augustijn-Beckers et al. 1994; Hornsby et al. 1996)
1.67; 2.98, 2.04 (soil, quoted exptl.; estimated-class-specific model, estimated-general model, Gramatica et al. 2000)

Environmental Fate Rate Constants, k, or Half-Lives, $t_{1/2}$:

Volatilization: based on the Henry's law constant, $t_{1/2}$ ~ 57 d from a model river (Lyman et al. 1982; quoted, Howard 1991);

$t_{1/2}$ ~ 400 yr from an model pond, which considered the effect of adsorption (Howard 1991).

Photolysis:

Oxidation: rate constant k, for gas-phase second order rate Constants, k_{OH} for reaction with OH radical, k_{NO3} with NO_3 radical and k_{O3} with O_3 or as indicated, *data at other temperatures see reference:

atmospheric $t_{1/2}$ = 320 d, based on an estimated rate constant $k_{O3} = 3.58 \times 10^{-20}$ cm^3·molecule^{-1} s^{-1} at 25°C for the vapor-phase reaction with ozone of concn 7×10^{11}/cm^3 in air (Atkinson & Carter 1984; quoted, Howard 1991) atmospheric $t_{1/2}$ = 2 d, based on an estimated rate constant $k_{OH} = 9.24 \times 10^{-12}$ cm^3 molecule^{-1} s^{-1} at 25°C for the vapor-phase reaction with hydroxyl radical of 5×10^5/cm^3 in air (Atkinson 1987; quoted, Howard 1991).

$k_{OH} = 9.4 \times 10^{-12}$ cm^3·molecule^{-1} s^{-1} with calculated tropospheric lifetime about 1.2 d at 298 K assuming an average OH concn of 1×10^6 molecule/cm^3 (Gautier et al. 2003)

Hydrolysis: $t_{1/2}$ = 462 min at pH 7 and $t_{1/2}$ = 30 min at pH 8 (Montgomery 1993);

$t_{1/2}$ ~ 31.9 d at pH 4, $t_{1/2}$ ~ 2.9 d at pH 7, and $t_{1/2}$ ~ 2.0 d at pH 9 at 22°C (Tomlin 1994)

$t_{1/2}$ = 3800 d at pH 7 in natural waters (Capel & Larson 1995).

Biodegradation: the presence of active microorganisms reduced the $t_{1/2}$ = 0.9–0.75 and 0.85 to 0.70 d in autoclaved clay and calcareous soil, respectively (Guirguis & Shafik 1975; quoted, Howard 1991);

rate constant k(aerobic) = 0.20 d^{-1} with $t_{1/2}$ = 3.5 d at 20°C by aerobic activated sludge, and k(anaerobic) = 0.20 d^{-1} with $t_{1/2}$ = 3.5 d at 20°C by anaerobic microorganisms (batch contacting method, Kawamoto & Urano 1990).

$t_{1/2}$(aerobic) = 180 d, $t_{1/2}$(anaerobic) = 1 d in natural waters (Capel & Larson 1995)

Biotransformation:

Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants

Half-Lives in the Environment:

Air: $t_{1/2}$ = 320 d, based on an estimated rate constant $k = 3.58 \times 10^{-20}$ cm^3 molecule^{-1} s^{-1} at 25°C for the vapor-phase reaction with ozone of 7×10^{11}/cm^3 in air (Atkinson & Carter 1984; quoted, Howard 1991)

atmospheric $t_{1/2}$ = 2 d, based on an estimated rate constant k =$.24 \times 10^{-12}$ cm^3 molecule^{-1} s^{-1} at 25°C for the vapor-phase reaction with hydroxyl radical of 5×10^5/cm^3 in air (Atkinson 1987; quoted, Howard 1991)

atmospheric transformation lifetime was estimated to be <1 d (Kelly et al. 1994)

Calculated tropospheric lifetime of 0.5 d for reaction with OH radicals, wet deposition lifetime estimated to be 5.6 d in the atmosphere by rainfall (Gautier et al. 2003)

Surface water: half-lives in lakes and rivers are reported to be approximately 4 d (Lamoreaux & Newland 1978; quoted, Howard 1991)

Biodegradation $t_{1/2}$ = 3.5 d by aerobic activated sludge or anaerobic microorganisms cultivated by a an artificial sewage (Kawamoto & Urano 1990)

Biodegradation $t_{1/2}$(aerobic) = 180 d, $t_{1/2}$(anaerobic) = 1 d, hydrolysis $t_{1/2}$ = 3800 d at pH 7 in natural waters (Capel & Larson 1995)

Ground water:

Sediment:

Soil: average degradation rate constant k = 0.0423 d^{-1} in silty clay with $t_{1/2}$ = 16 d and average degradation rate constant k = 0.0444 d^{-1} in sandy clay with $t_{1/2}$ = 16 d (Sattar 1990);

selected field $t_{1/2}$ = 0.5 d (Augustijn-Beckers et al. 1994; Hornsby et al. 1996).

Biota:

TABLE 18.1.1.28.1
Reported vapor pressures and Henry's law constants of dichlorvos at various temperatures

Vapor pressure				Henry's law constant	
Gückel et al. 1973		Gückel et al. 1982		Gautier et al. 2003	
evaporation rate		evaporation rate		gas stripping-GC/MS	
t/°C	P/Pa	t/°C	P/Pa	t/°C	H/(Pa m^3/mol)
20	1.60	20	0.947	10	0.00322
30	4.0	40	7.30	10	0.00367
40	9.33	60	40.0	11	0.00378
50	-			12	0.00520
60	-			12	0.00504
				15	0.00209
				18	0.0109
				20	0.0151
				20	0.0163
				22.5	0.0181
				23	0.0230
				25	0.0230
				25	0.0247
				25	0.0289
				20.0	0.0253
				Arrhenius expression:	
				ln H=/(M atm^{-1}) = –A + B/(T/K)	
				A	28.904
				B	11100

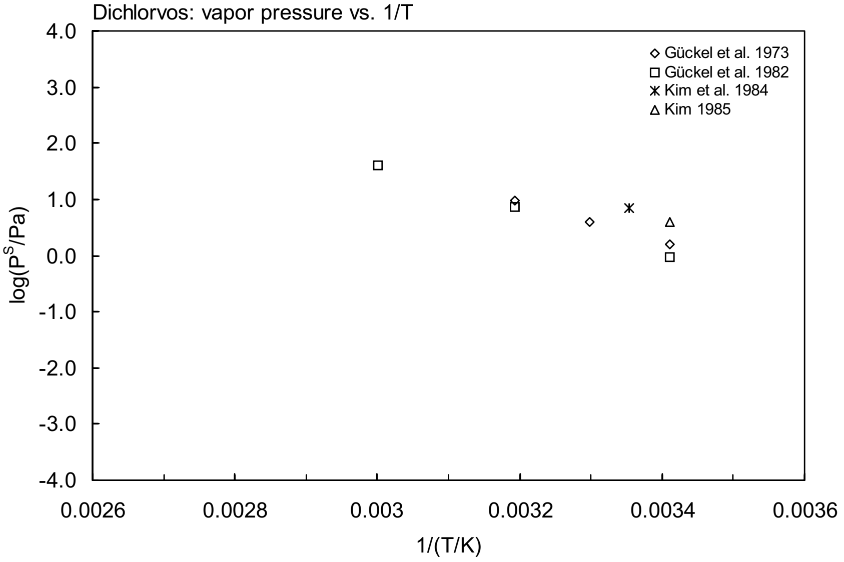


FIGURE 18.1.1.28.1 Logarithm of vapor pressure versus reciprocal temperature for dichlorvos.

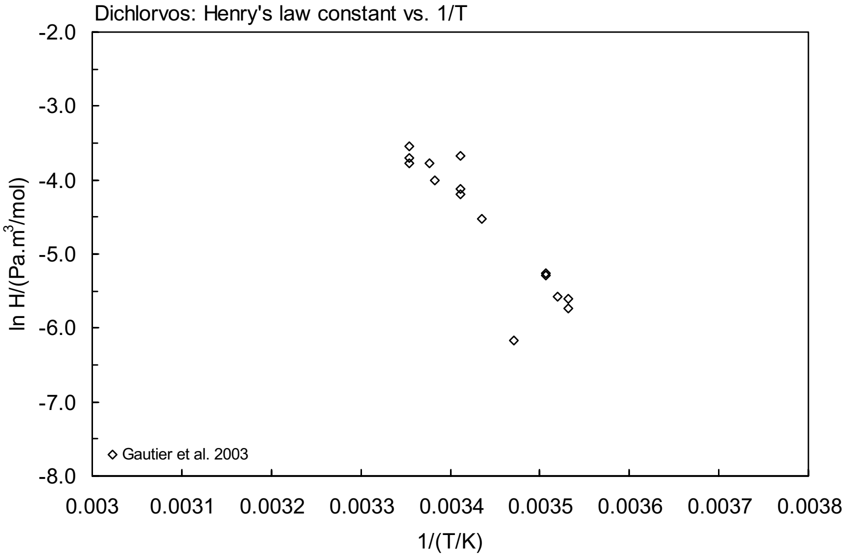
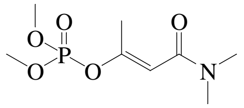


FIGURE 18.1.1.28.2 Logarithm of Henry's law constant versus reciprocal temperature for dichlorvos.

18.1.1.29 Dicrotophos



Common Name: Dicrotophos

Synonym: Bidirl, Bidrin, C 709, Cabicron, Carbomicron, CIBA 709, Diapadrin, Dicrotofos, Ektafos, ENT 24,482, Karbicron, Shell SD-3562

Chemical Name: (*E*)-2-dimethylcarbamoyl-1-methylvinyl dimethyl phosphate; (*E*)-3-(diethylamino)-1-methyl-3-oxo-1-propenyl dimethyl phosphate

Uses: contact and systemic insecticide and acaricide to control pests on rice, cotton, maize, soybeans, coffee, citrus, and potatoes.

CAS Registry No: 141-66-2 *cis*-dicrotophos

Molecular Formula: $C_8H_{16}NO_5P'$

Molecular Weight: 237.191

Melting Point (°C): liquid

Boiling Point (°C):

130	(at 0.1 mmHg, Worthing & Hance 1991; Montgomery 1993; Milne 1995)
400	(Tomlin 1994; Milne 1995)

Density (g/cm^3 at 20°C):

1.216	(Hartley & Kidd 1987)
1.216	(15°C, Merck Index 1989; Milne 1995)
1.21	(technical grade, Worthing & Hance 1991)
1.216	(Worthing & Hance 1991; Montgomery 1993; Tomlin 1994)

Molar Volume (cm^3/mol):

Dissociation Constant, pK_a:

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

Entropy of Fusion, ΔS_{fus} (J/mol K):

Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F: 1.0

Water Solubility (g/m^3 or mg/L at 25°C):

miscible	(Spencer 1973)
miscible	(Hartley & Kidd 1987; Budavari 1989; Milne 1995)
miscible	(Worthing & Walker 1987; Montgomery 1993; Tomlin 1994)
1000000	(20–25°C, estimated, Wauchope et al. 1992; Hornsby et al. 1996)

Vapor Pressure (Pa at 25°Cor as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):

0.0115*	(20°C, extrapolated, gas saturation-GC, measured range 32.3–77°C, Grayson & Fosbracey 1982)

$\ln (P/Pa) = 21.6 - 7631/(T/K)$; temp range 32.3–77°C, (Antoine eq., gas saturation-GC, Grayson & Fosbracey 1982)

0.0093	(20°C, Hartley & Kidd 1987)
0.0093	(20°C, Worthing & Hance 1991; Montgomery 1993; Tomlin 1994)
0.0213	(20–25°C, estimated, Wauchope et al. 1992; Hornsby et al. 1996)

Henry's Law Constant (Pa·m^3/mol at 25°C):

5.05×10^{-6} (20–25°C, calculated-P/C)

Octanol/Water Partition Coefficient, log K_{OW}:

–0.260	(calculated as per Broto et al. 1984, Karcher & Devillers 1990)
–0.49	(shake flask, Log P Database, Hansch & Leo 1987)
–0.49	(recommended, Sangster 1993)
–0.50	(Montgomery 1993)
0.0	(Hansch et al. 1995)

Bioconcentration Factor, log BCF:

Sorption Partition Coefficient, log K_{OC}:

1.88 (soil, 20–25°C, estimated, Wauchope et al. 1992; Hornsby et al. 1996)
1.04–2.27 (Montgomery 1993)
1.66 (soil, calculated-MCI $^1\chi$, Sabljic et al. 1995)
1.66; 1.49, 1.67 (soil, quoted exptl.; estimated-class-specific model, estimated-general model, Gramatica et al. 2000)

Environmental Fate Rate Constants, k, or Half-Lives, $t_{½}$:

Hydrolysis: $t_{½}$ = 117, 72, and 28 d in buffer solutions of pH 5, 7, and 9, respectively, at 25°C (Lee et al. 1989; quoted, Montgomery 1993);
calculated $t_{½}$ = 88 d in water at 20°C at pH 5 and = 23 d at pH 9 (Worthing & Hance 1991; Montgomery 1993; Tomlin 1994).

Half-Lives in the Environment:

Soil: $t_{½}$ = 3 d in sandy loam soil (Lee et al. 1989; quoted, Montgomery 1993);
selected field $t_{½}$ = 20 d (Wauchope et al. 1992; Hornsby et al. 1996).

TABLE 18.1.1.29.1
Reported vapor pressures of dicrotophos at various temperatures

Grayson & Fosbracey 1982	
gas saturation-GC	
t/°C	**P/Pa**
32.3	0.034
33.7	0.036
41.0	0.055
45.2	0.106
51.0	0.136
60.1	0.287
65.8	0.405
69.5	0.424
77.0	0.820
30	0.0115
ln P = A – B/(T/K)	
	P/Pa
A	7631
B	21.6

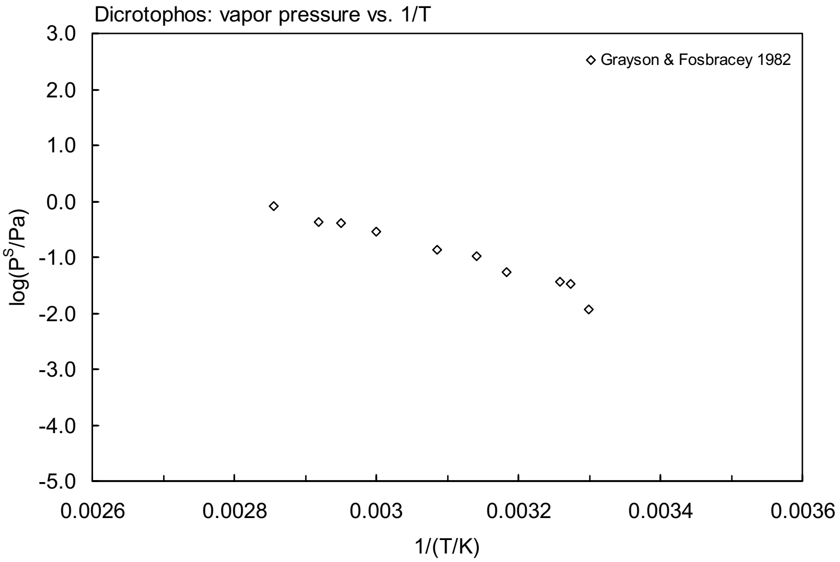
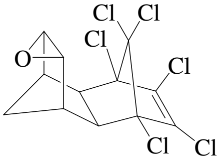


FIGURE 18.1.1.29.1 Logarithm of vapor pressure versus reciprocal temperature for dicrotophos.

18.1.1.30 Dieldrin



Common Name: Dieldrin
Synonym: Aldren, Alvit, Alyran, Compound 497, Dieldrite, Dieldrix, Dorytox, ENT 16225, HEOD, Illoxol, Insectlack, Kombi-Albertan, NA 2761, NCI-C00124, Octalox, Panoram D-31, Quintox
Chemical Name: 1,2,3,4,10,10-hexachloro-6,7-epoxy-1,4,4*a*,5,6,7,8, 8*a*-octahydroendo-1,4-*exo*-5,8-dimethano-naphthalene; 3,4,5,6,9,9-hexachloro-1*a*,2,2*a*,3,6,6*a*,7,7*a*-octahydro-2,7:3,6-dimethanonaphth[2,3-b]oxirene
Uses: insecticide to control public health insect pests, termites, locusts, and tropical disease vectors.
CAS Registry No: 60-57-1
Molecular Formula: $C_{12}H_8Cl_6O$
Molecular Weight: 380.909
Melting Point (°C):
175.5 (Lide 2003)
Boiling Point (°C):
265, 352, 404 (estimated from structure, Tucker et al. 1983)
Density (g/cm^3 at 20°C):
1.75 (Hartley & Kidd 1987; Montgomery 1993)
Molar Volume (cm^3/mol):
318.2 (calculated-Le Bas method at normal boiling point)
253.6 (Ruelle & Kesselring 1997)
Dissociation Constant, pK$_a$:
Enthalpy of Vaporization, ΔH_V (kJ/mol):
76.6 (Rordorf 1989)
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
21.4 (Rordorf 1989)
18.41 (Ruelle & Kesselring 1997)
Entropy of Fusion, ΔS_{fus} (J/mol K):
41.34, 48.12 (Plato 1972)
47 (Rordorf 1989)
44.77 (Hinckley et al. 1990)
Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 K/mol K), F:
0.026 (20°C, Suntio et al. 1988)
0.033 (Mackay et al. 1986)

Water Solubility (g/m^3 or mg/L at 25°C or as indicated. Additional data at other temperatures designated * are compiled at the end of this section):
0.19 (colorimetric method, Lipke & Kearns 1960)
0.25* (shake flask-GC/UV, measured range 25–45°, Richardson & Miller 1960)
0.14–0.18 (particle size of 0.04–5.0μ, shake flask-GC, Robeck et al. 1965)
0.15 (Eye 1968; quoted, Freed 1976; Jury et al. 1983,84)
0.20 (Günther et al. 1968)
0.186 (25–29°C, shake flask-GC/ECD, Park & Bruce 1968)
0.022 (Biggar & Riggs 1974)
0.195* (particle size of ≤ 5.0μ, shake flask-GC/ECD, measured range 15–45°C, Biggar & Riggs 1974)
0.022*, 0.15*, 0.195* (particle size: 0.01, 0.05 & 5.0μ; shake flask-GC/ECD, measured range 15–45°C, Biggar & Riggs 1974)
0.20 (generator column-GC/ECD, Weil et al. 1974)
0.187 (Martin & Worthing 1977; Worthing & Walker 1987)
0.10–0.25 (Wauchope 1978)

0.022 (Kenaga 1980a, b; Garten & Trabalka 1983; Isnard & Lambert 1989)
0.10 (Weber et al. 1980; Eadie & Robbins 1987)
0.468 (20–25°C, shake flask-GC, Kanazawa 1981)
0.19 (20°C, Hartley & Kidd 1987)
0.14, 0.20 (20°C, 30°C, Montgomery 1993)
0.20 (20–25°C, selected, Augustijn-Beckers et al. 1994; Hornsby et al. 1996)
4.57, 4.95 (supercooled liquid: LDV derivation of literature-derived value, FAV final-adjusted value, Shen & Wania 2005)
log $[C_L/(\text{mol m}^{-3})] = -1158/(T/K) + 1.94$ (supercooled liquid, linear regression of literature data, Shen & Wania 2005)

Vapor Pressure (Pa at 25°C or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):

1.04×10^{-4} (20°C, Porter 1964)
1.04×10^{-4}, 1.91×10^{-4}, 3.65×10^{-4} (20, 30, 40°C, effusion method, Porter 1964 as quoted in Spencer & Cliath 1969)
2.40×10^{-5} (Eichler 1965; Martin 1972; Melnikov 1971)
3.47×10^{-4}, 1.33×10^{-3}, 4.63×10^{-3} (20, 30, 40°C, gas saturation method, Spencer & Cliath 1969)
6.59×10^{-4} (calculated from vapor pressure eq. apparent vapor pressure, Spencer & Cliath 1969)
$\log (P/\text{mmHg}) = 12.07 - 5178/(T/K)$; for temp range 20–40°C (gas saturation, apparent vapor pressure, Spencer & Cliath 1969)
6.77×10^{-4} (gas saturation, Spencer & Cliath 1969)
3.87×10^{-4} (20°C, partition coeff., Atkins & Eggleton 1971)
4.13×10^{-4} (20°C, Khan 1980)
2.40×10^{-5} (20–25°C, Weber et al. 1980)
8.90×10^{-4} (20°C, GC, Seiber et al. 1981)
4.20×10^{-4}* (20°C, gas saturation-GC, extrapolated, measured range 35–75°C, Grayson & Fosbracey 1982)
$\ln (P/\text{Pa}) = 30.7 - 11285/(T/K)$; temp range 35 to 75.2°C (Antoine eq., gas saturation-GC, Grayson & Fosbracey 1982)
0.00532, 0.0597 (P_{GC} by GC-RT correlation, different stationary phases, Bidleman 1984)
0.0215 (supercooled liquid P_L, converted from literature P_S with ΔS_{fus} Bidleman 1984)
4.00×10^{-4} (20°C, Hartley & Kidd 1987)
7.90×10^{-4}* (gas saturation-GC, measured range 25–125°C, Rordorf 1989)
$\log (P_S/\text{Pa}) = 14.37 - 5210.07/(T/K)$; measured range 32.4–125°C (solid, gas saturation-GC, Rordorf 1989)
$\log (P_L/\text{Pa}) = 11.66013 - 4001.62/(T/K)$; temp range not specified (liquid, gas saturation-GC, Rordorf 1989)
0.0215, 0.0101 (supercooled P_L, converted from literature P_S with different ΔS_{fus} values, Hinckley et al. 1990)
0.00532, 0.0318 (P_{GC} by GC-RT correlation with different reference standards, Hinckley et al. 1990)
$\log (P_L/\text{Pa}) = 12.46 - 4310/(T/K)$ (GC-RT correlation, supercooled liquid, Hinckley et al. 1990)
2.37×10^{-5} (20°C, Montgomery 1993)
4.00×10^{-4} (20–25°C, selected, Augustijn-Beckers et al. 1994; Hornsby et al. 1996)
0.010 (supercooled liquid P_L, Wania & Mackay 1996)
3.24×10^{-4} (liquid P_L, GC-RT correlation., Donovan 1996)
0.016, 0.014 (supercooled liquid P_L: LDV literature derived value, FAV final adjusted value, Shen & Wania 2005)
$\log (P_L/\text{Pa}) = -3995/(T/K) + 11.62$ (supercooled liquid, linear regression of literature data, Shen & Wania 2005)

Henry's Law Constant (Pa·m^3/mol at 25°C):

4.59 (gas stripping, Atkins & Eggleton 1971)
0.02 (calculated-P/C, Mackay & Leinonen 1975)
0.0171 (20°C, calculated-P/C, Kavanaugh & Trussell 1980)
5.84 (exptl., Warner et al. 1980)
0.0456 (calculated-P/C, Levins 1981)
1.10 (20°C, Mackay & Shiu 1981)
2.94 (20°C, measured, Slater & Spedding 1981)
0.172 (estimated-group method per Hine & Mookerjee 1975, Tucker et al. 1983)
1.66 (calculated-P/C, Jury et al. 1984, 1987a; Jury & Ghodrati 1989)
0.78 (calculated-P/C, Mackay et al. 1986)

0.74	(WERL Treatability Database, quoted, Ryan et al. 1988)
1.12	(20°C, calculated-P/C, Suntio et al. 1988)
1.0	(calculated-P/C, Nash 1989)
5.88	(Montgomery 1993)
1.016	(wetted wall column-GC, Altschuh et al. 1999)
1.0, 1.1	(LDV literature-derived value, FAV final adjusted value, Shen & Wania 2005)

Octanol/Water Partition Coefficient, log K_{OW}:

2.60	(Hansch & Leo 1979)
5.48	(calculated, Kenaga 1980a, b)
6.20	(TLC-retention time correlation, Lord et al. 1980)
4.32	(shake flask-GC, Kanazawa 1981)
6.20	(20°C, shake flask-GC, Briggs 1981)
5.11	(HPLC-RT correlation, Hammers et al. 1982)
5.30	(RP-HPLC correlation, Hermens & Leeuwangh 1982)
5.10	(shake flask-GC, Platford 1982)
4.32	(Hansch & Leo 1985; Medchem Database 1988)
4.51, 4.49, 4.60, 4.55	(shake flask, Brooke et al. 1986)
4.51	(HPLC-RT correlation, De Kock & Lord 1987)
5.40	(shake flask/slow-stirring method, De Bruijn et al. 1989)
3.69–6.20	(Montgomery 1993)
4.76	(RP-HPLC-RT correlation, Sicbaldi & Finizio 1993)
5.20	(selected, Hansch et al. 1995)
4.76	(RP-HPLC-RT correlation, Finizio et al. 1997)
5.40, 5.58	(LDV literature-derived value, FAV final-adjusted value, Shen & Wania 2005)

Octanol/Air Partition Coefficient, log K_{OA} at 25°C and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section:

7.40	(calculated-K_{OW}/K_{AW}, Wania & Mackay 1996)
8.837*, 8.898	(gas saturation-GC/MS, calculated, measured range 5–45°C, Shoeib & Harner 2002)

log $K_{OA} = -3.82 + 3790/(T/K)$, temp range: 5–45°C (gas saturation-GC, Shoeib & Harner 2002)

8.89, 8.84	(LDV literature-derived value, FAV final adjusted value, Shen & Wania 2005)

Bioconcentration Factor, log BCF:

3.08, 4.14, 4.69	(algae, daphnia, guppies, Reinert 1967)
3.65–4.69	(earthworms, Wheatley & Hardman 1968)
0.230	(bioaccumulation factor log BF, adipose tissue in male Albino rats, Robinson et al. 1969)
0.322	(bioaccumulation factor log BF, adipose tissue in male Albino rats, Walker et al. 1969)
3.04–3.66	(*Saccharomyces cerevisiae*, Voerman & Tammes 1969)
3.0–5.48	(benthic algae, Rose & McIntire 1970)
0.301	(bioaccumulation factor log BF, adipose tissue in male Albino rats, Baron & Walton 1971)
3.24	(soft clam, Butler 1971)
3.11, 3.54, 2.37	(*Scenedemus obliquus*, *Daphnia magna*, Reinert 1972)
2.37	(wet-wt. basis, *Scenedemus obliquus*, Reinert 1972)
3.43, 4.79, 2.66–4.60	(*Gambusia, Physa*, *Oedogonium sp.*, Metcalf et al. 1973)
4.51	(wet-wt. basis, *Ankistrodesmus,* Neudorf & Khan 1975)
3.39	(oyster, Mason & Rowe 1976)
3.20	(mussel, steady state, Ernst 1977)
2.30	(*Anabaena cylindrica*, Schauberger & Wildman 1977)
2.70; 3.26	(*Anacystis nidulans*, *Nostoc muscorum*, Schauberger & Wildman 1977)
2.0–4.0	(Callahan et al. 1979; quoted, Howard 1991)
3.76, 3.65	(fish: flowing water, static water; Kenaga 1980a, b; Kenaga & Goring 1980)
0.362	(average beef fat diet, Kenaga 1980b)
3.54	(pulex, Kenaga & Goring 1980)
3.62	(earthworms, Lord et al. 1980)

2.00 (*Triaenodes tardus,* Belluck & Felsot 1981)
3.65 (*Pseudorasbora parva*, flow-through conditions, Kanazawa 1981)
1.0–5.0 (selected, Schnoor & McAvoy 1981)
3.37 (mussel, quoted average, Geyer et al. 1982)
4.23–4.98 (earthworms, Gish & Hughes 1982)
4.16 (fish, correlated, Mackay 1982)
3.52 (trout, Verschueren 1983)
3.55 (clam fat, 60-d expt., Hartley & Johnson 1983)
4.10 (guppy, Davies & Dobbs 1984)
4.25 (activated sludge, Freitag et al. 1984)
3.36, 3.48, 4.25 (algae, golden ide, activated sludge, Freitag et al. 1985)
3.33, 3.29 (mussel, calculated values, Zaroogian et al. 1985)
3.33, 3.29 (oyster, calculated values, Zaroogian et al. 1985)
3.70, 3.90 (oyster, quoted from Zaroogian et al. 1985; Hawker & Connell 1986)
1.72–1.95 (human fat lipid basis, Geyer et al., 1987)
1.56–1.78 (human fat wet wt. basis, Geyer et al., 1987)
4.10 (quoted, Isnard & Lambert 1988; Howard 1991)
–2.10 (beef biotransfer factor log B_b, correlated-K_{OW}, Potter et al. 1974)
–1.97 (milk biotransfer factor log B_m, correlated-K_{OW}, Saha 1969; Wilson & Cook 1972)
–1.01 (vegetation, correlated-K_{OW}, Beall & Nash 1972; quoted, Travis & Arms 1988)
2.96–4.11 (aquatic food web, Fordham & Reagan 1991)
3.81 (fish, Fordham & Reagan 1991)
3.88 (selected, Chessells et al. 1992)
3.36, 4.06 (algae *Chlorella*: wet wt basis, dry wt basis, Geyer et al. 2000)
3.49, 5.49 (mussel *Mytilus edulis*: wet wt basis, lipid wt basis, Geyer et al. 2000)
3.54, 5.57 (*Daphnia*: wet wt basis, lipid wt basis, Geyer et al. 2000)
3.46, 5.54 (oyster *Crassostrea virginica*: wet wt basis, lipid wt basis, Geyer et al. 2000)
3.32, 5.34 (oyster *Crassostrea virginica*: wet wt basis, lipid wt basis, Geyer et al. 2000)
3.70, 5.62 (oyster *Crassostrea virginica*: wet wt basis, lipid wt basis, Geyer et al. 2000)
4.10, 5.26 (guppy female: wet wt basis, lipid wt basis, Geyer et al. 2000)
4.41, 5.41 (carp: wet wt basis, lipid wt basis, Geyer et al. 2000)
3.32, 5.34 (oyster *Crassostrea virginica*: wet wt basis, lipid wt basis, Geyer et al. 2000)
1.69; 1.85 (human: wet wt basis, lipid wt basis, Geyer et al. 2000)
3.65; 3.66 (*Oncorhynchus mykiss*, wet wt. basis: quoted exptl.; calculated-QSAR model based on quantum chemical parameters, Wei et al. 2001)

Sorption Partition Coefficient, log K_{OC}:
4.55 (soil, calculated-S as per Kenaga & Goring 1978, Kenaga 1980)
4.08 (calculated-K_{OW}, Rao & Davidson 1980)
3.87 (extrapolated from RP-TLC and reported as log K_{OM}, Briggs 1981)
4.0 (selected, Schnoor & McAvoy 1981; Schnoor 1992)
3.36–3.85 (reported as log K_{OM}, Mingelgrin & Gerstl 1983)
4.08 (soil, screening model calculations, Jury et al. 1984, 1987a, b; Jury & Ghodrati 1989)
4.36 (calculated-K_{OW} as per Kenaga & Goring 1980, Chapman 1989)
4.15 (soil: clay loam/kaolinite, 20°C, batch equilibrium-sorption isotherm, Kishi et al. 1990)
4.50 (sediment, Fordham & Reagan 1991)
4.10 (soil, quoted exptl., Meylan et al. 1992)
4.03 (soil, calculated-MCI χ and fragment contribution, Meylan et al. 1992)
5.08 (estimated-QSAR and SPARC, Kollig 1993)
4.08–4.55 (Montgomery 1993)
4.08 (20–25°C, estimated, Augustijn-Beckers et al. 1994; Hornsby et al. 1996)
4.55 (soil, calculated-MCI $^1\chi$, Sabljic et al. 1995)
4.55; 4.71 (soil, quoted exptl.; estimated-general model, Gramatica et al. 2000)
4.90; 4.10 (soil, calculated-universal solvation model; quoted exptl., Winget et al. 2000)
4.08, 4.06 (soils: organic carbon OC $\geq$ 0.1%, OC $\geq$ 0.5%, average, Delle Site 2001)

Environmental Fate Rate Constants, k, or Half-Lives, $t_{½}$:

Volatilization: $t_{½}$ ~ 1.4 d from a model river of depth 1 m flowing at 1 m/s with a wind velocity of 3 m/s by using Henry's law constant (Lyman et al. 1982; quoted, Howard 1991).

Photolysis: rate constant $k = 4.8 \times 10^{-4}\ h^{-1}$ by direct sunlight at 40° latitude (Mabey et al. 1982); using fungus and 254 nm UV, more than 90% initial added amounts were degraded in 4 weeks of incubation (Katayama & Matsumura 1991).

Oxidation: rate constant for singlet oxygen, $k < 3600\ M^{-1}\ h^{-1}$ and for RO_2 radicals $k < 30\ M^{-1}\ h^{-1}$ (Mabey et al. 1982);

photooxidation $t_{½}$ = 4–40.5 h, based on an estimated rate constant for vapor-phase reaction with hydroxyl radical in air (Atkinson 1987; quoted, Howard et al. 1991);

calculated tropospheric lifetimes of 1.1 d due to gas-phase reaction with OH radical (Atkinson et al. 1992).

Hydrolysis: first-order $t_{½}$ = 10.5 yr based on a first-order rate constant $k = 7.5 \times 10^{-6}\ h^{-1}$ at pH 7.0 and 25°C (Ellington et al. 1986, 1987, 1988; quoted, Howard et al. 1991; Montgomery 1993);

rate constant $k = 6.3 \times 10^{-2}\ yr^{-1}$ at pH 7 and 25°C (Kollig 1993).

Biodegradation: aqueous aerobic $t_{½}$ = 4200–25,920 h, based on unacclimated aerobic soil grab sample data (Castro & Yoshida 1971; quoted, Howard et al. 1991; Howard 1991) and reported soil field test data (Kearney et al. 1969; quoted, Howard et al. 1991);

$t_{½}$ = 868 d (Nash 1980; quoted, Jury et al. 1983);

rate constant $k = 0.013\ d^{-1}$ from soil incubation studies by die-away tests (Rao & Davidson 1980; quoted, Scow 1982);

aqueous anaerobic $t_{½}$ = 24–168 h, based on soil and freshwater mud grab sample data (Maule et al. 1987; quoted, Howard et al. 1991);

$t_{½}$ = 870 d in soil by 100-d leaching screening simulation in 0–10 cm depth of soil (Jury et al. 1984, 1987a, b; Jury & Ghodrati 1989).

Biotransformation:

Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants:

$k_1 = 20.40\ h^{-1}$; $k_2 = 0.013\ h^{-1}$ (Ernst 1977; quoted, Hawker & Connell 1986)

$k_2 = 0.017\ d^{-1}$ (fish, Fordham & Reagan 1991)

$k_2 = 0.014\ d^{-1}$ (birds, Fordham & Reagan 1991)

Half-Lives in the Environment:

Air: $t_{½}$ = 4–40.5 h, based on an estimated rate constant for vapor-phase reaction with hydroxyl radical in air (Atkinson 1987; quoted, Howard et al. 1991; Mortimer & Connell 1995);

calculated life-time of 1.1 d in troposphere (Atkinson et al. 1992).

Surface water: estimated $t_{½} \geq 300$ d in lake waters (Zoeteman et al. 1980);

$t_{½}$ = 4200–25920 h, based on estimated aqueous aerobic biodegradation half-life (Howard et al. 1991; quoted, Mortimer & Connell 1995).

Ground water: $t_{½}$ = 24–51840 h, based on estimated aqueous aerobic and anaerobic biodegradation half-lives (Howard et al. 1991).

Sediment: $t_{½}$ = 15100 h (mean value quoted from Howard et al. 1991).

Soil: field $t_{½}$ = 49 d in nondisked soil (Nash 1983);

$t_{½}$ ~ 7 yr persistence in soil (Nash & Woolson 1967);

estimated persistence of 3 yr in soil (Kearney et al. 1969; Edwards 1973; quoted, Morrill et al. 1982; Jury et al. 1987);

$t_{½}$ = 4200–25920 h, based on unacclimated aerobic soil grab sample data (Castro & Yoshida 1971; quoted, Howard et al. 1991) and reported soil field test data (Kearney et al. 1969; quoted, Howard et al. 1991);

"best estimate" of 10 yr for 95% disappearance, the "true value" lies between 8.2–13.6 yr in experimental field (Freeman et al. 1975)

persistence of more than 36 months (Wauchope 1978);

first-order $t_{½}$ ~ 53.3 d from rate constant $k = 0.013\ d^{-1}$ from soil incubation studies by die-away tests (Rao & Davidson 1980; quoted, Scow 1982);

moderately persistent in soils with $t_{½}$ = 20–100 d (Willis & McDowell 1982);

microagroecosystem $t_{½}$ = 19–26 d in moist fallow soil (Nash 1983);

measured dissipation rate $k = 0.055\ d^{-1}$ (Nash 1983; quoted, Nash 1988);

estimated dissipation rate k = 0.034 and $0.049\ d^{-1}$ (Nash 1988);

biodegradation $t_{½}$ = 868 d (Jury et al. 1984, 1987a, b; Jury & Ghodrati 1989; quoted, Montgomery 1993);
$t_{½}$ > 50 d and subject to plant uptake via volatilization (Ryan et al. 1988);
estimated field $t_{½}$ = 1000 d (Augustijn-Beckers et al. 1994; Hornsby et al. 1996);
$t_{½}$ = 5 – 9 yr in soil (Geyer et al. 2000)
$t_{½}$ = 21.7 and 25 yr for control and sludge-amended Luddington soils, respectively (Meijer et al. 2001).

Biota: estimated $t_{½}$ ~ 1.3 and 10.2 d in rat's liver, and similar values estimated $t_{½}$ = 10.3 d for the blood in rat and $t_{½}$ = 3 d in adipose tissue of rat (Robinson et al. 1969);
$t_{½}$ = 53.1 h in mussels (Ernst 1977; quoted, Hawker & Connell 1986);
biochemical $t_{½}$ = 868 d from screening model calculations (Jury et al. 1987a, b; Jury & Ghodrati 1989)

TABLE 18.1.1.30.1
Reported aqueous solubilities and octanol-air partition coefficients of dieldrin at various temperatures

Aqueous solubility						log K_{OA}	
Richardson & Miller 1960		Biggar & Riggs 1974				Shoeib & Harner 2002	
shake flask-UV spec.		shake flask-GC				generator column-GC/MS	
t/°C	S/g·m^{-3}	t/°C	S/g·m^{-3}	S/g·m^{-3}	S/g·m^{-3}	t/°C	log K_{OA}
		particle size	0.01μ	0.05μ	5.0μ		
25	0.25	15	0.010	0.065	0.090	15	9.359
35	0.54	25	0.022	0.150	0.195	25	8.837
45	1.0	35	0.047	0.270	0.400	35	8.550
		45	0.090	0.480	0.650	45	8.075
						25	8.898
						log K_{OA} = A + B/(T/K)	
						A	–3.82
						B	3790
						enthalpy of phase change ΔH_{OA}/(kJ mol^{-1}) = 72.6	

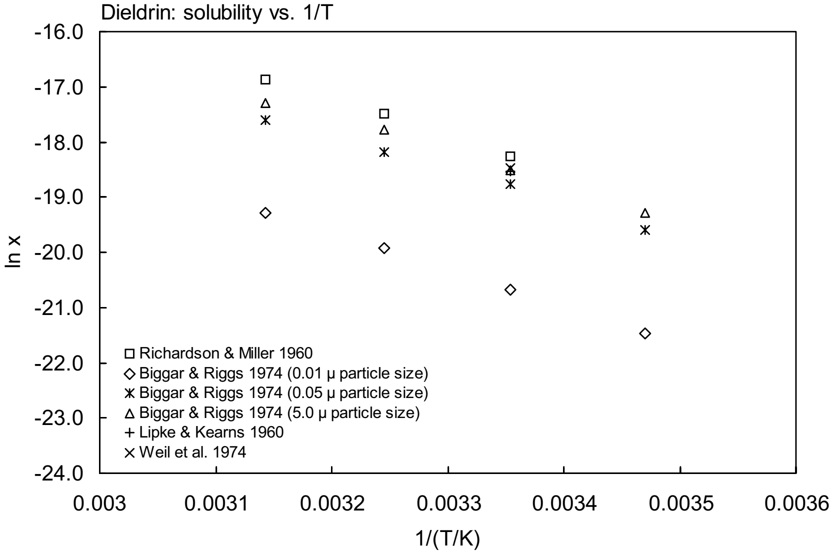


FIGURE 18.1.1.30.1 Logarithm of mole fraction solubility (ln *x*) versus reciprocal temperature for dieldrin.

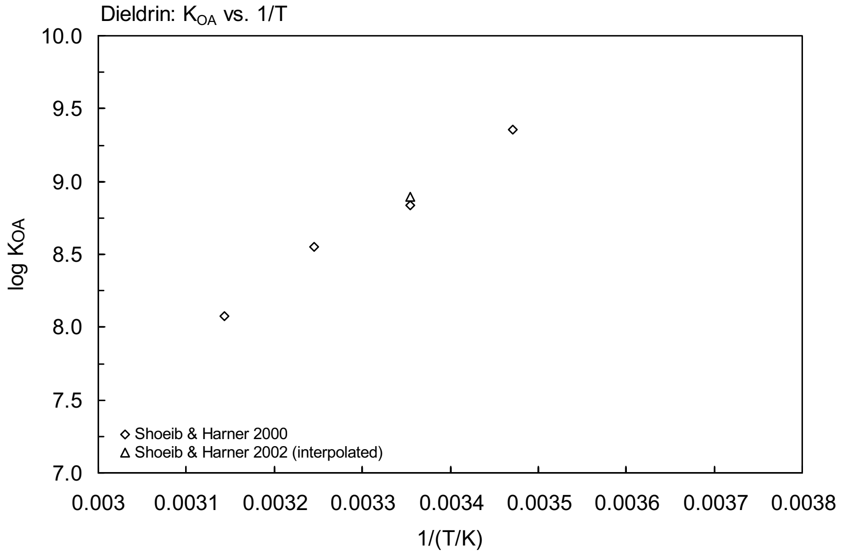


FIGURE 18.1.1.30.2 Logarithm of K_{OA} versus reciprocal temperature for dieldrin.

TABLE 18.1.1.30.2
Reported vapor pressures of dieldrin at various temperatures and the coefficients for the vapor pressure equations

$\log P = A - B/(T/K)$ (1)
$\log P = A - B/(C + t/°C)$ (2)
$\log P = A - B/(C + T/K)$ (3)
$\log P = A - B/(T/K) - C \cdot \log (T/K)$ (4)
$\ln P = A - B/(T/K)$ (1a)
$\ln P = A - B/(C + t/°C)$ (2a)

Spencer & Cliath 1969		Grayson & Fosbracey 1982		Rordorf 1989			
gas saturation-GC		gas saturation-GC		gas saturation-GC			
t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa
wet				set 1		set 2	
20	3.47×10^{-4}	35.0	0.0026	25	0.00079	25	0.0051
30	1.32×10^{-3}	38.2	0.0042	50	0.018	50	0.064
40	4.68×10^{-3}	51.5	0.017	75	0.25	75	0.55
dry		62.8	0.059	100	2.60	100	3,60
20	3.73×10^{-4}	70.0	0.114	125	19.0	125	18.0
30	1.35×10^{-3}	75.2	0.182				
40	4.52×10^{-3}	20	0.00042	eq. 1	P_S/Pa	eq. 1	PS/Pa
				A	14.37	A	11.867
eq.1	P/mmHg	eq. 1a	P/Pa	B	5210.07	B	4220.71
A	12.07	A	11285				
B	5178	B	30.7	eq. 1	P_L/Pa	eq. 1	PL/Pa
				A	11.6603	A	9.519590
				B	4001.62	B	3280.59
				ΔH_V = 76.6 kJ/mol		ΔH_V = 62.8 kJ/mol	

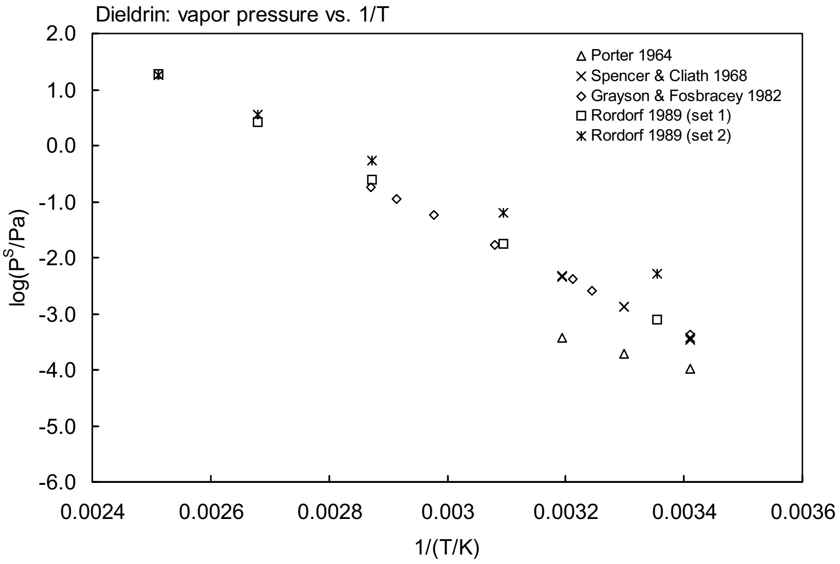
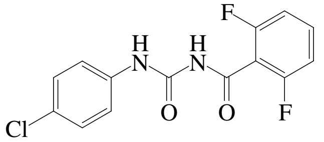


FIGURE 18.1.1.30.3 Logarithm of vapor pressure versus reciprocal temperature for dieldrin.

18.1.1.31 Diflubenzuron



Common Name: Diflubenzuron

Synonym: Deflubenzon, difluron, Dimilin, DU 112307, Duphacid, ENT 29054, OMS 1804, Largon, Micromite, PDD 60401, PH 60–40, TH-6040

Chemical Name: 1-(4-chlorophenyl)-3-(2,6-difluorobenzol) urea; *N*-[[(4-chlorophenyl)-amino]carbonyl]-2,6-difluorobenzamide

Uses: nonsystemic insecticide to control leaf-eating larvae and leaf miners in forestry, woody ornamentals and fruit trees.

CAS Registry No: 35367-38-5

Molecular Formula: $C_{14}H_9ClF_2N_2O_2$

Molecular Weight: 310.683

Melting Point (°C):

230–232	(pure, Hartley & Kidd 1987; Montgomery 1993; Milne 1995)
230–232	(dec., Tomlin 1994)
239	(Lide 2003)

Boiling Point (°C):

dec. on distillation (Montgomery 1993)

Density (g/cm³ at 20°C):

288.3	(calculated-Le Bas method at normal boiling point)

Molar Volume (cm³/mol):

Dissociation Constant, pK_a:

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

Entropy of Fusion, ΔS_{fus} (J/mol K):

Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F: 0.00795 (mp at 239°C)

Water Solubility (g/m³ or mg/L at 25°C or as indicated):

0.25	(Ivie et al. 1980; quoted, Belluck & Felsot 1981)
0.20	(Spencer 1982; Wauchope 1989)
0.14	(20°C, Hartley & Kidd 1987; Milne 1995)
0.10	(20°C, Worthing & Walker 1987, 1991)
14.0	(Montgomery 1993)
0.30	(Milne 1995)
0.08	(selected, Lohninger 1994)
0.08	(20–25°C, selected, Hornsby et al. 1996)

Vapor Pressure (Pa at 25°C or as indicated):

$< 3.3 \times 10^{-5}$	(50°C, Hartley & Kidd 1987)
$< 1.3 \times 10^{-5}$	(Worthing & Hance 1991)
3.33×10^{-5}	(20°C, Montgomery 1993)
1.20×10^{-7}	(gas saturation method, Tomlin 1994)
1.20×10^{-7}	(20–25°C, selected, Hornsby et al. 1996)

Henry's Law Constant (Pa·m³/mol at 25°C or as indicated):

7.40×10^{-4}	(20–25°C, calculated-P/C, Montgomery 1993)
4.70×10^{-4}	(20–25°C, calculated-P/C, this work)

Octanol/Water Partition Coefficient, log K_{OW}:

5.06	(Belluck & Felsot 1981)
3.88	(shake flask-UV, Sotomatsu et al. 1987)

2.12	(shake flask-UV, Nakagawa et al. 1991)
3.10	(selected, Nendza 1991)
3.29	(calculated, Montgomery 1993)
3.89	(Tomlin 1994)

Bioconcentration Factor, log BCF:

2.88	(calculated-S as per Kenaga & Goring, this work)
2.44	(calculated-K_{OW} as per Kenaga & Goring, this work)

Sorption Partition Coefficient, log K_{OC}:

3.01	(calculated, Montgomery 1993)
4.00	(average value, Dowd et al. 1993)
4.00	(20–25°C, selected, Hornsby et al. 1996)
4.06	(estimated-chemical structure, Lohninger 1994)

Environmental Fate Rate Constants, k, or Half-Lives, $t_{1/2}$:

Volatilization:

Photolysis:

Oxidation:

Hydrolysis: half-lives at 20°C: $t_{1/2}$ > 150 d at pH 5 and 7 and $t_{1/2}$ = 42 d at pH 9 (Tomlin 1994).

$t_{1/2}$ > 300 d at pH 2, $t_{1/2}$ = 100 d at pH 7 and $t_{1/2}$ = 0.48 d at pH 12 in natural waters at 20–25°C (Capel & Larson 1995)

Biodegradation: $t_{1/2}$(aerobic) = 3 d, $t_{1/2}$(anaerobic) = 12 d in natural waters (Capel & Larson 1995)

Biotransformation:

Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants:

Half-Lives in the Environment:

Air:

Surface water: stable at pH 5 and 7 with $t_{1/2}$ > 150 d, and $t_{1/2}$ = 42 d at pH 9 and 20°C (Tomlin 1994)

biodegradation $t_{1/2}$(aerobic) = 3 d, $t_{1/2}$(anaerobic) = 12 d, hydrolysis $t_{1/2}$ > 300 d at pH 2, $t_{1/2}$ = 100 d at pH 7 and $t_{1/2}$ = 0.48 d at pH 12 in natural waters at 20–25°C (Capel & Larson 1995)

Ground water:

Sediment:

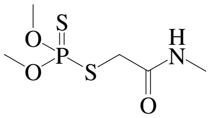
Soil: $t_{1/2}$ < 7 d (Hartley & Kidd 1987; quoted, Montgomery 1993; Tomlin 1994);

$t_{1/2}$ = 10 d in forest soil (Dowd et al. 1993);

field $t_{1/2}$ = 10 d (20–25°C, selected, Hornsby et al. 1996).

Biota:

18.1.1.32 Dimethoate



Common Name: Dimethoate

Synonym: AC 12880, AC 18682, American Cynamid 12880, BI 58, Cekuthoate, Chemathoate, CL 12880, Cygon, Daphene, De-fend, Demos-L40, Devigon, Dimetate, Dimeton, Dimevur, ENT 24650, Ferkethion, Fip, Fortion NM, Fosfamid, Fosfotox, Fostion MM, L 395, Lurgo, NC 262, Perfekthion, Phosphamid, Rebelate, Rogodial, Rogor, Roxion, Sinoratox, Trimetion

Chemical Name: *O,O*-dimethyl *S*-methylcarbamoyl-methyl phosphorodithioate; *O,O*-dimethyl *S*-(*N*-monomethyl)carbamylmethyl dithiophosphate; 2-dimethoxyphosphinothioylthio-*N*-methylacetamide

Uses: systemic and contact insecticide to control thrips and red spider mites on many agricultural crops, sawflies on apples and plums, also wheat bulb and olive flies.

CAS Registry No: 60-51-5

Molecular Formula: $C_5H_{12}NO_3PS_2$

Molecular Weight: 229.258

Melting Point (°C):
51–52 (Hartley & Kidd 1987)
49.0 (Worthing & Hance 1991; Tomlin 1994; Milne 1995)
52 (Lide 2003)

Boiling Point (°C):
107 (at 0.05 mmHg, Melnikov 1971; Freed et al. 1977)
117 (at 0.1 mmHg, Hartley & Kidd 1987; Tomlin 1994; Milne 1995)
117 (tech. grade at 0.1 mmHg, Worthing & Hance 1991)

Density (g/cm^3 at 20°C):
1.277 (65°C, Hartley & Kidd 1987; Montgomery 1993; Tomlin 1994; Milne 1995)
1.281 (50°C, Worthing & Hance 1991; Montgomery 1993)

Molar Volume (cm^3/mol):
205.6 (calculated-Le Bas method at normal boiling point)

Dissociation Constant, pK_a:

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
23.43 (DSC method, Plato & Glasgow 1969)

Entropy of Fusion, ΔS_{fus} (J/mol K):

Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F: 0.543 (mp at 52°C)

Water Solubility (g/m^3 or mg/L at 25°C at normal boiling point):
39000 (Melnikov 1971)
25000 (Martin & Worthing 1977; Worthing 1979; Kenaga 1980a)
25140 (Briggs 1981)
7000–30000 (20–25°C, selected, Willis & McDowell 1982)
> 5000 (20°C, shake flask-GC, Bowman & Sans 1983a)
25020 (20°C, shake flask-GC, Bowman & Sans 1983b)
25000 (22°C, Verschueren 1983)
25000 (21°C, Hartley & Kidd 1987; Worthing & Walker 1987, 1991; Montgomery 1993)
25120 (Kanazawa 1989)
39800 (20–25°C, selected, Wauchope et al. 1992; Hornsby et al. 1996)
23300, 23800, 25000 (20°C, at pH 5, 7, 9, Tomlin 1994)
21000 (21°C, Milne 1995)

Vapor Pressure (Pa at 25°C or as indicated):
11.3×10^{-4} (20°C, Wolfdietrich 1965; Melnikov 1971; Khan 1980)
3.73×10^{-4} (20°C, vaporization rate-gravimetric method, Gückel et al. 1973)

11.0×10^{-4} (Worthing 1979; Hartley & Kidd 1987)
8.90×10^{-4} (20°C, GC, Seiber et al. 1981)
6.80×10^{-4} (gas saturation-GC, Kim et al. 1984, Kim 1985)
3.87×10^{-4} (20°C, extrapolated-Clausius-Clapeyron eq. with vapor pressures at several temperatures, Kim et al. 1984)
85.0×10^{-4} (20°C, GC-RT correlation without mp correlation, Kim et al. 1984; Kim 1985)
41.0×10^{-4} (20°C, GC-RT correlation with mp correction, Kim et al. 1984; Kim 1985)
2.90×10^{-4} (20°C, Worthing & Hance 1991)
33.3×10^{-4} (20–25°C, selected, Wauchope et al. 1992; Hornsby et al. 1996)
6.75×10^{-4} (20°C, Montgomery 1993)
11.0×10^{-4} (Tomlin 1994)
0.0363 (gradient GC method; Tsuzuki 2000)
0.0363; 0.11, 0.083 (gradient GC method; estimation using modified Watson method: Sugden's parachor, McGowan's parachor, Tsuzuki 2000)

Henry's Law Constant ($Pa{\cdot}m^3/mol$ at 25°C or as indicated):
6.23×10^{-6} (calculated-P/C, Lyman et al. 1982; quoted, Howard 1991)
1.10×10^{-4} (20°C, calculated-P/C, Suntio et al. 1988; quoted, Majewski & Capel 1995)
2.66×10^{-6} (20–21°C, calculated-P/C, Montgomery 1993)
1.15×10^{-4} (calculated-P/C, this work)

Octanol/Water Partition Coefficient, log K_{OW}:
–0.29 (Hamaker 1975; Kenaga & Goring 1980)
–0.294 (shake flask-GC, Freed et al. 1979)
0.79 (20 ± 2°C, shake flask-UV, Briggs 1981)
0.70 (22°C, shake flask-GC, Bowman & Sans 1983)
0.50, 0.78 (recommended, Hansch & Leo 1985)
2.71 (Kanazawa 1989)
0.699 (Worthing & Hance 1991; Milne 1995)
0.51–0.78 (Montgomery 1993)
0.50 (recommended, Sangster 1993)
0.704 (Tomlin 1994)
0.78 (selected, Hansch et al. 1995)

Bioconcentration Factor, log BCF:
2.00 (estimated-S, Howard 1991)

Sorption Partition Coefficient, log K_{OC}:
1.23 (soils, calculated, Kenaga 1980a; quoted, Howard 1991)
0.72 (20 ± 2°C, shake flask-UV and reported as log K_{OM}, Briggs 1981)
1.43 (average of 2 soils, Kanazawa 1989)
1.26, 1.56 (clay loam soil, Kanazawa 1989)
0.716 (clay soil, Kanazawa 1989;)
0.72, 1.47 (reported as log K_{OM}, estimated as log K_{OM}, Magee 1991)
1.20, 1.39 (soil, quoted exptl., calculated-χ and fragment contribution, Meylan et al. 1992)
1.30 (soil, 20–25°C, selected, Wauchope et al. 1992; Hornsby et al. 1996)
0.132 (estimated-QSAR and SPARC, Kollig 1993)
0.96 (Montgomery 1993)
1.00 (estimated-chemical structure, Lohninger 1994)
1.21; 1.72 (sandy loam soil, sandy loam sand, Tomlin 1994)
1.20 (soil, calculated-MCI $^1\chi$, Sabljic et al. 1995)
1.20; 1.70, 1.85 (soil, quoted exptl.; estimated-class-specific model, estimated-general model, Gramatica et al. 2000)

Environmental Fate Rate Constants, k, or Half-Lives, $t_{½}$:

Volatilization:

Photolysis:

Oxidation: photooxidation $t_{½}$ = 0.469–4.69 h in air, based on estimated rate constant for the reaction with hydroxyl radical in air (Atkinson 1987; quoted, Howard et al. 1991).

Hydrolysis: $t_{½}$ = 0.8 h at pH 9 and $t_{½}$ = 21 h at pH 2 both at 70°C (Melnikov 1971; quoted, Freed et al. 1977)

neutral rate constant k = 1.7×10^{-4} h^{-1} with a calculated $t_{½}$ = 118 h at pH 7 and 25°C (Ellington et al. 1987, 1988; quoted, Montgomery 1993);

first-order $t_{½}$ = 2822 h, based on measured neutral and base catalyzed hydrolysis rate constants (Ellington et al. 1987; quoted, Howard et al. 1991);

rate constant k = 1.68 yr^{-1} at pH 7.0 and 25°C (Kollig 1993);

$t_{½}$ = 12 d at pH 9 (Tomlin 1994)

$t_{½}$ = 120 d at pH 2, $t_{½}$ = 120 d at pH 7 and $t_{½}$ = 0.0038 d at pH 12 in natural waters (Capel & Larson 1995)

Biodegradation: aqueous aerobic $t_{½}$ = 264–1344 h, based on river die-away test data (Eichelberger & Lichtenburg 1971; quoted, Howard et al. 1991) and soil die-away test data for two soils (Bro-Rasmussen et al. 1970; quoted, Howard et al. 1991); aqueous anaerobic $t_{½}$ = 1056–5376 h, based on estimated unacclimated aqueous aerobic biodegradation half-life (Howard et al. 1991)

$t_{½}$(aerobic) = 11 d, $t_{½}$(anaerobic) = 44 d in natural waters (Capel & Larson 1995)

Biotransformation:

Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants:

Half-Lives in the Environment:

Air: $t_{½}$ = 0.469–4.69 h, based on estimated rate constant for the reaction with hydroxyl radical in air (Atkinson 1987; quoted, Howard et al. 1991).

Surface water: $t_{½}$ = 264–1344 h, based on estimated unacclimated aqueous aerobic biodegradation half-life (Howard et al. 1991)

Biodegradation $t_{½}$(aerobic) = 11 d, $t_{½}$(anaerobic) = 44 d, hydrolysis $t_{½}$ = 120 d at pH 2, $t_{½}$ = 120 d at pH 7 and $t_{½}$ = 0.0038 d at pH 12 in natural waters (Capel & Larson 1995)

$t_{½}$ = 423 d at 6°C, 193h at 23°C in darkness for Milli-Q water; $t_{½}$ = 171 d at 6°C, $t_{½}$ = 43 d at 22°C in darkness, $t_{½}$ = 29 d under sunlight conditions for river water at pH 7.3; $t_{½}$ = 173 d at 6°C, $t_{½}$ = 29 d at 22°C in darkness for filtered river water, pH 7.3; $t_{½}$ = 219 d at 6°C, $t_{½}$ = 36 d at 22°C in darkness, $t_{½}$ = 74 d under sunlight conditions for seawater, pH 8.1 (Lartiges & Garrigues 1995).

Ground water: $t_{½}$ = 528–2688 h, based on estimated unacclimated aqueous aerobic biodegradation half-life (Howard et al. 1991).

Sediment:

Soil: $t_{½}$ = 264–888 h, based on soil die-away test data for two soils (Bro-Rasmussen et al. 1970; quoted, Howard et al. 1991);

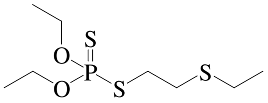
selected $t_{½}$ = 7.0 d (Wauchope et al. 1992; Hornsby et al. 1996);

aerobic $t_{½}$ = 2–4.1 d in soil and photolytic $t_{½}$ = 7–16 d on soil surface (Tomlin 1994);

$t_{½}$ = 7.0 d (selected, Halfon et al. 1996).

Biota: disappearance rate and half-life from treated plants: $t_{½}$ = 2.95 d for cabbage, $t_{½}$ = 3.40 d for tomato leaves and $t_{½}$ = 2.40 d for tomato fruits (Othman et al. 1987).

18.1.1.33 Disulfoton



Common Name: Disulfoton

Synonym: Di-Syston, Dimaz, Disipton, Disystox, Dithiosystox, Frumin AL, Glebofos, Solvirex

Chemical Name: *O,O*-diethyl *S*-[2-(ethylthio) ethyl] phosphorodithioate; phosphorodithioic acid, *O,O*-diethyl *S*-[2-(ethylthio)ethyl] ester

Uses: insecticide to control aphids, thrips, mealybugs, and other sucking insects, and spider mites in potatoes, vegetables, cereals, maize, sorghum, rice, soybeans, groundnuts, lucerne, clover, sugar cane, sugar beet, hops, strawberries, cotton, coffee, pineapples, tobacco, ornamentals, fruit and nut crops, and forestry nurseries; also used as acaricide.

CAS Registry No: 298-04-4

Molecular Formula: $C_8H_{19}O_2PS_3$

Molecular Weight: 274.405

Melting Point (°C):

–25	(Milne 1995; Lide 2003)

Boiling Point (°C):

62.0	(at 0.01 mmHg, Hartley & Kidd 1987)
128	(at 1 mmHg, Worthing & Hance 1991; Tomlin 1994; Milne 1995)

Density (g/cm^3 at 20°C):

1.144	(Hartley & Kidd 1987; Tomlin 1994)
1.14	(Worthing & Hance 1991)

Molar Volume (cm^3/mol):

282.1	(calculated-Le Bas method at normal boiling point)

Dissociation Constant, pK_a:

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

Entropy of Fusion, ΔS_{fus} (J/mol K):

Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F: 1.0

Water Solubility (g/m^3 or mg/L at 25°C or as indicated):

66	(Günther 1968)
25	(20°C, Melnikov 1971; Spencer 1973)
25	(Martin & Worthing 1977)
16.3	(19.5°C, shake flask-GC, Bowman & Sans 1979, 1983b)
25	(22°C, Khan 1980; Worthing & Walker 1983)
15–66	(20–25°C, selected, Willis & McDowell 1982)
25	(22°C, Hartley & Kidd 1987)
12	(22°C, Worthing & Hance 1991)
25	(20–25°C, selected, Wauchope et al. 1992; Hornsby et al. 1996)
12	(20°C, Tomlin 1994)
12	(22°C, Milne 1995)
29.9, 29.9	(supercooled liquid S_L: literature-derived value LDV, final adjusted value FAV, Muir et al. 2004)

Vapor Pressure (Pa at 25°C or as indicated):

0.024	(20°C, vapor density, MacDougall & Archer 1964)

log (P/mmHg) = 10.20 – 4084.80/(T/K); temp range 10–40°C (vapor density, MacDougall & Archer 1964)

0.024	(20°C, Eichler 1965)
0.024	(20°C, Melnikov 1971; Khan 1980)
0.024	(Worthing 1983)
0.0041	(20°C, GC-Rt correlation, Kim et al. 1984; Kim 1985)
0.024	(20°C, Hartley & Kidd 1987)
0.020	(20°C, selected, Suntio et al. 1988)

0.024 (20°C, Worthing & Hance 1991)
0.020 (20–25°C, selected, Wauchope et al. 1992; Hornsby et al. 1996)
0.013 (Tomlin 1994)
0.010, 0.0099 (supercooled liquid P_L: literature-derived value LDV, final adjusted value FAV, Muir et al. 2004)

Henry's Law Constant ($Pa{\cdot}m^3/mol$ at 25°C or as indicated):
0.404 (calculated-P/C, Lyman et al. 1982; quoted, Howard 1991)
0.22 (20°C, calculated-P/C, Suntio et al. 1988)
0.101, 0.253 (10°, 20°C, Wanner et al. 1989)
0.090 (final adjusted value FAV, Muir et al. 2004)

Octanol/Water Partition Coefficient, log K_{OW}:
3.04 (Callahan et al. 1979)
3.88 (shake flask-UV, Hermens & Leeuwangh 1982)
4.02 (shake flask-GC, Bowman & Sans 1983b)
4.02 (recommended, Hansch & Leo 1985)
3.84 (RP-HPLC correlation, Saito et al. 1993)
3.95 (Tomlin 1994)
4.02 (recommended, Hansch et al. 1995)
3.95 (literature-derived value LDV, Muir et al. 2004)

Octanol/Air Partition Coefficient, log K_{OA}:
8.39 (final adjusted value FAV, Muir et al. 2004)

Bioconcentration Factor, log BCF:
2.00 (calculated-S, Kenaga 1980; quoted, Pait et al. 1992)
2.04 (calculated-K_{OC}, Kenaga 1980)
2.00, 2.83 (estimated-S, estimated-K_{OW}, Lyman et al. 1982; quoted, Howard 1991)
2.65 (carp, Takase & Oyama 1985; quoted, Howard 1991)

Sorption Partition Coefficient, log K_{OC}:
3.25 (soil, Hamaker & Thompson 1972; Kenaga 1980; Kenaga & Goring 1980)
2.81, 3.04, 3.72 (Hamaker & Thompson 1972)
2.87 (soil, calculated-S as per Kenaga & Goring 1978, Kenaga 1980)
3.20 (av. soils/sediments, Rao & Davidson 1980)
2.67–3.70 (reported as log K_{OM}, Mingelgrin & Gerstl 1983)
2.90 (calculated- MCI χ, Gerstl & Helling 1987)
3.20 (soil, screening model calculations, Jury et al. 1987b)
3.36 (estimated as log K_{OM}, Magee 1991)
3.22 (soil, quoted exptl., Meylan et al. 1992)
2.91 (soil, calculated-MCI χ and fragments contribution, Meylan et al. 1992)
2.78 (soil, 20–25°C, estimated, Wauchope et al. 1992; Hornsby et al. 1996)
2.94 (estimated-QSAR and SPARC, Kollig 1993)
2.91 (soil, HPLC-screening method, mean value, Kördel et al. 1993, 1995)
3.49 (estimated-chemical structure, Lohninger 1994)
3.22 (soil, calculated-MCI $^1\chi$, Sabljic et al. 1995)
2.91; 2.91 (HPLC-screening method; calculated-PCKOC fragment method, Müller & Kördel 1996)
3.66, 3.146, 3.11, 3.37, 4.146 (first generation Eurosoils ES-1, ES-2, ES-3, ES-4, ES-5, shake flask/batch equilibrium-HPLC/UV, Gawlik et al. 1998)
3.417, 3.333, 3.151, 2.782, 3.127 (second generation Eurosoils ES-1, ES-2, ES-3, ES-4, ES-5, HPLC-k′ correlation, Gawlik et al. 2000)
3.22; 3.15, 3.40 (soil, quoted exptl.; estimated-class-specific model, estimated-general model, Gramatica et al. 2000)
2.92 (soil: organic carbon OC $\geq$ 0.5%, average, Delle Site 2001)

Environmental Fate Rate Constants, k, or Half-Lives, $t_{½}$:

Volatilization: gas exchange $t_{½}$ = of 900 d for winter and $t_{½}$ = 360 d for summer in Rhine River (Wanner et al. 1989).

Photolysis: photolytic $t_{½}$ = 1000 d for winter and $t_{½}$ = 100 d for summer in the Rhine River (Wanner et al. 1989);

$t_{½}$ = 1–4 d (Tomlin 1994)

Apparent first-order rate constant phototransformation at $\lambda > 285$ nm, $k = (1.38 \pm 0.12) \times 10^{-2}\ h^{-1}$ in purified water, and $k = (1.68 \pm 0.12) \times 10^{-2}\ h^{-1}$ in Capot river water with $t_{½}$ ~ 40 h (Zamy et al. 2004)

Oxidation: half-life ranged from $t_{½}$ ~ 5 h of midday sunlight during summer to $t_{½}$ = 12 h during winter estimated from kinetic data for oxygenation reactions photosensitized by humic substances in water exposed to sunlight (Zepp et al. 1981);

photooxidation $t_{½}$ = 0.50–4.80 h in air, based on estimated rate constant for the reaction with hydroxyl radical in air (Atkinson 1987; quoted, Howard et al. 1991).

Hydrolysis: first-order $t_{½}$ = 103 d, based on measured overall rate constant $k = 2.8 \times 10^{-4}\ h^{-1}$ at pH 7, 25°C (Ellington et al. 1986, 1987, 1988; quoted, Howard et al. 1991);

abiotic hydrolysis $k = 1.3 \times 10^{-7}\ s^{-1}$ under neutral condition, $k = 2.0 \times 10^{-3}\ s^{-1}$ under base-catalyzed condition at 20°C and hydrolysis $t_{½}$ = 170 d at 11°C, pH 9 and $t_{½}$ = 62 d in summer were predicted in Rhine River (Wanner et al. 1989);

$t_{½}$ = 3.04 yr in water at pH 1–5 and at 20°C; 1.2 d at pH 7 and $t_{½}$ = 7.2 h at pH 9 both at 70°C (Worthing & Hance 1991);

rate constant $k = 3.23\ yr^{-1}$ at pH 7.0 and 25°C (Kollig 1993);

$t_{½}$ = 133 d at pH 4, $t_{½}$ = 169 d at pH 7, and $t_{½}$ = 131 d at pH 9 at 22°C (Tomlin 1994).

Biodegradation: $t_{½}$ < 14 d, rapidly oxidized in soil (Szeto et al. 1983)

primary biodegradation rate constant $k = 0.2\ \mu g^2\ L^2\ d^{-1}$ with $t_{½}$ = 41 d, and the degradation $t_{½}$ = 7–41 d for winter and $t_{½}$ = 4–28 d for summer in Rhine River (Wanner et al. 1989);

aqueous aerobic $t_{½}$ = 72–504 h, based on aerobic soil field data and reported half-lives for soil (Howard et al. 1991);

aqueous anaerobic $t_{½}$ = 288–2016 h, based on estimated unacclimated aqueous aerobic biodegradation half-life (Howard et al. 1991).

Biotransformation:

Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants:

Half-Lives in the Environment:

Air: $t_{½}$ = 0.50–4.80 h, based on estimated rate constant for the reaction with hydroxyl radical in air (Atkinson 1987; quoted, Howard et al. 1991).

Surface water: gas exchange $t_{½}$ = 900 d for winter, $t_{½}$ = 360 d for summer; abiotic hydrolysis half-lives of 170 d for winter, 62 d for summer; photolytic transformation $t_{½}$ = 1000 d for winter, $t_{½}$ = 200 d for summer and primary biodegradation $t_{½}$ = 7–41 d for winter, $t_{½}$ = 8–28 d for summer in Rhine River under environmental conditions (Wanner et al. 1989);

overall $t_{½}$ = 72–504 h, based on estimated unacclimated aqueous aerobic biodegradation half-life (Howard et al. 1991).

$t_{½}$ ~ 40 h upon photolysis in Capot river water (Zamy et al. 2004)

Ground water: $t_{½}$ = 144–1008 h, based on estimated unacclimated aqueous aerobic biodegradation half-life (Howard et al. 1991).

Sediment:

Soil: estimated persistence of 4 wk in soil (Kearney et al. 1969; Edwards 1973; quoted, Morrill et al. 1982);

$t_{½}$ = 72–504 h, based on aerobic soil field data (Szeto et al. 1983; quoted, Howard et al. 1991) and reported half-lives for soil (Domsch 1984; quoted, Howard et al. 1991);

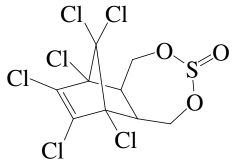
$t_{½}$ = 5 d from screening model calculations (Jury et al. 1987b);

estimated $t_{½}$ = 30 d (Wauchope et al. 1992; Hornsby et al. 1996);

soil $t_{½}$ = 9 d (Pait et al. 1992).

Biota: biochemical $t_{½}$ = of 5 d from screening model calculations (Jury et al. 1987b).

18.1.1.34 Endosulfan



Common Name: Endosulfan

Synonym: Benzoepin, Beosit, Bio 5462, Chlorthiepin, Crissulfan, Cyclodan, Endocel, ENT 23979, FMC 5462, Hildan, Hoe 2671, Insectophene, KOP-thiodan, Malix, NCI-C00566, Niagara 5462, OMS-570, Thifor, Thimul, Thiodan, Thiofor, Thionex, Thiosulfan, Tionel, Tiovel

Chemical Name: 1,4,5,6,7,7-hexachloro-5-norbornene-2,3-dimethyl cyclic sulfite; 1,2,3,4,7,7-hexachlorobicyclo-2,2,1-hepten-5,6-bisoxymethylene sulfite; (1,4,5,6,7,7-hexachloro-8,9,10-trinorborn-5-en-2,3-ylene-bismethylene)-sulfite; 6,7,8,9,10,10-hexachloro-1,5,5*a*,6,9,9*a*-hexahydro-6,9-methano-2,4,3-benzodioxathiepine 3-oxide

Uses: insecticide for vegetable crops and also used as acaricide.

CAS Registry No: 115-29-7; 959-98-8 (α-endosulfan, endosulfan I); 33213-65-9 (β-endosulfan, endosulfan II)

Molecular Formula: $C_9H_6Cl_6O_3S$

Molecular Weight: 406.925

Melting Point (°C):

70–100	(tech. grade, Worthing & Hance 1991; Milne 1995)
70–100, 108–110	(α-endosulfan, β-endosulfan, Suntio et al. 1988)
106, 207–209	(α-endosulfan, β-endosulfan, Montgomery 1993)
109.2, 213.3	(α-endosulfan, β-endosulfan, Tomlin 1994)
106, 109.2	(Milne 1995)

Boiling Point (°C):

106	(at 0.7 mmHg, Hartley & Kidd 1987; Milne 1995)

Density (g/cm^3 at 20°C):

1.80	(tech. grade, Tomlin 1994)
1.745	(Milne 1995; Montgomery 1993)

Molar Volume (cm^3/mol):

312.8	(calculated-Le Bas method at normal boiling point,)

Dissociation Constant, pK_a:

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

Entropy of Fusion, ΔS_{fus} (J/mol K):

Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F:

0.22. 0.13	(20°C, α-, β-endosulfan, Suntio et al. 1988)

Water Solubility (g/m^3 or mg/L at 25°C pr as indicated):

0.53	(α-endosulfan, generator column-GC, Weil et al. 1974)
0.286	(β-endosulfan, generator column-GC, Weil et al. 1974)
<1.0	(Wauchope 1978)
0.050	(Weber et al. 1980)
0.510	(α-endosulfan, 20°C, shake flask-GC, Bowman & Sans 1983a)
0.45	(β-endosulfan, 20°C, shake flask-GC, Bowman & Sans 1983a)
0.06–0.15	(U.S. EPA 1984; McLean et al. 1988)
0.32	(22°C, Hartley & Kidd 1987)
0.15	(20°C, selected, Suntio et al. 1988)
0.32	(α-endosulfan at 22°C, Worthing & Hance 1991; Tomlin 1994; Milne 1995)
0.33	(β-endosulfan at 22°C, Worthing & Hance 1991; Tomlin 1994)
0.32	(20–25°C, selected, Wauchope et al. 1992; Hornsby et al. 1996)
0.53	(α-endosulfan, Montgomery 1993)
0.28	(β-endosulfan, Montgomery 1993)

3.75, 3.63 (α-endosulfan, supercooled liquid S_L: literature-derived value LDV, final adjusted value FAV, Muir et al. 2004)

1.71, 2.56 (α-endosulfan, supercooled liquid: LDV derivation of literature-derived value, FAV final-adjusted value, Shen & Wania 2005)

32.1, 36.2 (β-endosulfan, supercooled liquid: LDV derivation of literature-derived value, FAV final-adjusted value, Shen & Wania 2005)

Vapor Pressure (Pa at 25°C or as indicated):

0.00133 (Martens 1972; Khan 1980)

0.013 (endosulfan I, Barlow 1978)

$>$ 0.00013 (20–25°C, Weber et al. 1980)

1.20 (80°C, Hartley & Kidd 1987)

0.0061 (endosulfan I, GC-RT correlation, supercooled liquid value, Hinckley et al. 1990)

0.0032 (endosulfan II, GC-RT correlation, supercooled liquid value, Hinckley et al. 1990)

0.0011 (20°C, selected, Suntio et al. 1988)

1.20 (tech. grade at 80°C, Worthing & Hance 1991)

2.27×10^{-5} (20–25°C, selected, Wauchope et al. 1992; Hornsby et al. 1996)

0.00133 (Montgomery 1993)

8.3×10^{-5} (20°C, 2 to 1 mixture of α- and β-endosulfan, Tomlin 1994)

2.3×10^{-5} (selected, Halfon et al. 1996)

0.0061, 0.0063 (α-endosulfan, supercooled liquid P_L: literature-derived value LDV, final adjusted value FAV, Muir et al. 2004)

0.0060, 0.0044 (α-endosulfan, supercooled liquid P_L: LDV literature-derived value, FAV final adjusted value, Shen & Wania 2005)

0.0043, 0.0040 (β-endosulfan, supercooled liquid P_L: LDV literature-derived value, FAV final adjusted value, Shen & Wania 2005)

Henry's Law Constant (Pa·m^3/mol at 25°C and reported temperature dependence equations):

1.09 (calculated-P/C, Mabey et al. 1982)

2.98 (20°C, calculated-P/C, Suntio et al. 1988)

0.679, 0.0627 (endosulfan I, II, calculated, Cotham & Bidleman 1989)

1.135 (calculated-P/C an average of α- and β-endosulfan, Howard 1991)

10.23 (α-endosulfan, Montgomery 1993)

1.935 (β-endosulfan, calculated-P/C, Montgomery 1993)

6.45, 13.23 (20°C, tech. grade: distilled water, salt water 33.3l%, wetted wall column-GC, Rice et al. 1997a, b)

6.63, 0.788 (20°C, endosulfan I, II, distilled water, wetted wall column-GC, Rice et al. 1997a, b)

log $K_{AW} = -876.14/(T/K) + 0.4463$; temp range: 8.3–38.2°C, (endosulfan I, distilled water, wetted-wall column-GC, Rice et al. 1997a)

12.89, 2.12 (20°C, endosulfan I, II, salt water 33.3l%, wetted wall column-GC, Rice et al. 1997a, b)

8.65, 8.48; 9.31 (20°C, endosulfan I: microlayer, subsurface natural water of salinity 17l% and TOC 0.4–1.0 ppm, from Pt. Lookout, Chesapeake Bay; estimated value adjusted to salinity, Rice et al. 1997b)

8.77, 8.04; 9.12 (20°C, endosulfan I: microlayer, subsurface natural water of salinity 16l% and TOC 0.5–0.6 ppm, from Solomons, Chesapeake Bay; estimated adjusted to salinity, Rice et al. 1997b)

7.14, 9.21; 8.43 (20°C, endosulfan I: microlayer, subsurface natural water of salinity 12l%, TOC 0.6 ppm, from Sandy Point, Chesapeake Bay; estimated value adjusted to salinity, Rice et al. 1997b)

0.719, 0.040 (α-, β-endosulfan, wetted wall column-GC, Altschuh et al. 1999)

6.99 (20°C, Endosulfan I, selected from literature experimentally measured data, Staudinger & Roberts 2001)

log $K_{AW} = 0.446 - 876/(T/K)$, (Endosulfan I, van't Hoff eq. derived from literature data, Staudinger & Roberts 2001)

0.715, 0.699 (α-endosulfan, literature-derived value LDV, final adjusted value FAV, Muir et al. 2004)

0.72, 0.70 (α-endosulfan, LDV literature-derived value, FAV final adjusted value, Shen & Wania 2005)

0.040, 0.045 (β-endosulfan, LDV literature-derived value, FAV final adjusted value, Shen & Wania 2005)

Octanol/Water Partition Coefficient, log K_{OW}:

3.55, 3.62 (α-, β-endosulfan, Ali 1978)
3.83 (α-endosulfan, shake flask-GC, Hermens & Leeuwangh 1982)
3.83 (α-endosulfan, Hansch & Leo 1985)
4.74, 4.78 (α-, β-endosulfan, calculated-fragment const., Noegrohati & Hammers 1992)
3.55, 3.62 (α-, β-endosulfan, Montgomery 1993)
4.74, 4.79 (α-, β-endosulfan at pH 5, Tomlin 1994)
3.62, 3.83 (α-, β-endosulfan, Hansch et al. 1995)
3.84 (Pomona-database, Müller & Kördel 1996)
5.09 (α-endosulfan, literature-derived value LDV, Muir et al. 2004)
4.74, 4.94 (α-endosulfan, LDV literature-derived value, FAV final adjusted value, Shen & Wania 2005)
4.78, 4.78 (β-endosulfan, LDV literature-derived value, FAV final adjusted value, Shen & Wania 2005)

Octanol/Air Partition Coefficient, log K_{OA} at 25°C and reported temperature dependence equation. Additional data at other temperatures designated * are compiled at the end of this section:

8.677*, 8.638 (gas saturation-GC/MS, calculated, measured range 5–25°C, Shoeib & Harner 2002)
log $K_{OA} = -5.90 + 4333/(T/K)$, temp range: 5–25°C (gas saturation-GC, Shoeib & Harner 2002)
8.64 (α-endosulfan, final adjusted value FAV, Muir et al. 2004)
8.63, 8.49 (α-endosulfan, LDV literature derived value, FAV final adjusted value, Shen & Wania 2005)

Bioconcentration Factor, log BCF:

–3.66 (beef biotransfer factor log B_b, correlated-K_{OW}, Beck et al. 1966)
2.78 (α-endosulfan for mussel, Ernst 1977;)
–1.52, –1.22 (α-, β-endosulfan, bioaccumulation factor log BF, adipose tissue in female Albino rats, Dorough et al. 1978)
2.63, 2.44 (α-, β-endosulfan, paddy field fish, Soon & Hock 1987)
1.91, 2.33 (α-, β-endosulfan, paddy field fish, Tejada 1995)
3.55; 3.65 (α-endosulfan for *Oncorhynchus mykiss*, wet wt. basis: quoted exptl.; calculated-QSAR model based on quantum chemical parameters, Wei et al. 2001)

Sorption Partition Coefficient, log K_{OC}:

3.46 (α-endosulfan, estimated, Lyman et al. 1982; quoted, Howard 1991)
3.83 (β-endosulfan, calculated-S, Lyman et al. 1982; quoted, Howard 1991)
4.09 (soil, 20–25°C, selected, Wauchope et al. 1992; Hornsby et al. 1996)
4.00 (α- or β-endosulfan, estimated-QSAR & SPARC, Kollig 1993)
3.31, 3.37 (α-endosulfan, β-endosulfan, calculated, Montgomery 1993)
4.09 (soil, α-endosulfan, HPLC-screening method, mean value of different stationary and mobile phases, Kördel et al. 1993)
4.09 (estimated-chemical structure, Lohninger 1994)
3.48–4.30 (Tomlin 1994)
4.09 (α-endosulfan, HPLC-screening method, Kördel et al. 1995)
4.09; 5.24 (HPLC-screening method; calculated-PCKOC fragment method, Müller & Kördel 1996)
3.90 (soil, estimated-general model, Gramatica et al. 2000)

Environmental Fate Rate Constants, k, or Half-Lives, $t_{1/2}$:

Volatilization:
Photolysis:
Oxidation: photooxidation $t_{1/2}$ = 2.5–24.8 h, based on an estimated rate constant for the vapor-phase reaction with hydroxyl radical in air with a deoxygenated endosulfan analog (Atkinson 1987; quoted, Howard et al. 1991).
Hydrolysis: first-order $t_{1/2}$ = 218 h, based on neutral aqueous hydrolysis rate constant $k = (3.2 \pm 2.0) \times 10^{-3}\ h^{-1}$ for α-Endosulfan at pH 7 and 25°C (Ellington et al. 1986, 1987, 1988; quoted, Howard et al. 1991; Montgomery 1993);
first-order $t_{1/2}$ = 187 h, based on neutral aqueous hydrolysis rate constant $k = (3.7 \pm 2.0) \times 10^{-3}\ h^{-1}$ for β-endosulfan at pH 7 and 25°C (Ellington et al. 1987, 1988; quoted, Howard et al. 1991; Montgomery

1993); rate constant k = 6.1 × 10^{-2} yr^{-1} for α-endosulfan at pH 7 and 25°C and rate constant k = 8.9 × 10^{-2} yr^{-1} for β-endosulfan at pH 7 and 25°C (Kollig 1993).

$t_{½}$ = 360 d at pH 2, $t_{½}$ = 9.1 d at pH 7 and $t_{½}$ = 0.00029 d at pH 12 in natural waters (Capel & Larson 1995)

Biodegradation: aqueous aerobic $t_{½}$ = 48–336 h, based on unacclimated aerobic river die-away test data (Eichelberger & Lichtenburg 1971; quoted, Howard et al. 1991) and reported soil grab sample data (Bowman et al. 1965; quoted, Howard et al. 1991);

first-order rate constant k = –0.00502 h^{-1} in nonsterile sediment, k = –0.00796 h^{-1} in sterile sediment by shake-tests at Range Point, first-order k = –0.0157 h^{-1} in nonsterile water, and k = –0.0325 h^{-1} in sterile water by shake-tests at Range Point (Walker et al. 1988);

first-order rate constants k = –0.00165 to –0.00296 h^{-1} in nonsterile sediment, k = –0.00426, –0.00545 h^{-1} in sterile sediment by shake-tests at Davis Bayou and first-order rate constants k = –0.00335 to –0.00490 h^{-1} in nonsterile water and k = –0.0130, –0.00866 h^{-1} in sterile water by shake-tests at Davis Bayou (Walker et al. 1988)

$t_{½}$(aerobic) = 2 d, $t_{½}$(anaerobic) = 8 d in natural waters (Capel & Larson 1995).

Biotransformation:

Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants:

k_1 = 12.3 h^{-1}; k_2 = 0.0205 h^{-1} (mussel from α-endosulfan, Ernst 1977; quoted, Hawker & Connell 1986)

Half-Lives in the Environment:

Air: $t_{½}$ = 2.5–24.8 h, based on an estimated rate constant for the vapor-phase reaction with hydroxyl radicals in air with a deoxygenated Endosulfan analog (Atkinson 1987; quoted, Howard et al. 1991);

$t_{½}$ = 9.2 ± 4 yr at Eagle Harbor in the Great Lake's atmosphere. (Buehler et al. 2004).

Surface water: persistence of up to 4 weeks in river water (Eichelberger & Lichtenberg 1971);

$t_{½}$ = 30 d and 45 d for α- and β-endosulfan respectively for surface waters in case of first order reduction process may be assumed and estimated $t_{½}$ ~ 30–300 d for β-endosulfan in lakes in the Netherlands (Zoeteman et al. 1980);

$t_{½}$ = 4.5–218 h, based on aqueous hydrolysis half-lives for both α- and β-endosulfan at pH 7 and 9 and 25°C, respectively (Ellington et al. 1987; quoted, Howard et al. 1991)

$t_{½}$ = 1.3 d in rice paddy water (Tejada et al. 1993; quoted, Abdullah et al. 1997)

$t_{½}$(aerobic) = 2 d, $t_{½}$(anaerobic) = 8 d, hydrolysis $t_{½}$ = 360 d at pH 2, $t_{½}$ = 9.1 d at pH 7 and $t_{½}$ = 0.00029 d at pH 12 in natural waters (Capel & Larson 1995)

Ground water: estimated $t_{½}$ = 30–300 d in lakes and Ground water (β-Endosulfan, Zoeteman et al. 1980);

$t_{½}$ = 4.5–218 h, based on aqueous hydrolysis half-lives for both α- and β-endosulfan at pH 7 and 9 and 25°C respectively (Ellington et al. 1987; quoted, Howard et al. 1991).

Sediment:

Soil: $t_{½}$ = 4.5–218 h, based on aqueous hydrolysis half-lives for both α- and β-endosulfan at pH 7 and 9 and 25°C, respectively (Ellington et al. 1987; quoted, Howard et al. 1991);

$t_{½}$ > 50 d and subject to plant uptake via volatilization (Ryan et al. 1988);

selected $t_{½}$ = 50 d (Wauchope et al. 1992; Hornsby et al. 1996);

$t_{½}$ = 1.2 d in rice soil (Tejada et al. 1993; quoted, Abdullah et al. 1997);

soil $t_{½}$ = 120 d (Pait et al. 1992);

degraded in soil with $t_{½}$ = 30–70 d (Tomlin 1994); 50 d (selected, Halfon et al. 1996)

$t_{½}$ = 5 – 7 yr in soil (Geyer et al. 2000)

Biota: $t_{½}$ = 33.8 h in mussels (α-endosulfan, Ernst 1977);

$t_{½}$ = 1.0 d in rice leaves (Tejada et al. 1993; quoted, Abdullah et al. 1997).

TABLE 18.1.1.34.1
Reported octanol-air partition coefficients of *α*-endosulfan at various temperatures

Shoeib & Harner 2002	
generator column-GC/MS	
t/°C	log K_{OA}
5	9.7188
10	9.3591
15	9.1651
20	8.8316
25	8.6772
25	8.638

log K_{OA} = A + B/(T/K)

A	–5.902
B	4333

enthalpy of phase change

$\Delta H_{OA}/(\text{kJ mol}^{-1}) = 83.0$

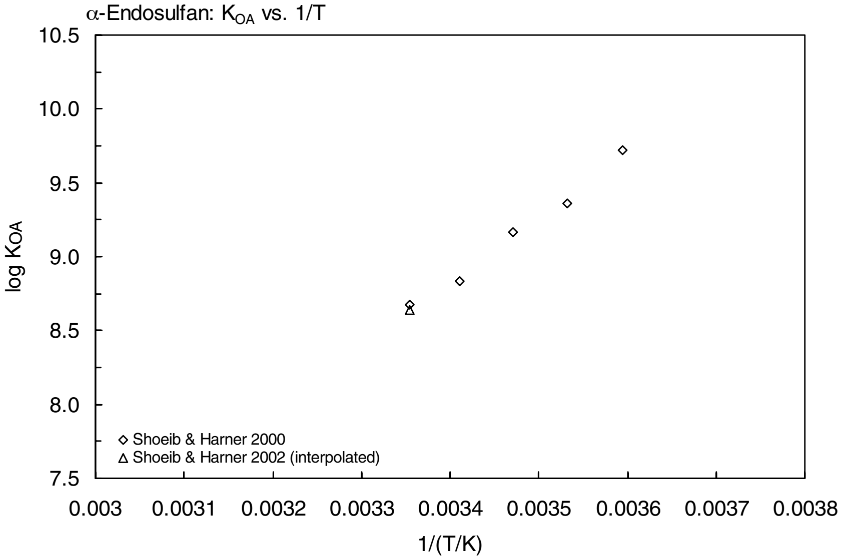
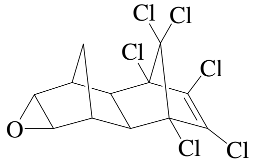


FIGURE 18.1.1.34.1 Logarithm of K_{OA} versus reciprocal temperature for α-endosulfan.

18.1.1.35 Endrin



Common Name: Endrin
Synonym: Endrex, ENT 17521, Hexadrin, Isodrin epoxidek, Mendrin, NA 2761, NCI-C00157, Nendrin, RCRA
Chemical Name: 1,2,3,4,10,10-hexachloro-6,7-epoxy-1,4,4*a*,5,6,7,8,8*a*-octahydro-*exo*-1,4-*exo*-5,8-dimethano-naphthalene
Uses: Insecticide/Avicide/Rodenticide
CAS Registry No: 72-20-8
Molecular Formula: $C_{12}H_8Cl_6O$
Molecular Weight: 380.909
Melting Point (°C):
 226–230 (Hartley & Kidd 1987; Howard 1991)
 245 (dec, Lide 2003)
Boiling Point (°C):
 245 (dec. Montgomery 1993)
Density (g/cm^3 at 20°C):
 1.70, 1.65 (pure, technical, at 25°C, Montgomery 1993)
Molar Volume (cm^3/mol):
 318.2 (calculated-Le Bas method at normal boiling point)
Dissociation Constant, pK_a:
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
 23.88 (Ruelle & Kesselring 1997)
Entropy of Fusion, ΔS_{fus} (J/mol K):
Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F: 0.00694 (mp at 245°C)

Water Solubility (g/m^3 or mg/L at 25°C or as indicated. Additional data at other temperatures designated * are compiled at the end of this section):
 0.23* (shake flask-UV, measured range 25–45°C, Richardson & Miller 1960)
 0.26 (rm. temp., shake flask-GC, Robeck et al. 1965)
 0.23 (Günther et al. 1968)
 0.25* (shake flask-GC/ECD, measured range 15–45°C, Biggar & Riggs 1974)
 0.022*, 0.15*, 0.195* (particle size: 0.01, 0.05 and 5.0μ, shake flask-GC/ECD, measured range 15–45°C, Biggar & Riggs 1974)
 0.26 (generator column-GC/ECD, Weil et al. 1974)
 0.10 (Weber et al. 1980)
 0.024 (Bruggeman et al. 1981)
 0.25 (misquoted as 0.25 μg/L from Biggar & Riggs, Howard 1991)
 0.22–0.26 (Montgomery 1993)
 0.23 (20–25°C, selected, Augustijn-Beckers et al. 1994; Hornsby et al. 1996)
 15.85 (20–25°C, supercooled liquid value, Majewski & Capel 1995)
 0.105, 0.000065 (predicted-molar volume, mp and mobile order thermodynamics, Ruelle & Kesselring 1997)
 1.03, 1.14 (supercooled liquid: LDV derivation of literature-derived value, FAV final-adjusted value, Shen & Wania 2005)
 $\log [C_L/(\text{mol m}^{-3})] = -1022/(T/K) + 0.86$ (supercooled liquid, linear regression of literature data, Shen & Wania 2005)

Vapor Pressure (Pa at 25°C or as indicated):
 4.00×10^{-4} (20°C, Bowery 1964)
 2.67×10^{-5} (Eichler 1965; Melnikov 1971; Martin 1972; Quellette & King 1977)

2.67×10^{-5} (20–25°C, Weber et al. 1980)
1.17×10^{-5} (20°C, selected exptl. value, Kim 1985)
2.00×10^{-5} (20°C, selected, Suntio et al. 1988)
9.33×10^{-5} (25°C, Montgomery 1993)
2.67×10^{-5} (20–25°C, selected, Augustijn-Beckers et al. 1994; Hornsby et al. 1996)
1.38×10^{-3} (20–25°C, supercooled liquid value, Majewski & Capel 1995)
0.0052, 0.0031 (supercooled liquid P_L: LDV literature derived value, FAV final adjusted value, Shen & Wania 2005)

Henry's Law Constant ($Pa{\cdot}m^3/mol$ at 25°C or as indicated):
1.8×10^{-4} (calculated-P/C, Mabey et al. 1982)
0.042 (Ryan et al. 1988)
0.033 (20°C, calculated-P/C, Suntio et al. 1988)
0.762 (calculated, Howard 1991)
0.0507 (calculated-P/C, Montgomery 1993)
0.644 (wetted wall column-GC, Altschuh et al. 1999)
0.64, 1.1 (LDV literature-derived value, FAV final adjusted value, Shen & Wania 2005)

Octanol/Water Partition Coefficient, log K_{OW}:
5.60 (calculated, Neely et al. 1974)
4.56 (RP-HPLC-RT correlation, Veith et al. 1979)
5.34 (Kenaga & Goring 1980;)
3.21 (Rao & Davidson 1980)
4.82 (Veith & Kosian 1982)
5.01 (HPLC-RT correlation, Eadsforth 1986)
5.28 (HPLC-RT correlation, Liu & Qian 1988)
5.195 ± 0.005 (slow-stirring method, De Bruijn et al. 1989)
3.21–5.34 (Montgomery 1993)
4.71 (RP-HPLC-RT correlation, Sicbaldi & Finizio 1993)
5.20 (recommended, Hansch et al. 1995)
4.71 (RP-HPLC-RT correlation, Finizio et al. 1997)
5.20, 4.94 (LDV literature-derived value, FAV final-adjusted value, Shen & Wania 2005)

Octanol/Air Partition Coefficient, log K_{OA} at 25°C and reported temperature dependence equation. Additional data at other temperatures designated * are compiled at the end of this section:
8.338*, 8.609 (gas saturation-GC/MS, calculated, measured range 5–35°C, Shoeib & Harner 2002)
log $K_{OA} = -11.75 + 6067/(T/K)$, temp range: 5–35°C (gas saturation-GC, Shoeib & Harner 2002)
8.13, 8.32 (LDV literature derived value, FAV final adjusted value, Shen & Wania 2005)

Bioconcentration Factor, log BCF:
2.40–2.18 (bluegills, Bennett & Day 1970)
2.60–2.88 (channel catfish, Argyle et al. 1973)
3.21 (channel catfish, 55-d exposure, Argyle et al. 1973)
3.13, 4.69 (*Gambusia, Physa*, Metcalf et al. 1973)
3.11, 4.69, 3.66 (fish, snail, algae, Metcalf et al. 1973)
2.83, 2.49, 2.48 (fish, mosquitoes, Daphnia, 3-d expt. with no dietary routes, Metcalf et al. 1973)
3.43 (oyster, Mason & Rowe 1976)
3.28 (mussel, Ernst 1977)
3.24 (calculated-K_{OW}, Mackay 1982)
4.02; 4.18; 3.85 (flagfish, 30-d exposure; 65-d exposure; 110-d exposure, Hermanutz 1978)
3.70 (fathead minnow, Jarvinen & Tyo 1978)
3.17 (mosquito fish, 35-d exposure, Veith et al. 1979; Veith & Kosian 1983)
3.66 (fathead minnow, 300-d exposure, Veith et al. 1979; Veith & Kosian 1983)
3.66 (*Oedogonium sp.*, Baughman & Paris 1981)
3.85–4.18 (flag fish, mosquito fish, Veith & Kosian 1983)

3.24, 3.18	(mussel, calculated-K_{OW} & models, Zaroogian et al. 1985)
3.17	(fathead minnow, quoted from Veith et al. 1979, Zaroogian et al. 1985)
3.40	(Isnard & Lambert 1988)
3.13–4.0	(fish, quoted, Howard 1991)
3.85	(fathead minnow, whole body, after 300-d exposure, Howard 1991)
3.21–3.30	(channel catfish, after 41- and 55-d exposure, Howard 1991)
4.18	(flagfish, whole body after 65-d exposure, Howard 1991)
3.52–3.68	(sheepshead minnow, 33-d exposure for embryojuveniles, Howard 1991)
3.40–3.81	(sheepshead minnow, adults, after 28–161 d, Howard 1991)
2.70–3.10	(shellfish, Howard 1991)
4.69, 3.22–3.44, 3.48	(snail, oyster, grass shrimp, mussel, Howard 1991)
2.15–2.30	(algae, Howard 1991)
3.83	(fish, reported as log BAF_w, LeBlanc 1996)
3.28, 5.28	(mussel *Mytilus edulis*: wet wt basis, lipid wt basis, Geyer et al. 2000)
3.22, 5.14	(oyster *Crasssostrea virginica*: wet wt basis, lipid wt basis, Geyer et al. 2000)
3.44, 5.37	(oyster *Crasssostrea virginica*: wet wt basis, lipid wt basis, Geyer et al. 2000)
3.42	(clam: wet wt basis, Geyer et al. 2000)
3.66, 5.18	(fathead minnow, uptake 300-d: wet wt basis, lipid wt basis, Geyer et al. 2000)

Sorption Partition Coefficient, log K_{OC} at 25°C or as indicated:

4.53	(calculated, Kenaga 1980, quoted, Howard 1991)
5.36	(calculated-S, Mill et al. 1980; quoted, Adams 1987)
4.00	(20–25°C, selected, Augustijn-Beckers et al. 1994; Hornsby et al. 1996)
5.00; 4.10	(soil, calculated-universal solvation model; quoted exptl., Winget et al. 2000)

Environmental Fate Rate Constants, k, or Half-Lives, $t_{1/2}$:

Volatilization: $t_{1/2}$ ~ 9.6 d from a model river 1-m deep, flowing 1 m/s with a wind speed of 3 m/s, and $t_{1/2} > 14$ yr from a model pond (Howard 1991).

Photolysis:

Oxidation:

k(aq.) = $(2.7 \pm 0.7) \times 10^8$ M^{-1} s^{-1} for the reaction with OH radical in aqueous solution (Fenton reaction) at 24 ± 1°C and pH 2.8 (Haag & Yao 1992) with reference to 4.2×10^8 M^{-1} s^{-1} for the reaction of DPCP with OH radical in aqueous solution (Buxton et al. 1988; quoted, Haag & Yao 1992);

k(aq.) = $(1.3 \pm 0.4) \times 10^9$ M^{-1} s^{-1} (Fenton reaction) and k = $(1.1 \pm 0.2) \times 10^9$ M^{-1} s^{-1} (photo-Fenton reaction) for the reaction with OH radical in aqueous solution at 24 ± 1°C and pH 3.4 (Haag & Yao 1992) with reference to 8×10^8 M^{-1} s^{-1} for the reaction of lindane with OH radical in aqueous solution (Buxton et al. 1988; quoted, Haag & Yao 1992)

k(aq.) < 0.02 M^{-1} s^{-1} for direct reaction with ozone in water at pH 2.7–6.4 and 23 ± 3°C, with $t_{1/2} > 20$ d at pH 7 (Yao & Haag 1991).

Hydrolysis: $t_{1/2}$ = 4 yr at least (Callahan et al. 1979).

Biodegradation: $t_{1/2}$ = 5–14 d in thick anaerobic sewage sludge (Howard 1991).

Biotransformation:

Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants:

–log k_2 = 1.99 h (oyster, Mason & Rowe 1976; quoted, Hawker & Connell 1986)

log k_1 = 1.5 h^{-1}; –log k_2 = 1.78 h (mussel, Ernst 1977; quoted, Hawker & Connell 1986)

Half-Lives in the Environment:

Air: $t_{1/2}$ = 1.45 h was predicted for reaction with hydroxyl radical (Howard 1991).

Surface water: $t_{1/2} > 8$ wk in river water (Eichelberger & Lichtenberg 1971);

measured k_{O3}(aq.) < 0.02 M^{-1} s^{-1} for direct reaction with ozone in water at pH 2.7–6.4 and 23 ± 3°C, with $t_{1/2} > 20$ d at pH 7 (Yao & Haag 1991).

Ground water:

Sediment:

Soil: $t_{1/2}$ ~ 12 yr in Congaree sandy loam soil (Nash & Woolson 1967);
field $t_{1/2}$ = 63 d for sugar cane in soil (Willis & Hamilton 1973; quoted, Nash 1983);
moderately persistent in soil with $t_{1/2}$ = 20–100 d (Willis & McDowell 1982);
microagroecosystem $t_{1/2}$ = 33 d in moist fallow soil (Nash 1983);
$t_{1/2}$ > 50 d in soil (Ryan et al. 1988);
selected field $t_{1/2}$ = 4300 d (Augustijn-Beckers et al. 1994; Hornsby et al. 1996)
$t_{1/2}$ ~ 12 yr in soil (Geyer et al. 2000)
Biota: elimination $t_{1/2}$ = 24 h (Ernst 1977, quoted, Callahan et al. 1979).

TABLE 18.1.1.35.1
Reported aqueous solubilities and octanol-air partition coefficients of endrin at various temperatures

Aqueous solubility						log K_{OA}	
Richardson & Miller 1960		Biggar & Riggs 1974				Shoeib & Harner 2002	
shake flask-UV spec.		shake flask-GC				generator column-GC/MS	
t/°C	S/g·m^{-3}	t/°C	S/g·m^{-3}	S/g·m^{-3}	S/g·m^{-3}	t/°C	log K_{OA}
		particle size	0.01µ	0.05µ	5.0µ		
25	0.23	15	0.010	0.090	0.130	5	10.2787
35	0.38	25	0.0245	0.180	0.250	15	9.3548
45	0.51	35	0.058	0.315	0.420	20	8.6528
		45	0.120	0.518	0.625	25	8.3377
						35	8.2855
						25	8.609
						log K_{OA} = A + B/(T/K)	
						A	–11.75
						B	6067
						enthalpy of phase change ΔH_{OA}/(kJ mol^{-1}) = 84.9	

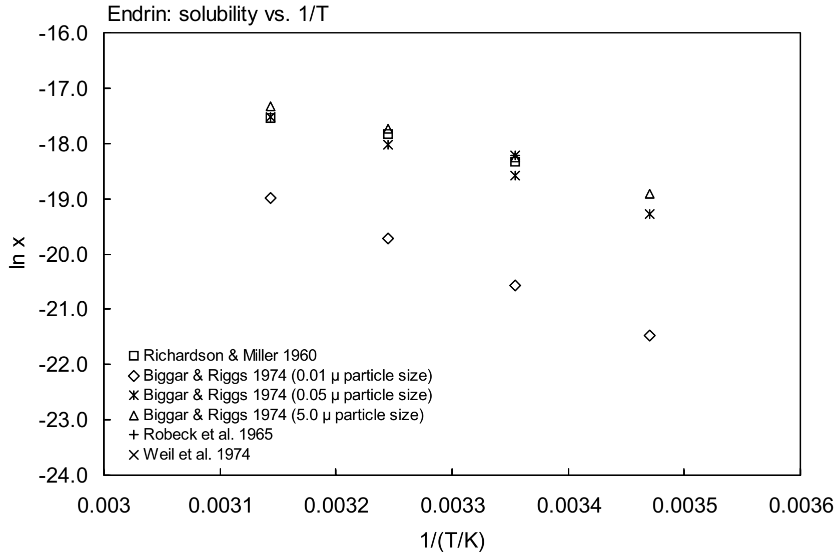


FIGURE 18.1.1.35.1 Logarithm of mole fraction solubility (ln *x*) versus reciprocal temperature for endrin.

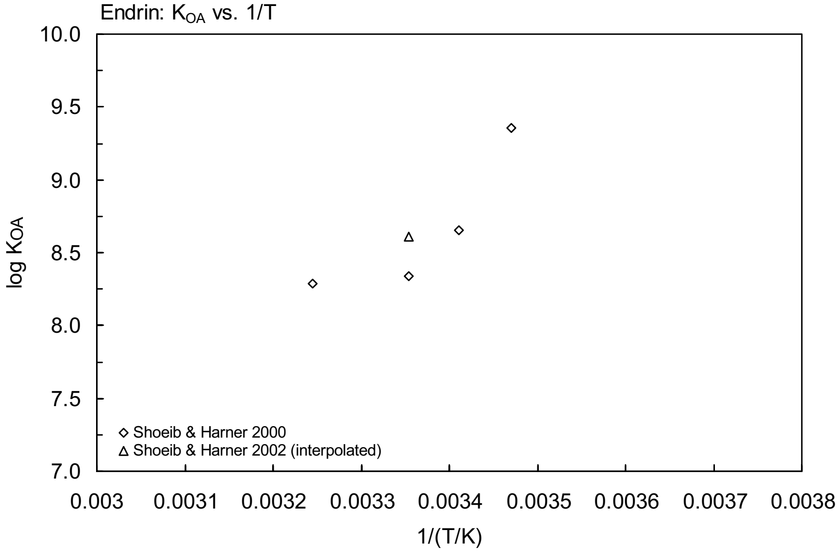
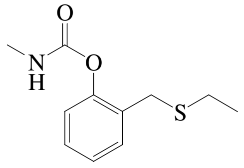


FIGURE 18.1.1.35.2 Logarithm of K_{OA} versus reciprocal temperature for endrin.

18.1.1.36 Ethiofencarb



Common Name: Ethiofencarb
Synonym: Croneton, Bay-Hox-1901
Chemical Name: α-ethylthio-*o*-tolyl methylcarbamate
CAS Registry No: 29973-13-5
Uses: insecticide
Molecular Formula: $C_{11}H_{15}NO_2S$
Molecular Weight: 225.307
Melting Point (°C):
33.4 (Spencer 1982; Hartley & Kidd 1987, Montgomery 1993, Tomlin 1994)
Boiling Point (°C):
decomposes on distillation (Hartley & Kidd 1987, Tomlin 1994)
Density (g/cm^3 at 20°C):
1.1473 (Hartley & Kidd 1987, Worthing & Walker 1987; Montgomery 1993)
1.231 (20°C, Tomlin 1994)
Molar Volume (cm^3/mol):
Dissociation Constant, pK_a:
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
Entropy of Fusion, ΔS_{fus} (J/mol K):
Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F: 0.827 (mp at 33.4°C)

Water Solubility (g/m^3 or mg/L at 25°C):
1900 (20°C, Spencer 1982, Hartley & Kidd 1987, Montgomery 1993)
1820 (20°C, Worthing & Walker 1987)
1800 (20°C, Tomlin 1994)

Vapor Pressure (Pa at 25°C):
6.67×10^{-4} (Spencer 1982)
0.013 (30°C, Hartley & Kidd 1987; Worthing & Walker 1987)
4.506×10^{-4} (20°C, Montgomery 1993)
0.00045, 0.00094, 0.026 (20, 25, 50°C, Tomlin 1994)

Henry's Law Constant (Pa·m^3/mol):
5.37×10^{-5} (calculated-P/C, Montgomery 1993)

Octanol/Water Partition Coefficient, log K_{OW}:
0.98 (calculated-Montgomery 1993)
2.04 (Tomlin 1994)
4.20 (RP-HPLC-RT correlation, Nakamura et al. 2001)

Octanol/Air Partition Coefficient, log K_{OA}:

Bioconcentration Factor, log BCF or log K_B:

Sorption Partition Coefficient, log K_{OC}:
1.84 (calculated, Montgomery 1993)

Environmental Fate Rate Constants or Half-Lives:

Volatilization:

Photolysis: photodegradation in sunlight is very rapid (Tomlin 1994).

Oxidation:

Hydrolysis: hydrolyzed in alkaline solution (Tomlin 1994).

Biodegradation:

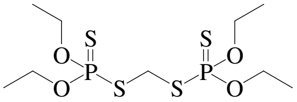
Biotransformation:

Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants:

Half-Lives in the Environment:

Surface water: in isopropanol/water (1:1, 37–40°C) solutions, half-lives were $t_{½}$ = 300 d at pH 2, $t_{½}$ = 45 h at pH 7 and $t_{½}$ = 5 min at pH 11.4 (Hartley & Kidd 1987; Montgomery 1993; Tomlin 1994).

18.1.1.37 Ethion



Common Name: Ethion

Synonym: AC 3422, Bladan, diethion, Embathion, ENT 24105, Ethanox, Ethiol, Ethodan, Ethopaz, FMC 1240, Fosfono 50, Hylemax, Hylemox, Itopaz, KWIT, NA 2783, NIA 1240, Niagara 1240, Nialate, Vegfru fosmite

Chemical Name: bis(*S*-(dimethoxyphosphinothioyl)mercapto)methane; *O,O,O′,O′*-tetraethyl-*S,S′*-methylene bis(phosphorodithioate); *O,O,O′,O′*-tetraethyl-*S,S′*-methylene-bisphosphorothiolothionate

Uses: nonsystemic insecticide and acaricide used on apples.

CAS Registry No: 563-12-2

Molecular Formula: $C_9H_{22}O_4P_2S_4$

Molecular Weight: 384.476

Melting Point (°C):

–12 to –15	(Montgomery 1993; Tomlin 1994; Milne 1995)
–13	(Lide 2003)

Boiling Point (°C):

164–165	(at 0.3 mmHg, Hartley & Kidd 1987; Howard 1991; Tomlin 1994; Milne 1995)

Density (g/cm^3 at 20°C):

1.22	(Hartley & Kidd 1987; Worthing & Hance 1991; Montgomery 1993; Tomlin 1994; Milne 1995)

Molar Volume (cm^3/mol):

350.2	(calculated-Le Bas method at normal boiling point)

Dissociation Constant, pK_a:

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

Entropy of Fusion, ΔS_{fus} (J/mol K):

Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F: 1.0

Water Solubility (g/m^3 or mg/L at 25°C or as indicated):

2.0	(Metcalf 1971, 1974)
0.60	(Miles 1976; Miles & Harris 1978)
1.0	(20–25°C, selected, Willis & McDowell 1982; Gerstl & Helling 1987)
1.1	(19.5°C, shake flask-GC, Bowman & Sans 1983b)
1.1	(20–25°C, selected, Wauchope et al. 1992; Hornsby et al. 1996)
0.68, 0.76	(20°C, 30°C, Montgomery 1993)
2.0	(Tomlin 1994)

Vapor Pressure (Pa at 25°C):

0.0002	(Khan 1980; Merck Index 1983, 1989)
0.0002	(Worthing 1983, Worthing & Hance 1991)
0.0002	(Hartley & Kidd 1987; Montgomery 1993; Tomlin 1994)
1.50×10^{-4}	(20°C, selected, Suntio et al. 1988)
3.20×10^{-4}	(20–25°C, selected, Wauchope et al. 1992; Hornsby et al. 1996)
1.58×10^{-4}	(gradient GC method; quoted lit., Tsuzuki 2000)

1.58×10^{-4}; 4.17×10^{-5}, 1.58×10^{-4} (gradient GC method; estimation using modified Watson method: Sugden's parachor, McGowan's parachor, Tsuzuki 2000)

Henry's Law Constant ($Pa \cdot m^3/mol$ at 25°C or as indicated):

0.0699	(calculated-P/C, Lyman et al. 1982; quoted, Howard 1991)
0.032	(20°C, calculated-P/C, Suntio et al. 1988)
0.0384	(calculated-P/C, Montgomery 1993)

Octanol/Water Partition Coefficient, log K_{OW}:

5.07	(Hansch & Leo 1979)
5.073	(shake flask-GC, Bowman & Sans 1983b)
5.07	(recommended, Sangster 1993)
4.28, 5.07	(Montgomery 1993)
5.07	(selected, Hansch et al. 1995)

Bioconcentration Factor, log BCF:

2.77	(estimated-log K_{OW}, Howard 1991)
2.77	(estimated-S, Howard 1991)

Sorption Partition Coefficient, log K_{OC} at 25°C or as indicated:

4.19	(average of 4 soils, King & McCarthy 1968)
4.19	(soil, Hamaker & Thompson 1972; Kenaga & Goring 1980)
3.81, 3.94. 4.0	(organic soil, Beverley sandy loam, Plainsfield sand, Sharom et al. 1980)
3.66	(calculated-MCI χ, Gerstl & Helling 1987)
4.19; 4.28	(reported as log K_{OM}, estimated as log K_{OM}, Magee 1991)
4.06, 4.12	(soil, quoted exptl., calculated-MCI χ and fragment contribution, Meylan et al. 1992)
4.00	(soil, 20–25°C, selected, Wauchope et al. 1992; Hornsby et al. 1996)
3.54–4.34	(Montgomery 1993)
4.43	(estimated-chemical structure, Lohninger 1994)
4.06	(calculated-MCI $^1\chi$, Sabljic et al. 1995)
3.70, 3.95	(soil, estimated-class-specific model, estimated-general model, Gramatica et al. 2000)

Environmental Fate Rate Constants, k, or Half-Lives, $t_{½}$:

Volatilization: using Henry's law constant, $t_{½}$ ~ 102 d from a model river 1-m deep, flowing 1 m/s with wind velocity of 3 m/s (Lyman et al. 1982; quoted, Howard 1991).

Photolysis:

Oxidation: photooxidation $t_{½}$ ~ 6.95 h for the vapor-phase reaction with hydroxyl radicals in air (Howard 1991).

Hydrolysis: half-lives in water at 25°C and pHs of 4.5, 5.0, 6.0, 7.0 and 8.0 were 99, 63, 58, 25, and 8.4 wk, respectively (Chapman & Cole 1982; quoted, Montgomery 1993);

$t_{½}$(exptl) = 20.8 wk was determined in buffered distilled water at 30°C between pH 4 and 7, $t_{½}$ = 8.9 wk at pH 8 and $t_{½}$ = 1 d at pH 10 (Dierberg & Pfeuffer 1983; quoted, Howard 1991);

$t_{½}$ = 390 d at pH 9 (Tomlin 1994).

Biodegradation: $t_{½}$ > 24 wk in sterile sandy loam and $t_{½}$ = 7 wk in nonsterile sandy loam; $t_{½}$ > 24 wk in sterile organic soil and $t_{½}$ = 8.0 wk in nonsterile organic soil (Miles et al. 1979; quoted, Howard 1991);

$t_{½}$ = 24–26 d in both sterilized and unsterilized Florida canal water over 12 wk observation (Dierberg & Pfeuffer 1983; quoted, Howard 1991).

Biotransformation:

Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants:

Half-Lives in the Environment:

Air: $t_{½}$ ~ 6.95 h for the vapor-phase reaction with hydroxyl radical in air (Howard 1991).

Surface water: $t_{½}$ = 4 wk in river water (Eichelberger & Lichtenberg 1971).

Ground water:

Sediment:

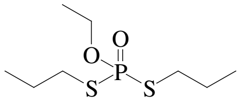
Soil: $t_{½}$ > 24 wk in sterile sandy loam and $t_{½}$ = 7 wk in nonsterile sandy loam; $t_{½}$ > 24 wk in sterile organic soil and $t_{½}$ = 8.0 wk in nonsterile organic soil (Miles et al. 1979; quoted, Howard 1991);

selected field $t_{½}$ = 150 d (Wauchope et al. 1992; Hornsby et al. 1996);

$t_{½}$ = 90 d in soil (Tomlin 1994).

Biota:

18.1.1.38 Ethoprop



Common Name: Ethoprop
Synonym: ethoprophos
Chemical Name: *O*-ethyl *S*,*S*-dipropylphosphorodithioate
CAS Registry No: 13194-48-4
Uses: insecticide/nematicide
Molecular Formula: $C_8H_{19}O_2PS_2$
Molecular Weight: 242.340
Melting Point (°C): liquid

20	(Montgomery 1993)

Boiling Point (°C):

86–91/0.2 mmHg	(Spencer 1982; Hartley & Kidd 1987; Worthing & Walker 1987; Montgomery 1993; Tomlin 1994)

Density (g/cm^3 at 20°C):

1.094	(Spencer 1982; Hartley & Kidd 1987; Worthing & Walker 1987; Montgomery 1993; Tomlin 1994)

Molar Volume (cm^3/mol):
Dissociation Constant, pK_a:
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
Entropy of Fusion, ΔS_{fus} (J/mol K):
Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F: 1.0

Water Solubility (g/m^3 or mg/L at 25°C):

700	(20°C, Hartley & Kidd 1987; Tomlin 1994)
750	(Worthing & Walker 1987)
700	(Montgomery 1993)
750	(selected, Wauchope et al. 1992; Hornsby et al. 1996)

Vapor Pressure (Pa at 25°C):

0.0465	(26°C, Hartley & Kidd 1987)
0.0465	(20°C, Montgomery 1993)
0.0507	(selected, Wauchope et al. 1992; Hornsby et al. 1996)

Henry's Law Constant (Pa·m^3/mol at 25°C):

0.0161	(calculated-P/C, Montgomery 1993; Majewski & Capel 1995)

Octanol/Water Partition Coefficient, log K_{OW}:

3.59	(21°C, Montgomery 1993; Tomlin 1994)
3.59	(quoted, Sabljic et al. 1995)

Octanol/Air Partition Coefficient, log K_{OA}:

Bioconcentration Factor, log BCF or log K_B:

Sorption Partition Coefficient, log K_{OC}:

1.41–2.20	(soil, quoted values, Wauchope et al. 1992)
1.85	(soil, Wauchope et al. 1992; Hornsby et al. 1996)
1.82–2.27	(Montgomery 1993)
1.80	(soil, calculated-MCI, Sabljic et al. 1995)

Environmental Fate Rate Constants, k, or Half-Lives, $t_{½}$:

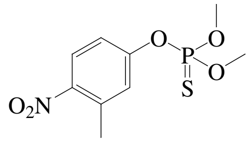
Hydrolysis: stable in water up to 100°C at pH 7, but rapidly hydrolyzed at 25°C at pH 7 (Worthing 1987; Tomlin 1994).

Half-Lives in the Environment:

Soil: $t_{½}$ ~ 87 d in humus-containing soil at pH 4.5 and $t_{½}$ = 14–28 d in sandy loam at pH 7.2–7.3 (Hartley & Kidd 1987; Montgomery 1993; Tomlin 1994);

field $t_{½}$ = 87 d in organic soil, $t_{½}$ = 1–28 d in sandy soil; others $t_{½}$ = 3–63 d; recommended $t_{½}$ = 25 d (Wauchope et al. 1992; Hornsby et al. 1996).

18.1.1.39 Fenitrothion



Common Name: Fenitrothion

Synonym: Accothion, Agria 1050, Agrothion, Arbogal, Cyfen, Cytel, Dybar, Falithion, Fenitox, Kotion, Sumithion

Chemical Name: *O,O*-dimethyl *O*-4-nitro-*m*-tolyl phosphorothioate; phosphorothioic acid *O,O*-dimethyl *O*-4-nitro-*m*-tolyl ester; *O,O*-dimethyl *O*-(3-methyl-4-nitrophenyl) phosphorothioate

Uses: insecticide to control boring, chewing and sucking insects in cereals, cotton, maize, sorghum, citrus fruit, pome fruit, stone fruit, soft fruit, vines, bananas, olives, rice, soybeans, beet, sugar cane, oilseed rape, vegetables, lucerne, coffee, cocoa, tea, tobacco, ornamentals and forestry; also used as a public health insecticide to control household insects, flies in animal houses, mosquito larvae, and locusts.

CAS Registry No: 122-14-5

Molecular Formula: $C_9H_{12}NO_5PS$

Molecular Weight: 277.234

Melting Point (°C):

3.4	(Tomlin 1994)

Boiling Point (°C):

164	(at 1 mmHg, Worthing & Hance 1991; Milne 1995)
140–145	(at 0.1 mmHg, dec., Tomlin 1994)

Density (g/cm^3 at 20°C):

1.328	(Worthing & Hance 1991; Tomlin 1994)
1.3227	(25°C, Milne 1995)

Molar Volume (cm^3/mol):

229.7	(calculated-Le Bas method at normal boiling point)

Dissociation Constant, pK_a:

7.20	(Kortum et al. 1961; Wolfe 1980)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

Entropy of Fusion, ΔS_{fus} (J/mol K):

Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F: 1.0

Water Solubility (g/m^3 or mg/L at 25°C or as indicated):

30	(Macy 1948; Hamaker 1975; Kenaga 1980; Kenaga & Goring 1980)
30	(20°C, Bright et al. 1950; Melnikov 1971; Hamaker 1975)
25.2	(20°C, shake flask-GC, Bowman & Sans 1979)
38.7	(20–25°C, shake flask-GC, Kanazawa 1981)
21	(20°C, Worthing & Hance 1991; Tomlin 1994)
30	(20–25°C, selected, Augustijn-Beckers et al. 1994; Hornsby et al. 1996)
30	(21°C, Milne 1995)

Vapor Pressure (Pa at 25°C or as indicated):

8.0×10^{-3}	(20°C, Melnikov 1971)
7.2×10^{-3}	(20°C, Freed et al. 1979)
8.0×10^{-4}	(20°C, Hartley & Graham-Bryce 1980; Khan 1980)
5.5×10^{-3}	(gas saturation method, Addison 1981)
5.4×10^{-3}	(gas saturation-extrapolated, Addison 1981)
8.0×10^{-3}	(Budavari 1989)
1.1×10^{-2}	(GC-RT correlation, supercooled liquid value, Hinckley et al. 1990)
1.5×10^{-4}	(20°C, Worthing & Hance 1991)
1.3×10^{-4}	(20–25°C, estimated, Augustijn-Beckers et al. 1994; Hornsby et al. 1996)
0.0180	(20°C, Tomlin 1994)

0.00316 (gradient GC method, Tsuzuki 2000)
3.23×10^{-3}; 3.47×10^{-3}, 2.18×10^{-3} (gradient GC method; estimation using modified Watson method: Sugden's parachor, McGowan's parachor, Tsuzuki 2000)

Henry's Law Constant (Pa·m^3/mol at 25°C):
0.0942, 0.0669 (exptl., estimated Metcalf et al. 1980)
0.0962 (calculated-bond contribution method, Meylan & Howard 1991)
0.0012 (calculated-P/C, this work)

Octanol/Water Partition Coefficient, log K_{OW}:
3.38 (20°C, shake flask-GC, Chiou et al. 1977)
3.30 (shake flask, Mundy et al. 1978)
3.38 (shake flask-GC, Freed et al. 1979)
3.36 (Rao & Davidson 1980)
3.44 (shake flask-GC, Kanazawa 1981, 1989)
3.397 (shake flask-GC, Bowman & Sans 1983b)
3.16 (shake flask-HPLC, Moody et al. 1987)
3.466 ± 0.003 (shake flask/slow-stirring method, De Bruijn & Hermens 1991; De Bruijn et al. 1993)
3.43 (20°C, Worthing & Hance 1991; Tomlin 1994)
2.96 (RP-HPLC-RT correlation, Saito et al. 1993)
3.03 (RP-HPLC-RT correlation, Sicbaldi & Finizio 1993)
3.30 (recommended, Sangster 1993)
3.43 (Milne 1995)
3.30 (selected, Hansch et al. 1995)
3.03 (RP-HPLC-RT correlation, Finizio et al. 1997)

Bioconcentration Factor, log BCF:
1.00 (fish in static water, Leo et al. 1971; Kenaga & Goring 1980)
2.23 (motsugo, Kanazawa 1975)
2.34 (rainbow trout, Takimoto & Miyamoto 1976)
2.02 (mussel, McLeese et al. 1979)
1.96 (calculated-S, Kenaga 1980)
2.39 (*Pseudorasbora parva*, Kanazawa 1981)
2.34, 2.17 (mussel, calculated-K_{OW} & models, Zaroogian et al. 1985)
2.11 (mussel, Zaroogian et al. 1985)
2.74, 2.75 (*Oryzias latipes*, Takimoto et al. 1984)
2.48 (*Oryzias latipes*, Takimoto et al. 1987)
2.60 (willow shiner, Tsuda et al. 1989)
3.36 ± 0.04 (guppy, calculated on an extractable lipid wt. basis, De Bruijn & Hermens 1991)
2.37, 2.72 (killifish, De Bruijn & Hermens 1991)
2.18, 2.31, 1.48 (minnow, motsugo, mullet, De Bruijn & Hermens 1991)
3.54 (*Poecilia reticulata,* De Bruijn & Hermens 1991)
2.30, 2.39 (rainbow trout, topmouth gudgeon, De Bruijn & Hermens 1991)
1.65, 1.68 (*Oryzias latipes*, Tsuda et al. 1995)

Sorption Partition Coefficient, log K_{OC}:
2.83 (soil, calculated-S as per Kenaga & Goring 1978, Kenaga 1980)
2.63 (average of 2 soils, Kanazawa 1989)
3.30 (20–25°C, selected, Augustijn-Beckers et al. 1994; Hornsby et al. 1996)
2.54, 2.76 (soil, estimated-class-specific model, estimated-general model, Gramatica et al. 2000)

Environmental Fate Rate Constants, k, or Half-Lives, $t_{½}$:
Volatilization: $t_{½}$ = 6.3 d from the bottom of Palfrey Lake and $t_{½}$ = 7.2 d from the surface of Palfrey Lake vs. a calculated $t_{½}$ = 20.6 d; 0.9 d from Palfrey Brook vs. a calculated $t_{½}$ = 5.40 d (Metcalf et al. 1980).

Photolysis: disappearance rate constant k = 0.053 h^{-1} with calculated first-order $t_{½}$ = 13 h (Lacorte & Barcelo 1994).

Oxidation:

Hydrolysis: second-order alkaline hydrolysis rate constant k = 4.2 × 10^{-3} M^{-1} s^{-1} at 27°C (Maquire & Hale 1980; quoted, Wolfe 1980);

estimated half-lives at 22°C: $t_{½}$ ~ 108.8 d at pH 4, $t_{½}$ ~ 84.3 d at pH 7, and $t_{½}$ ~ 75 d at pH 9 (Tomlin 1994).

Biodegradation: aerobic degradation k = 2.3 × 10^{-3} h^{-1} with $t_{½}$ = 13.0 d for control system, k = 0.4 × 10^{-3} h^{-1} with $t_{½}$ = 73.0 d for metabolism, k = 5.3 × 10^{-3} h^{-1} with $t_{½}$ = 8.50 d for co-metabolism; anaerobic degradation k = 1.7 × 10^{-3} h^{-1} with $t_{½}$ = 17.0 d for control system, k = 3.9 × 10^{-3} h^{-1} with $t_{½}$ = 9.6 d for metabolism, k = 38.0 × 10^{-3} h^{-1} with $t_{½}$ = 1.0 d for co-metabolism, by a mixture of microorganisms from activated sludge, soil and sediment in cyclone fermentors (Liu et al. 1981)

Biotransformation:

Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants:

k_1 = 88 d^{-1} (rainbow trout, Takimoto & Miyamoto 1976; quoted, McLeese et al. 1976)
k_2 = 0.4 d^{-1} (rainbow trout, Takimoto & Miyamoto 1976; quoted, McLeese et al. 1976)
k_2 = 0.070 h^{-1} (willow shiner, Tsuda et al. 1989)
k_1 = (3.89 ± 1.39) × 10^{-3} mL g^{-1} d^{-1} (guppy, De Bruijn & Hermens 1991)
k_2 = (1.13 ± 0.07) d^{-1} (guppy, De Bruijn & Hermens 1991)
k_2 = 1.01 d^{-1} (guppy, calculated-K_{OW}, De Bruijn & Hermens 1991)
k_2 = (0.28 ± 0.02) × 10^{-3} (NADPH) min^{-1}·mg $protein^{-1}$ (rainbow trout, De Bruijn et al. 1993)
k_2 = (0.15 ± 0.02) × 10^{-3} (GSH) min^{-1}·mg $protein^{-1}$ (rainbow trout, De Bruijn et al. 1993)

Half-Lives in the Environment:

Air:

Surface water: $t_{½}$ = 15–168 h in summer, Palfrey Lake, Canada at pH 6.7, 11°C under sunlight conditions (Metcalfe et al. 1980);

$t_{½}$ = 36–48 h at pH 7.0–7.5, 19–23°C under sunlight conditions, $t_{½}$ = 518–1188 h at pH 7.5, 23°C under dark conditions in Lac Bourgeous, Quebec (Greenhalgh et al. 1980);

$t_{½}$ = 5.5 d and 1.0 d under aerobic and anaerobic co-metabolism conditions, $t_{½}$ = 73 d under aerobic metabolism condition (Liu et al. 1981)

$t_{½}$ = 13 h in winter, irrigation ditch from Ebre Delta, Spain under sunlight conditions, at pH 7.8, 11°C (Lacorte & Barcelo 1994);

$t_{½}$ = 202 d at 6°C, $t_{½}$ = 62 d at 22°C in darkness for Milli-Q water at pH 6.1; $t_{½}$ = 103 d at 6°C, $t_{½}$ = 31 d at 22°C in darkness, $t_{½}$ = 4 d under sunlight conditions for river water at pH 7.3; $t_{½}$ = 143 d at 6°C, $t_{½}$ = 27 d at 22°C in darkness for filtered water at pH 7.3; $t_{½}$ = 224 d at 6°C, $t_{½}$ = 34 d at 22°C in darkness, $t_{½}$ = 3 d under sunlight conditions in seawater (Arcachon Bay, France) at pH 8.1, 22–25°C (Lartiges & Garri gues 1995);

$t_{½}$ = 11–19.3 h at pH 7.8–8.2, 25–20°C under sunlight conditions in rice crop field; $t_{½}$ = 70–74 h at pH 8.2, 15–18°C under dark conditions from Ebre Delta, Spain (Oubina et al. 1996).

Ground water:

Sediment:

Soil: selected field $t_{½}$ = 4 d (Augustijn-Beckers et al. 1994; Hornsby et al. 1996);

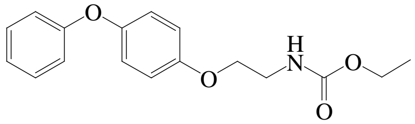
$t_{½}$ = 12–28 d under upland conditions and $t_{½}$ = 4–20 d under submerged conditions (Tomlin 1994).

Biota: excretion $t_{½}$ = 9.9 h (willow shiner, Tsuda et al. 1989);

elimination rate constants k = (0.28 ± 0.02) × 10^3 (NADPH) and (0.15 ± 0.02) × 10^3 (GSH) min^{-1}·mg $protein^{-1}$ (rainbow trout, De Bruijn et al. 1993);

degradation $t_{½}$ = 4 d in balsam fir and spruce foliage (Tomlin 1994).

18.1.1.40 Fenoxycarb



Common Name: Fenoxycarb
Synonym: Insegar, Logic, Pictyl, Torus, Varikil
Chemical Name: ethyl 2-(4-phenoxyphenoxy)ethylcarbamate; ethyl[2-(*p*-phenoxy)ethyl]- carbamate
Uses: insecticide to control lepidoptera, scale insects, and psyllids on fruit, cotton and ornamentals; and also cockroaches, fleas, mosquito larvae, and fire ants in public health situations.
CAS Registry No: 79127-80-3
Molecular Formula: $C_{17}H_{19}NO_4$
Molecular Weight: 301.338
Melting Point (°C):
53 (Lide 2003)
Boiling Point (°C):
Density (g/cm^3 at 20°C):
1.23 (Tomlin 1994)
Molar Volume (cm^3/mol):
344.2 (calculated-Le Bas method at normal boiling point)
Dissociation Constant, pK_a:
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
Entropy of Fusion, ΔS_{fus} (J/mol K):
Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F: 0.531 (mp at 53°C)

Water Solubility (g/m^3 or mg/L at 25°C or as indicated):
6.0 (20°C, Hartley & Kidd 1987; Tomlin 1994; Milne 1995)
5.7 (Worthing & Hance 1991)
6.0 (20–25°C, selected, Hornsby et al. 1996)

Vapor Pressure (Pa at 25°C or as indicated):
1.7×10^{-6} (Hartley & Kidd 1987)
7.8×10^{-6} (20°C, Worthing & Hance 1991)
8.7×10^{-7} (Tomlin 1994)
1.7×10^{-6} (20–25°C, selected, Hornsby et al. 1996)

Henry's Law Constant (Pa·m^3/mol):
8.5×10^{-5} (calculated-P/C, this work)

Octanol/Water Partition Coefficient, log K_{OW}:
4.30 (Worthing & Hance 1991; Milne 1995)
4.07 (Tomlin 1994)
4.30 (selected, Hansch et al. 1995)

Bioconcentration Factor, log BCF:
2.35 (calculated-S as per Kenaga 1980, this work)
3.11 (calculated-K_{OW} as per Kenaga 1980, this work)

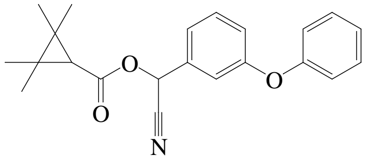
Sorption Partition Coefficient, log K_{OC}:
3.00 (20–25°C, estimated, Hornsby et al. 1996)

Environmental Fate Rate Constants, k, or Half-Lives, $t_{½}$:

Half-Lives in the Environment:

Soil: $t_{½}$ = 1.7–2.5 months in laboratory soil and water and $t_{½}$ = few days to 31 d in field soil and water (Tomlin 1994); field $t_{½}$ = 1 d (20–25°C, selected, Hornsby et al. 1996).

18.1.1.41 Fenpropathrin



Common Name: Fenpropathrin
Synonym: Rody, Danitol, Meothrin, S-3206, Ortho Danitol, Herald, Meothrin
Chemical Name: (*R,S*)-α-cyano-3-phenoxybenzyl 2,2,3,3-tetramethylcyclopropanecarboxylate
CAS Registry No: 64257-84-7 (racemate); 39515-41-8 (unstated stereochemistry)
Uses: insecticide/acaricide (pyrethroid)
Molecular Formula: $C_{22}H_{23}NO_3$
Molecular Weight: 349.423
Melting Point (°C):

47	(Lide 2003)

Boiling Point (°C):
Density (g/cm^3 at 20°C):

1.15	(Hartley & Kidd 1987; Tomlin 1994)

Molar Volume (cm^3/mol):
Dissociation Constant, pK$_a$:
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
Entropy of Fusion, ΔS_{fus} (J/mol K):
Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F: 0.608 (mp at 47°C)

Water Solubility (g/m^3 or mg/L at 25°C):

0.33	(Hartley & Kidd 1987)
0.0141	(Tomlin 1994)
0.33	(selected, Augustijn-Beckers et al. 1994)

Vapor Pressure (Pa at 25°C):

0.00073	(20°C, Hartley & Kidd 1987; Tomlin 1994)
0.00130, 0.00133	(quoted, Augustijn-Beckers et al. 1994)
7.33×10^{-4}	(selected, Augustijn-Beckers et al. 1994)

Henry's Law Constant (Pa·m^3/mol at 25°C):

Octanol/Water Partition Coefficient, log K_{OW}:

6.0	(20°C, Tomlin 1994)

Octanol/Air Partition Coefficient, log K_{OA}:

Bioconcentration Factor, log BCF or log K_B:

Sorption Partition Coefficient, log K_{OC}:

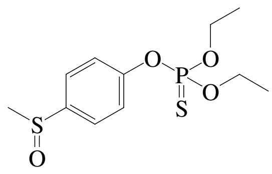
6.75, 3.70	(quoted, estimated, Augustijn-Beckers et al. 1994)
3.70	(soil, estimated and selected, Augustijn-Beckers et al. 1994)

Environmental Fate Rate Constants, k, or Half-Lives:
Volatilization:
Photolysis: degraded principally by photolysis, $t_{1/2}$ = 2.7 wk in river water (Hartley & Kidd 1987; Tomlin 1994).
Oxidation:
Hydrolysis: decomposed in alkaline solution (Hartley & Kidd 1987; Tomlin 1994).
Biodegradation:

Biotransformation:
Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants:

Half-Lives in the Environment:
Air:
Surface water: degraded principally by photolysis, $t_{½}$ = 2.7 wk in river water (Hartley & Kidd 1987; Tomlin 1994).
Ground water:
Sediment:
Soil: duration of activity in soil 1–5 d (Hartley & Kidd 1987; Tomlin 1994);
reported field $t_{½}$ = 8–144 d, recommended field $t_{½}$ = 5 d (Augustijn-Beckers et al. 1994).
Biota:

18.1.1.42 Fensulfothion



Common Name: Fensulfothion
Synonym: Dassnit, Terracur
Chemical Name: *O,O*-diethyl *O*-4-methylsulphinylphenyl phosphorothioate
Uses: insecticide/nematicide
CAS Registry No: 115-90-2
Molecular Formula: $C_{11}H_{17}O_4PS_2$
Molecular Weight: 308.354
Melting Point (°C):
yellow-brown oil (Spencer 1982; Hartley & Kidd 1987)
< 25 (Montgomery 1993)
Boiling Point (°C):
138–141/0.01 mmHg (Hartley & Kidd 1987, Worthing & Walker 1987; Howard 1991)
Density (g/cm^3):
1.202 (20°C, Spencer 1982, Hartley & Kidd 1987; Worthing & Walker 1987)
Acid Dissociation Constant, pK_a:
Molar Volume (cm^3/mol):
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
Entropy of Fusion, ΔS_{fus} (J/mol K):
Fugacity Ratio at 25°C, F: 1.0

Water Solubility (g/m^3 or mg/L at 25°C):
1600 (Spencer 1982)
2000 (20°C, shake flask, Bowman & Sans 1979, 1983b)
1540 (Hartley & Kidd 1987; Worthing & Walker 1987)
1540 (selected, Augustijn-Beckers et al. 1994; Hornsby et al. 1996)

Vapor Pressure (Pa at 25°C):
9.09×10^{-5} (Howard 1991)
6.67×10^{-3} (selected, Augustijn-Beckers et al. 1994; Hornsby et al. 1996)

Henry's Law Constant (Pa·m^3/mol):
1.40×10^{-5} (calculated-P/C, Howard 1991)

Octanol/Water Partition Coefficient, log K_{OW}:
2.23 (shake flask-concn ratio-GC, Bowman & Sans 1983)
2.23 (Montgomery 1993)
2.23 (recommended, Sangster 1993)
2.23 (recommended, Hansch et al. 1995)

Octanol/Air Partition Coefficient, log K_{OA}:

Bioconcentration Factor, log BCF or log K_B:
1.46, 0.93 (calculated-K_{OW}, solubility, Howard 1991)
1.68 (killifish *Oryzias latipes*, after 48–72 h exposure, Tsuda et al. 1995)

Sorption Partition Coefficient, log K_{OC}:

1.83, 2.11 (estimated, Howard 1991)
1.89 (calculated, Montgomery 1993)
2.09–2.57 (Augustijn-Beckers et al. 1994)
2.48 (soil, selected, Augustijn-Beckers et al. 1994; Hornsby et al. 1996)
2.52 (soil, calculated-MCI $^1\chi$, Sabljic et al. 1995)
3.45, 2.266, 2.11, 2.26, 2.85 (first generation EUROSOILS ES-1, ES-2, ES-3, ES-4, ES-5, shake flask/batch equilibrium-HPLC/UV, Gawlik et al. 1998, 1999)
3.05, 2.44, 2.15, 2.237, 2.85 (second generation EUROSOILS ES-1, ES-2, ES-3, ES-4, ES-5, shake flask/batch equilibrium-HPLC/UV, Gawlik et al. 1999)
3.053, 2.443, 2.150, 2.237, 2.848 (second generation EUROSOILS ES-1, ES-2, ES-3, ES-4, ES-5, shake flask/batch equilibrium-HPLC/UV and HPLC-k′ correlation, Gawlik et al. 2000)
2.52; 2.94, 2.62 (soil, quoted obs.; estimated-class-specific model, estimated-general model using molecular descriptors, Gramatica et al. 2000)

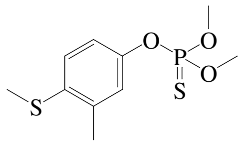
Environmental Fate Rate Constants, k, and Half-Lives, $t_{1/2}$:

Volatilization:
Photolysis:
Photooxidation:
Hydrolysis: $t_{1/2}$ = 58–87 d over pH range of 4.5–8.0 at 25°C in pure water (Howard 1991).
Biodegradation: field $t_{1/2}$ ~ 30 d (estimated, Augustijn-Becker et al. 1994).
Biotransformation:
Bioconcentration and Uptake and Elimination Rate Constants (k_1 and k_2):
$k_2 = 0.17\ h^{-1}$ (killifish *Oryzias latipes*, Tsuda et al. 1995)

Half-Lives in the Environment:

Air: $t_{1/2}$ = 7.03 h for reaction with OH radicals in the atmosphere (Howard 1991).
Surface water: $t_{1/2}$ = 58–87 d in pure water at 25°C over the pH range of 4.5–8.0 (Howard 1991).
Ground water:
Sediment:
Soil: $t_{1/2}$ < 1 wk to several weeks in soil (Howard 1991);
field $t_{1/2}$ = 3 to 182 d and $t_{1/2}$ ~ 30 d (estimated, Augustijn-Becker et al. 1994; Hornsby et al. 1996).
Biota:

18.1.1.43 Fenthion



Common Name: Fenthion

Synonym: Bay 29493, Baycid, Bayer 9007, Baytex, Baycid, DMTP, Ekalux, ENT 25540, Entex, Lebacid, Lebaycid, Mercaptophos, MPP, NCI-C08651, OMS 2, Queletox, Spottan, Talodex, Tiquvon

Chemical Name: *O,O*-dimethyl *O*-(3-methyl-4-(methylthio)phenyl) phosphorothioate; *O,O*-dimethyl *O*-4-methylthio-*m*-tolyl phosphorothioate

Uses: insecticide with contact, stomach and respiratory action and also used as acaricide and cholinesterase inhibitor.

CAS Registry No: 55-38-9

Molecular Formula: $C_{10}H_{15}O_3$PS2

Molecular Weight: 278.328

Melting Point (°C):

7.0	(Montgomery 1993)
7.5	(Tomlin 1994; Milne 1995)

Boiling Point (°C):

87.0	(at 0.01 mmHg, Hartley & Kidd 1987; Worthing & Hance 1991; Montgomery 1993; Tomlin 1994; Milne 1995)

Density (g/cm^3 at 20°C):

1.246	(Hartley & Kidd 1987; Tomlin 1994; Milne 1995)
1.25	(Worthing & Hance 1991; Montgomery 1993)

Molar Volume (cm^3/mol):

264.6	(calculated-Le Bas method at normal boiling point)

Dissociation Constant, pK_a:

Enthalpy of Vaporization, ΔH_V (kJ/mol):

89.31	(Rordorf 1989)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

Entropy of Fusion, ΔS_{fus} (J/mol K):

Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F: 1.0

Water Solubility (g/m^3 or mg/L at 25°C or as indicated):

55	(Günther et al. 1968; Martin & Worthing 1977; Budavari 1989)
54–56	(rm. temp., Spencer 1973, 1980)
56	(22°C, Khan 1980)
55	(22°C, Verschueren 1983)
7.51	(20°C, shake flask-GC, Bowman & Sans 1983a, b)
9.3	(20°C, shake flask-GC, Bowman & Sans 1985)
54–56	(20°C, Hartley & Kidd 1987)
2.0	(20°C, Worthing & Walker 1987; Worthing & Hance 1991; Milne 1995)
2.0, 4.2, 7.51, 9.3, 50	(20°C, literature data variability, Heller et al. 1989)
4.2	(20–25°C, selected, Wauchope et al. 1992; Lohninger 1994; Hornsby et al. 1996)
9.30, 11.3	(20°C, 30°C, Montgomery 1993)
4.2	(20°C, Tomlin 1994)

Vapor Pressure (Pa at 25°C or as indicated and reported temperature dependence equations):

4.0×10^{-3}	(20°C, Eichler 1965)
4.0×10^{-3}	(20°C, Melnikov 1971)
4.0×10^{-3}	(20°C, Hartley & Graham-Bryce 1980)
4.0×10^{-3}	(20°C, Khan 1980; Budavari 1989; Worthing & Hance 1991; Montgomery 1993)
8.4×10^{-3}	(20°C, GC-RT correlation, Kim et al. 1984; Kim 1985)

4.0×10^{-3}, 10×10^{-3} (20°C, 30°C, Hartley & Kidd 1987)
4.0×10^{-3} (20°C, selected, Suntio et al. 1988)
2.5×10^{-3}, 4.0×10^{-2}, 0.43, 3.40, 21.0 (25, 50, 70, 100, 125°C, gas saturation-GC, Rordorf 1989)
$\log (P_L/Pa) = 13.037 - 4665.2/(T/K)$; measured range 32.7–160°C (liquid, gas saturation-GC, Rordorf 1989)
3.7×10^{-4} (20–25°C, selected, Wauchope et al. 1992; Hornsby et al. 1996)
7.4×10^{-4} (Tomlin 1994)

Henry's Law Constant (Pa·m^3/mol at 25°C or as indicated):
0.022 (20°C, calculated-P/C, Suntio et al. 1988)
0.547 (Montgomery 1993)

Octanol/Water Partition Coefficient, log K_{OW}:
4.09 (shake flask-GC, Bowman & Sans 1983b)
4.167 ± 0.009 (shake flask/slow-stirring method, De Bruijn & Hermens 1991)
4.09, 4.84 (Montgomery 1993)
3.56 (RP-HPLC correlation, Saito et al. 1993)
4.09 (recommended, Sangster 1993)
4.84 (Tomlin 1994)
4.09 (selected, Hansch et al. 1995)
4.17 (RP-HPLC-RT correlation, Nakamura et al. 2001)

Bioconcentration Factor, log BCF:
1.81 (calculated-S, Kenaga 1980)
–4.50 (beef biotransfer factor log B_b, correlated-K_{OW}, MacDougall 1972)
–5.60 (milk biotransfer factor log B_m, correlated-K_{OW}, Johnson & Bowman 1972)
4.22 ± 0.08 (guppy, calculated on an extractable lipid wt. basis, De Bruijn & Hermens 1991)
4.17 (*Poecilia reticulata*, De Bruijn & Hermens 1991)
2.68 (whole body willow shiner after 24–168 h exposure, Tsuda et al. 1992)
1.34, 1.46, 1.43, 1.41 (whole body carp: 24 h, 72 h, 120 h, and 148 h; Tsuda et al. 1993)
1.96 (killifish *Oryzias latipes*, after 12–72 h exposure, Tsuda et al. 1995)
1.96, 2.02 (*Oryzias latipes*, Tsuda et al. 1995; quoted, Devillers et al. 1996)

Sorption Partition Coefficient, log K_{OC}:
2.68 (calculated-S, Kenaga 1980)
3.18 (soil, 20–25°C, selected, Wauchope et al. 1992; Hornsby et al. 1996)
3.31 (soil, HPLC-screening test, mean value of different stationary and mobile phases, Kördel et al. 1993, 1995a, b)
0.89–1.58 (Montgomery 1993)
3.18 (Tomlin 1994; Lohninger 1994)
3.31; 3.37 (HPLC-screening method; calculated-PCKOC fragment method, Müller & Kördel 1996)
4.35, 3.55, 3.46, 3.146, 3.64 (first generation Eurosoils ES-1, ES-2, ES-3, ES-4, ES-5, shake flask/batch equilibrium-HPLC/UV, Gawlik et al. 1998)
3.10 (sandy loam soil, column equilibrium method-HPLC/UV, 20°C, Xu et al. 1999)
3.716, 3.658, 3,450, 3.226, 3.292 (second generation Eurosoils ES-1, ES-2, ES-3, ES-4, ES-5, shake flask/batch equilibrium-HPLC/UV and HPLC-k′ correlation, Gawlik et al. 2000)
3.50, 3.00 (soil, estimated-class-specific model, estimated-general model using molecular descriptors, Gramatica et al. 2000)

Environmental Fate Rate Constants, k, or Half-Lives, $t_{½}$:
Volatilization:
Photolysis:
Oxidation:
Hydrolysis: $t_{½}$ = 223 d at pH 4, $t_{½}$ = 200 d at pH 7, and $t_{½}$ = 151 d at pH 9 at 22°C (Tomlin 1994).

Biodegradation: rate constants k = –0.00745 h^{-1} in nonsterile sediment and k = –0.00199 h^{-1} in sterile sediment by shake-tests at Range Point and k = –0.00129 h^{-1} in nonsterile water by shake-tests at Range Point (Walker et al. 1988).

Biotransformation:

Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants:

$k_1 = (8.81 \pm 0.72) \times 10^{-3}$ mL g^{-1} d^{-1} (guppy, De Bruijn & Hermens 1991)
$k_2 = (0.60 \pm 0.02)$ d^{-1} (guppy, De Bruijn & Hermens 1991)
$k_2 = 0.42$ d^{-1} (guppy, calculated-K_{OW}, De Bruijn & Hermens 1991)
$k_2 = 0.07$ h^{-1} (whole body willow shiner, Tsuda et al. 1992)
$k_2 = 0.34$ h^{-1} (carp, Tsuda et al. 1992)
$k_2 = (0.64 \pm 0.09) \times 10^{-3}$ (NADPH) min^{-1}·mg $protein^{-1}$ (rainbow trout, De Bruijn et al. 1993)
$k_2 = (0.12 \pm 0.02) \times 10^{-3}$ (GSH) min^{-1}·mg $protein^{-1}$ (rainbow trout, De Bruijn et al. 1993)
$k_2 = 0.14$ h^{-1} (killifish *Oryzias latipes*, Tsuda et al. 1995)

Half-Lives in the Environment:

Air:

Surface water: persistence of up to 4 wk in river water (Eichelberger & Lichtenberg 1971);
$t_{1/2}$ = 189 d at 6°C, 71 d at 2 2°C in darkness for Mill-Q water at pH 6.1; $t_{1/2}$ = 149 d at 6°C, $t_{1/2}$ = 42 d at 22°C in darkness, $t_{1/2}$ = 2 d under sunlight conditions for river water at pH 7.3; $t_{1/2}$ = 104 d at 6°C, $t_{1/2}$ = 33 d at 22°C in darkness for filtered river water, pH 7.3; $t_{1/2}$ = 227 d at 6°C, $t_{1/2}$ = 26 d at 22°C in darkness, $t_{1/2}$ = 5 d under sunlight conditions for seawater at pH 8.1 (Lartiges & Garrigues 1995).

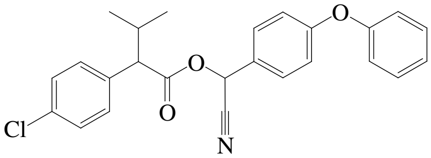
Ground water:

Sediment:

Soil: selected field $t_{1/2}$ = 34 d (Wauchope et al. 1992; Hornsby et al. 1996);
$t_{1/2}$ ~ 1 d in soil and water (Tomlin 1994).

Biota: excretion rate constant k = 0.07 h^{-1} from whole body willow shiner (Tsuda et al. 1992);
elimination rate constants k = $(0.64 \pm 0.09) \times 10^{-3}$ (NADPH) and k = $(0.12 \pm 0.02) \times 10^{-3}$ (GSH) min^{-1}·mg $protein^{-1}$ (rainbow trout, De Bruijn et al. 1993);
excretion rate constant k = 0.34 h^{-1} with $t_{1/2}$ = 2.0 d from carp (Tsuda et al. 1993).

18.1.1.44 Fenvalerate



Common Name: Fenvalerate

Synonym: Belmark, Ectrin, Pydrin, Pyrethroid, S 5602, Sanmarton, SD 43775, Sumicide, Sumicidin, Sumifly, Sumipower, WL 43775

Chemical Name: (*RS*)-α-cyano-3-phenoxybenzyl (*RS*)-2-(4-chlorophenyl)-3-methylbutyrate; cyano-(3-phenoxyphenyl)-methyl 4-chloro-α-(-1-methylethyl)benzeneacetate

Uses: non-systemic insecticide to control a wide variety of pests and also used as acaricide

CAS Registry No: 51630-58-1

Molecular Formula: $C_{25}H_{22}ClNO_3$

Molecular Weight: 419.901

Melting Point (°C): liquid

Boiling Point (°C):
  decomposes on distillation (Hartley & Kidd 1987; Tomlin 1994)

Density (g/cm^3 at 20°C):
  1.26 (22°C, Spencer 1982)
  1.17 (23°C, Hartley & Kidd 1987; Milne 1995)
  1.175 (tech. grade at 25°C, Worthing & Hance 1991; Montgomery 1993; Tomlin 1994)

Molar Volume (cm^3/mol):
  479.6 (calculated-Le Bas method at normal boiling point)

Dissociation Constant, pK_a:

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

Entropy of Fusion, ΔS_{fus} (J/mol K):

Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F: 1.0

Water Solubility (g/m^3 or mg/L at 25°C or as indicated):
  0.085 (shake flask-GC, Coats & O'Donnell-Jafferey 1979)
  0.085 (Verschueren 1983; quoted, Pait et al. 1992)
  0.024 (in seawater, Schimmel et al. 1983; Zaroogian et al. 1985; Clark et al. 1989)
  <1.0 (20°C, Worthing 1979, 1987; Spencer 1982)
  <1.0 (20°C, Hartley & Kidd 1987; Montgomery 1993; Milne 1995)
  < 0.02 (Davies & Lee 1987; quoted, Kawamoto & Urano 1989)
  <1.0 (tech. grade at 20°C, Worthing & Walker 1991)
  0.002 (20–25°C, selected, Wauchope 1989; Wauchope et al. 1992; Hornsby et al. 1996)

Vapor Pressure (Pa at 25°C or as indicated):
  4.90×10^{-7} (Barlow 1978)
  3.07×10^{-5} (Worthing 1979)
  1.33×10^{-5} (22°C, Spencer 1982)
  3.70×10^{-5} (Hartley & Kidd 1987)
  1.47×10^{-6} (Budavari 1989)
  3.73×10^{-5} (Kawamoto & Urano 1989)
  8.10×10^{-7} (GC-RT correlation, supercooled liquid value, Hinckley et al. 1990)
  3.70×10^{-5} (tech. grade, Worthing & Hance 1991)
  1.47×10^{-6} (20–25°C, selected, Wauchope et al. 1992; Hornsby et al. 1996)
  1.92×10^{-7} (20°C, Tomlin 1994)
  1.78×10^{-6} (solid P^S, converted from P_L determined by GC-RT correlation, Tsuzuki 2001)

Henry's Law Constant (Pa·m^3/mol at 25°C or as indicated):

0.0152	(20–25°C, calculated-P/C, Montgomery 1993)
0.308	(20–25°C, calculated-P/C as per Wauchope et al. 1992, Majewski & Capel 1995)
0.0211	(calculated-P/C, this work)

Octanol/Water Partition Coefficient, log K_{OW} at 25°C or as indicated:

4.42	(shake flask-GC, Coats & O'Donnell-Jafferey 1979)
6.20	(shake flask-GC, Schimmel et al. 1983)
5.2 ± 0.6	(HPLC-RT correlation, Muir et al. 1985)
6.65	(shake flask, Log P Database, Hansch & Leo 1987)
6.25	(HPLC-RT correlation, Kawamoto & Urano 1989)
4.09	(23°C, Worthing & Walker 1991)
6.25	(HPLC-RT correlation, Hu& Leng 1992)
4.09–6.25	(Montgomery 1993)
6.20	(recommended, Sangster 1993)
5.01	(23°C, Tomlin 1994)
6.20	(recommended, Hansch et al. 1995)
4.08	(23°C, Milne 1995)

Bioconcentration Factor, log BCF:

3.67	(quoted, Schimmel et al. 1983)
1.67–1.84	(sand, 24 h BCF for chironomid larvae in water, Muir et al. 1985)
2.01–2.24	(sand, 24 h BCF for chironomid larvae in sediment, Muir et al. 1985)
1.30–1.53	(sand, 24 h BCF for chironomid larvae in sediment/pore water, Muir et al. 1985)
1.62–1.87	(silt, 24 h BCF for chironomid larvae in water, Muir et al. 1985)
1.36–2.06	(silt, 24 h BCF for chironomid larvae in sediment, Muir et al. 1985)
1.26–1.97	(silt, 24 h BCF for chironomid larvae in sediment/pore water, Muir et al. 1985)
1.36–1.51	(clay, 24 h BCF for chironomid larvae in water, Muir et al. 1985)
2.09–2.19	(clay, 24 h BCF for chironomid larvae in sediment, Muir et al. 1985)
0.95–1.70	(clay, 24 h BCF for chironomid larvae in sediment/pore water, Muir et al. 1985)
4.48, 4.57	(oyster, calculated-K_{OW} & models, Zaroogian et al. 1985)
4.48, 4.57	(sheepshead minnow, calculated-K_{OW} & models, Zaroogian et al. 1985)
3.67	(oyster, Zaroogian et al. 1985; quoted, Hawker & Connell 1986)
–3.09	(milk biotransfer factor log B_m, correlated-K_{OW}, Wszolek et al. 1980; quoted, Travis & Arms 1988)
2.61, 2.96	(*Oncorhynchus mykiss*, Muir et al. 1994; quoted, Devillers et al. 1996)
2.70	(calculated, Pait et al. 1992)

Sorption Partition Coefficient, log K_{OC}:

2.58	(silt, reported as K_P on 78% DOC, Muir et al. 1985)
2.61	(clay, reported as K_P on 61% DOC, Muir et al. 1985)
1.30	(selected, USDA 1989; quoted, Neary et al. 1993)
3.72	(soil, 20–25°C, selected, Wauchope et al. 1992; Hornsby et al. 1996)
3.64	(calculated, Montgomery 1993)
3.72	(estimated-chemical structure, Lohninger 1994)
3.74	(soil, calculated-MCI $^1\chi$, Sabljic et al. 1995)

Environmental Fate Rate Constants, k, or Half-Lives, $t_{1/2}$:

Biodegradation: rate constant k(aerobic) = 0.055 d^{-1} with $t_{1/2}$ = 13 d at 20°C by aerobic activated sludge, and k(anaerobic) = 0.055 d^{-1} with $t_{1/2}$ = 13 d at 20°C by anaerobic microorganisms (batch contacting method, Kawamoto & Urano 1990).

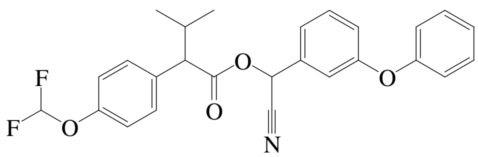
Half-Lives in the Environment:

Air:

Surface water: $t_{1/2}$ = 14 d in 100 mL of a pesticide-seawater solution under outdoor light, $t_{1/2}$ > 14 d under outdoor dark condition and $t_{1/2}$ > 28 d under indoor condition (Schimmel et al. 1983);

$t_{1/2}$ = 27–42 d in an estuary (Schimmel et al. 1983; quoted, Montgomery 1993).
$t_{1/2}$ = 13 d biodegradation by aerobic activated sludge or anaerobic microorganisms cultivated by an artificial sewage (Kawamoto & Urano 1990).
Ground water:
Sediment: $t_{1/2}$ = 34 d in 10 g of sediment/100 mL of a pesticide-seawater solution in untreated condition and $t_{1/2}$ > 28 d in sterile condition (Schimmel et al. 1983).
Soil: selected field $t_{1/2}$ = 35 d (Wauchope et al. 1992; Hornsby et al. 1996).
soil $t_{1/2}$ = 50 d (Pait et al. 1992).
Biota: average $t_{1/2}$ = 35 d in the forest (USDA 1989; quoted, Neary et al. 1993).

18.1.1.45 Flucythrinate



Common Name: Flucythrinate
Synonym: AC 222705, Cybolt, Cythrin, Pay-Off
Chemical Name: (*RS*)-α-cyano-3-phenoxybenzyl(*S*)-2-(4-difluoromethoxyphenyl)-3-methylbutyrate; cyano(3-phenoxy phenyl)methyl 4-(difluoromethoxy)-α-(1-methylethyl)benzeneacetate
Uses: non-systemic insecticide with contact and stomach action to control a wide range of insect pests in cotton, fruit trees, strawberries, vines, fruits, olives, coffee, cocoa, hops, vegetables, soybeans, cereals, maize, alfalfa, sugar beet, sunflowers and ornamentals
CAS Registry No: 70124-77-5
Molecular Formula: $C_{26}H_{23}F_2NO_4$
Molecular Weight: 451.463
Melting Point (°C):
    <25 (dark amber liquid, Montgomery 1993)
Boiling Point (°C):
    108.0 (at 0.35 mmHg, Hartley & Kidd 1987; Worthing & Hance 1991; Montgomery 1993; Tomlin 1994; Milne 1995)
Density (g/cm^3 at 20°C):
    1.189 (22°C, Hartley & Kidd 1987; Montgomery 1993; Tomlin 1994; Milne 1995)
    1.190 (22°C, Worthing & Hance 1991)

Molar Volume (cm^3/mol):
    499.9 (calculated-Le Bas method at normal boiling point)
    379.4 (22°C, calculated-density)
Dissociation Constant, pK$_a$:
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
Entropy of Fusion, ΔS_{fus} (J/mol K):
Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F: 1.0

Water Solubility (g/m^3 or mg/L at 25°C or as indicated):
    0.049 (in seawater, Schimmel et al. 1983)
    0.50 (21°C, Hartley & Kidd 1987; Worthing & Walker 1987, 1991; Tomlin 1994; Milne 1995)
    0.06 (20–25°C, selected, Wauchope 1989; Hornsby et al. 1996)
    0.50 (21°C, Montgomery 1993)

Vapor Pressure (Pa at 25°C or as indicated):
    1.2×10^{-6} (Hartley & Kidd 1987; Worthing & Hance 1991; Tomlin 1994)
    9.066 (Montgomery 1993)
    2.69×10^{-6}, 2.2×10^{-6} (liquid P_L, GC-RT correlation; Donovan 1996)
    1.2×10^{-6} (20–25°C, selected, Hornsby et al. 1996)
    2.82×10^{-6} (solid P^S, converted from P_L determined by GC-RT correlation method, Tsuzuki 2001)

Henry's Law Constant (Pa·m^3/mol at 25°C or as indicated):
    8187 (21–25°C, calculated-P/C, 8.08×10^{-2} atm·m^3/mol, Montgomery 1993)
    0.0011 (calculated-P/C, this work)

Octanol/Water Partition Coefficient, log K_{OW}:
    6.28 (shake flask-GC, Schimmel et al. 1983)
    6.20 (Clark et al. 1989)

2.08	(Worthing & Hance 1991; Tomlin 1994; Milne 1995)
5.55	(shake flask, Huang & Leng 1993)
4.70	(Montgomery 1993)
6.20	(recommended, Sangster 1993)
6.20	(selected, Hansch et al. 1995)

Bioconcentration Factor, log BCF:

2.96	(calculated-S as per Kenaga 1980, this work)

Sorption Partition Coefficient, log K_{OC}:

3.81	(calculated, Montgomery 1993)
5.00	(20–25°C, selected, Hornsby et al. 1996)

Environmental Fate Rate Constants, k, or Half-Lives, $t_{½}$:

Volatilization:

Photolysis: $t_{½}$ ~ 21 d for degradation on soil plates by simulated sunlight and $t_{½}$ = 4.0 d in aqueous solutions (Tomlin 1994).

Oxidation:

Hydrolysis: $t_{½}$ = 40, 52, and 6.3 d at pH 3, 5, 9 all at 27°C (Hartley & Kidd 1987; Montgomery 1993; Tomlin 1994).

Biodegradation:

Biotransformation:

Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants:

Half-Lives in the Environment:

Air:

Surface water: $t_{½}$ = 34 d in an estuarine environment (Schimmel et al. 1983; quoted, Montgomery 1993).

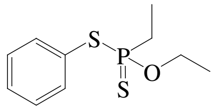
Ground water:

Sediment:

Soil: $t_{½}$ ~ 2 months in soil (Tomlin 1994);
field $t_{½}$ = 21 d (20–25°C, selected, Hornsby et al. 1996).

Biota:

18.1.1.46 Fonofos



Common Name: Fonofos
Synonym: Difonate, Dyfonate, ENT-25796, Fonophos, N 2788, N-2790, Stauffer NA 2790
Chemical Name: *O*-ethyl *S*-phenyl (*RS*)-ethylphosphorodithioate; (±)-*O*-ethyl *S*-phenyl ethylphosphorodithioate
Uses: soil insecticide to control rootworms, wireworms, crickets and similar crop pests in vegetables, sorghum, ornamentals, cereals, maize, vines, olives, sugar beet, sugar cane, potatoes, groundnuts, tobacco, turf, and fruit crops
CAS Registry No: 944-22-9 (unstated stereochemistry); 66767-39-3 (racemate); 62705-71-9 (*R*)-isomer; 62680-03-9 (*S*)-isomer
Molecular Formula: $C_{10}H_{15}OPS_2$
Molecular Weight: 246.329
Melting Point (°C): liquid
Boiling Point (°C):

130	(at 0.1 mmHg, Hartley & Kidd 1987; Worthing & Hance 1991; Montgomery 1993; Tomlin 1994; Milne 1995)

Density (g/cm^3 at 20°C):

1.160	(25°C, Hartley & Kidd 1987; Tomlin 1994; Milne 1995)
1.154	(Worthing & Hance 1991; Montgomery 1993)

Molar Volume (cm^3/mol):

213.4	(calculated-density)

Dissociation Constant, pK_a:
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
Entropy of Fusion, ΔS_{fus} (J/mol K):
Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F: 1.0

Water Solubility (g/m^3 or mg/L at 25°C or as indicated):

13	(22°C, Spencer 1973)
13	(Wauchope 1978)
15.7	(20°C, shake flask-GC, Bowman & Sans 1979, 1983b)
13	(Hartley & Kidd 1987; Worthing & Hance 1991; Milne 1995)
13	(20°C, Worthing & Walker)
16.9	(20–25°C, selected, Wauchope et al. 1992; Hornsby et al. 1996)
13	(rm. temp., Montgomery 1993)
13	(22°C, Tomlin 1994)

Vapor Pressure (Pa at 25°C or as indicated):

0.0267	(Menn 1969; Fuhrmann & Lichtenstein 1980)
0.028	(Khan 1980; Hartley & Kidd 1987; Montgomery 1993; Tomlin 1994)
0.028	(Worthing & Walker 1987; Worthing & Hance 1991)
0.0453	(20–25°C, selected, Wauchope et al. 1992; Hornsby et al. 1996)

Henry's Law Constant (Pa·m^3/mol at 25°C or as indicated):

0.5206	(calculated-P/C as per Worthing & Walker 1987, Schomburg et al. 1991)
0.5268	(20–25°C, calculated-P/C, Montgomery 1993)
0.530	(calculated-P/C as per Worthing & Walker 1987, Majewski & Capel 1995)

Octanol/Water Partition Coefficient, log K_{OW} at 25°C or as indicated:

3.892	(shake flask-GC, Bowman & Sans 1983b)
3.94	(shake flask, Log P Database, Hansch & Leo 1987)
3.90	(20°C, Worthing & Hance 1991)

3.89, 3.90	(Montgomery 1993)
3.94	(recommended, Sangster 1993)
3.94	(Tomlin 1994)
3.90	(Milne 1995)
3.94	(recommended, Hansch et al. 1995)

Bioconcentration Factor, log BCF:

1.89	(mosquito fish, wet wt. basis, De Bruijn & Hermens 1991)

Sorption Partition Coefficient, log K_{OC} at 25°C or as indicated:

2.3–2.7	(selected, sediment/water, Schnoor & McAvoy 1981; Schnoor 1992)
1.83	(screening model calculations, Jury et al. 1987b)
1.18	(loam soil, Worthing & Hance 1991)
2.94	(soil, 20–25°C, selected, Wauchope et al. 1992)
3.03	(calculated, Montgomery 1993)
2.94	(estimated-chemical structure, Lohninger 1994)
2.94	(soil, 20–25°C, selected, Hornsby et al. 1996)
3.44; 3.0, 3.04	(soil, quoted exptl.; estimated-class-specific model, estimated-general model, Gramatica et al. 2000)

Environmental Fate Rate Constants, k, or Half-Lives, $t_{½}$:

Volatilization:

Photolysis: $t_{½}$ = 12 d in water at pH 5 and 25°C (Worthing & Hance 1991; Tomlin 1994).

Oxidation:

Hydrolysis: alkaline chemical hydrolysis rate constant $k = 1 \times 10^{-4}\ M^{-1}\ s^{-1}$ with $t_{½}$ > 365 d (selected, sediment/water, Schnoor & McAvoy 1981; quoted, Schnoor 1992);

hydrolysis $t_{½}$ = 74–127 d in water at 40°C and pH 7, $t_{½}$ = 101 d at pH 4 (Worthing & Hance 1991; quoted, Montgomery 1993; Tomlin 1994).

Biodegradation:

Biotransformation:

Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants:

Half-Lives in the Environment:

Air:

Surface water:

Ground water:

Sediment:

Soil: persistence of less than one month in soil (Wauchope 1978);

$t_{½}$ > 24 wk in sterile sandy loam and $t_{½}$ = 3.0 wk in nonsterile sandy loam; $t_{½}$ > 24 wk in sterile organic soil and $t_{½}$ = 4.0 wk in nonsterile organic soil (Miles et al. 1979);

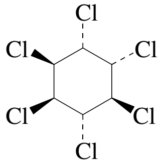
$t_{½}$ = 60 d from screening model calculations (Jury 1987b);

$t_{½}$ = 16.5–28 d at 24°C (Worthing & Hance 1991);

selected field $t_{½}$ = 40 d (Wauchope et al. 1992; quoted, Richards & Baker 1993; Hornsby et al. 1996).

Biota: biochemical $t_{½}$ = 60 d from screening model calculations (Jury et al. 1987b).

18.1.1.47 α-HCH



Common Name: α-HCH
Synonym: α-BHC, α-Hexachlorocyclohexane
Chemical Name: α-1,2,3,4,5,6-hexachlorocyclohexane, (1α, 2α, 3α, 4α, 5β, 6β-1, 2, 3, 4, 5, 6-hexachloro-cyclohexane
CAS Registry No: 319-84-6
Molecular Formula: $C_6H_6Cl_6$
Molecular Weight: 290.830
Melting Point (°C):
    158 (Lide 2003)
Boiling Point (°C): 288
Density (g/cm^3 at 20°C):
Molar Volume (cm^3/mol):
    243.6 (calculated-Le Bas method at normal boiling point)
Enthalpy of fusion, ΔH_{fus} (kJ/mol):
    30.96 (Ruelle & Kesselring 1997)
Entropy of fusion, ΔS_{fus} (J/mol K):
    72.0 (Passivirta et al. 1999)
Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F: 0.0496 (mp at 158°C)

Water Solubility (g/m^3 or mg/L at 25°C or as indicated and reported temperature dependence equations):
    10 (20°C, Slade 1945, Günther et al. 1968; Ulmann 1972; Horvath 1982)
    1.63 (shake flask-GC, Kanazawa et al. 1971)
    2.03, 1.21 (28°C, shake flask-centrifuge, membrane filter-GC, max. 0.1 μm particle size, Kurihara et al. 1973)
    1.77, 1.48 (28°C, shake flask-centrifuge, sonic and centrifuge-GC, max. 0.05 μm particle size, Kurihara et al. 1973)
    1.21–2.03 (28°C, Kurihara et al. 1973)
    2.0 (generator column-GC/ECD, Weil et al. 1974)
    4.34 (shake flask-GC/ECD, Malaiyandi et al. 1982)
    1.51 (20°C, Deutsche Forschungsgemeinschaft 1983; Ballschmiter & Wittlinger 1991; Fischer et al. 1991)
    21.6 (supercooled liquid value, Majewski & Capel 1995)
    0.666, 0.023 (calculated-molar volume, mp and mobile order thermodynamics, Ruelle & Kesselring 1997)
    $\log [S_L/(\text{mol/L})] = 2.790 - 1621/(T/K)$ (supercooled liquid, Passivirta et al. 1999)
    85.22, 96.85 (supercooled liquid values: LDV literature-derived value, FAV final-adjusted value, Xiao et al. 2004)
    $\log S_L/(\text{mol m}^{-3}) = -398.5/(T/K) + 0.859$ (supercooled liquid, final adjusted eq., Xiao et al. 2004)

Vapor Pressure (Pa at 25°C or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):
    2.67* (20°C, static method, measured range 20–60°C, Slade 1945)
    0.00333* (20°C, effusion manometer, measured range 15–30°C, Balson 1947)
    0.27 (supercooled liquid value from Balson 1947; quoted, Hinckley et al. 1990)
    0.0073 (20°C, Deutsche Forschungsgemeinschaft 1983; quoted, Ballschmiter & Wittlinger 1991; Fischer et al. 1991; Schreitmüller & Ballschmiter 1995)
    0.0840 (20°C, supercooled liquid value, Bidleman et al. 1986)
    0.313 (GC-RT correlation, Watanabe & Tatsukawa 1989)
    0.227 (supercooled liquid P_L, GC-RT correlation, Hinckley et al. 1990)
    $\log (P_L/\text{Pa}) = 10.49 - 3301/(T/K)$ (supercooled liquid, Hinckley et al. 1990)
    $\log (P_L/\text{Pa}) = 11.34 - 3375/(T/K)$ (supercooled liquid, Hinckley et al. 1990)
    0.003 (selected, Suntio et al. 1988, quoted, Calamari et al. 1991; Schreitmüller & Ballschmiter 1995)
    0.0060 (quoted, Howard 1991)
    0.00647 (quoted, supercooled liquid value, Majewski & Capel 1995)

0.159; 0.00464 (supercooled liquid P_L, GC-RT correlation; converted to solid P_S with fugacity ratio F, Passivirta et al. 1999)
log (P_S/Pa) = 14.53 – 4954/(T/K) (solid, Passivirta et al. 1999)
log (P_L/Pa) = 10.77 – 3335/(T/K) (supercooled liquid, Passivirta et al. 1999)
0.245, 0.245 (supercooled liquid P_L: LDV literature-derived value, FAV final adjusted value, Xiao et al. 2004)
log P_L/Pa = – 3434/(T/K) + 10.91 (supercooled liquid, linear regression of literature data, Xiao et al. 2004)
log P_L/Pa = – 3497/(T/K) + 11.12 (supercooled liquid, final adjusted eq., Xiao et al. 2004)

Henry's Law Constant (Pa·m^3/mol or at 25°C as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):

0.47–0.792 (Callahan et al. 1979)
2.16 (gas stripping-GC, Atlas et al. 1982)
0.55 (calculated-P/C, Mabey et al. 1982)
0.87 (calculated-P/C, Suntio et al. 1988)
1.10 (calculated-P/C, Ballschmiter & Wittlinger 1991; Fischer et al. 1991)
1.07 (calculated-P/C, Howard 1991)
0.43 (calculated-P/C, Calamari et al. 1991)
0.677* (23°C, gas stripping-GC/ECD, distilled water, measured range 0.5–45°C, Kucklick et al. 1991)
log [H/(Pa·m^3 mol^{-1}] = –2810/(T/K) + 9.31, temp range 0.5–45°C (gas stripping-GC measurements, distilled water, Kucklick et al. 1991, McConnell et al. 1993)
0.104, 0.257, 0.710, 2.10, 5.99 (0.5, 10, 25, 23, 35, 45°C, gas stripping-GC/ECD, artificial seawater, Kucklick et al. 1991)
log [H/(Pa·m^3 mol^{-1})] = –2969/(T/K) + 9.88, temp range 0.5–45°C (gas stripping-GC measurements, artificial seawater, Kucklick et al. 1991)
0.87 (20°C), 2.40, 1.10, 0.677, 0.710 (23°C) (quoted, Iwata et al. 1993)
0.215, 0.491, 0.373, 0.630, 0.630 (8.5°C in Green Bay, 18.9°C in Lake Michigan, 18.5°C in Lake Huron, 22.3°C in Lake Erie, 22.3°C in Lake Ontario, concn. ratio-GC, McConnell et al. 1993)
0.872 (calculated-P/C, this work)
1.239 (wetted wall column-GC, Altschuh et al. 1999)
log [H/(Pa m^3/mol)] = 8.98 – 1714/(T/K) (Passivirta et al. 1999)
0.43* (20°C, gas stripping-GC, measured range 10–40°C, Jantunen et al. 2000)
log [H/(Pa m^3/mol)] = 10.88 – 3298/(T/K); temp range 10–40°C (gas stripping-GC, Jantunen et al. 2000)
0.53 (20°C, selected from literature experimentally measured data, Staudinger & Roberts 1996, 2001)
log K_{AW} = 5.485 – 2682/(T/K) (van't Hoff eq. derived from literature data, Staudinger & Roberts 2001)
0.38* (20°C, dynamic headspace-GC, DHS method, measured range 5–35°C, Sahsuvar et al. 2003)
0.42* (20°C, gas stripping-GC, BS method, measured range 5–35°C, Sahsuvar et al. 2003)
0.39* (20°C, mean value of DHS and BS methods, temp range 5–35°C, Sahsuvar et al. 2003)
log [H/(Pa m^3/mol)] = 10.13 – 3088/(T/K); temp range 5–35°C (Sahsuvar et al. 2003)
0.646, 0.741 (LDV literature-derived value, FAV final adjusted value, Xiao et al. 2004)
log [H/(Pa m^3/mol)] = –3171/(T/K) + 10.45 (LDV linear regression of literature data, Xiao et al. 2004)
log [H/(Pa m^3/mol)] = –3099/(T/K) + 10.26 (FAV final adjusted eq., Xiao et al. 2004)

Octanol/Water Partition Coefficient, log K_{OW} at 25°C or as indicated. Additional data at other temperatures designated * are compiled at the end of this section:

3.81 (shake flask-GC, Kurihara et al. 1973)
3.81 (HPLC-RT correlation, Sugiura et al. 1979)
3.90 (Veith et al. 1979)
3.776 ± 0.025 (shake flask/slow stirring method; De Bruijn et al. 1989)
3.80 (recommended, Sangster 1993)
3.80 (recommended, Hansch et al. 1995)
3.79* ± 0.001 (shake flask-slow stirring-GC, measured range 5–45°C, Paschke & Schüürmann 1998)
3.81; 4.57 (quoted lit.; calculated, Passivirta et al. 1999)
3.81, 3.94 (LDV literature-derived value, FAV final-adjusted value, Xiao et al. 2004)
log K_{OW} = –374.5/(T/K) + 2.55 (LDV linear regression of literature data, Xiao et al. 2004)
log K_{OW} = –266.2/(T/K) + 3.04 (LDV linear regression of literature data, Xiao et al. 2004)

Octanol/Air Partition Coefficient, log K_{OA} at 25°C and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section:
6.90 (calculated-K_{OW}/K_{AW}, Wania & Mackay 1996)
7.26 (calculated, Finizio et al. 1997)
7.618*, 7.611 (gas saturation-GC/MS, calculated, measured range 5–25°C, Shoeib & Harner 2002)
log K_{OA} = –3.23 + 3231/(T/K), temp range: 5–25°C (gas saturation-GC, Shoeib & Harner 2002)
7.61, 7.464 (LDV literature-derived value, FAV final adjusted value, Xiao et al. 2004)
log K_{OA} = 3231/(T/K) – 3.23 (LDV linear regression of literature data, Xiao et al. 2004)
log K_{OA} = 3235/(T/K) – 3.90 (FAV final adjusted eq., Xiao et al. 2004)

Bioconcentration Factor, log BCF:
2.03 (mussels, Ernst 1977; quoted, Renberg & Sundström 1979; Hawker & Connell 1986)
3.08, 2.52, 2.78, 2.77 (golden orfe, carp, brown trout, guppy, Suguira et al. 1979)
2.20, 2.82 (mussels, Geyer et al. 1982)
2.97–3.38 mean 3.20; 2.97–3.45 mean 3.38 (rainbow trout, 15°C, steady-state BCF on 7- to 96-d laboratory study in 2 tanks with different water concn, Oliver & Niimi 1985)
3.20, 2.85 (rainbow trout: laboratory BCF, Lake Ontario field BCF, Oliver & Niimi 1985)
1.93 (paddy field fish, Soon & Hock 1987)
2.15 (calculated, Isnard & Lambert 1988)
6.01 (azalea leaves, Bacci et al. 1990)
3.04 (*Brachydanio rerio*, flow-through conditions, Butte et al. 1991)
2.33 (early juvenile of rainbow trout, Vigano et al. 1992)
5.72 (azalea leaves, calculated, Müller et al. 1994)
2.79; 2.606, 2.712 (fish, steady-state, quoted lit.; calculated-MCI χ, calculated-K_{OW}, Lu et al.1999)
2.33; 2.44 (*Oncorhynchus mykiss*, wet wt. basis: quoted exptl.; calculated-QSAR model based on quantum chemical parameters, Wei et al. 2001)

Sorption Partition Coefficient, log K_{OC}:
3.81 (calculated-S, Lyman et al. 1982)
4.10, 3.5 (field sediment trap material, calculated-K_{OW}, Oliver & Charlton 1984)
3.25 (av. lit. value, Gerstl 1991)
3.32 (derived from exptl., Meylan et al. 1992)
3.53 (calculated-MCI χ, Meylan et al. 1992)
3.25 (soil, calculated-MCI $^1\chi$, Sabljic et al. 1995)
5.50 (soil, calculated-universal solvation model, Winget et al. 2000)

Environmental Fate Rate Constants, k, or Half-Lives, $t_{1/2}$:
Volatilization: volatilization $t_{1/2}$ ~ 6 d from a model river of 1 m deep flowing 1 m/s with a wind speed of 3 m/s (Saleh et al. 1982);
$t_{1/2}$ ~ 500 d from a model pond (estimated, Howard 1991).
Photolysis:
Oxidation: photooxidation $t_{1/2}$ = 2.3 d for reaction with OH radical in the gas phase (Atkinson 1987).
Hydrolysis: hydrolytic $t_{1/2}$ = 26 yr at pH 8 and 5°C (Ngabe et al. 1993).
Biodegradation: overall degradation rate constant k = 0.0648 h^{-1} with $t_{1/2}$ = 10.7 h for (+)-α-HCH and rate constant k = 0.0298 h^{-1} with $t_{1/2}$ = 23.3 h for (–)-α-HCH were calculated from experiments S1–S3 of (35 ± 0.5) h for (+) enantiomer and 99 ± 3.5 h for (–) enantiomer in sewage sludge (Müller & Buser 1995).
Biotransformation:
Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants:
k_1 = 3.82 h^{-1}; k_2 = 0.036 h^{-1} (mussels, Ernst 1977; quoted, Hawker & Connell 1986)
k_1 = 0.52 d^{-1}, 0.56 d^{-1}, 0.91 d^{-1}, and 0.42 d^{-1} (golden orfe, carp, brown trout, and guppy at steady state, Sugiura et al. 1979)
k_2 = 0.0009 h^{-1} (azalea leaves, Peterson et al. 1991)
k_1 = 27.6 h^{-1}; k_2 = 0.13 h^{-1} (early juvenile of rainbow trout, Vigano et al. 1992)

Half-Lives in the Environment:
Air: atmospheric $t_{1/2}$ ~ 2.3 d based on reaction with OH radical at 25°C (Atkinson 1987);

half-lives in the Great Lake's atmosphere. $t_{½}$ = 4.4 ± 0.2 yr at Eagle Harbor, $t_{½}$ = 3.5 ± 0.2 yr at Sleeping Bear Dunes and $t_{½}$ = 3.3 ± 0.2 yr at Sturgeon Point (Buehler et al. 2004).

Surface water: $t_{½}$ = 1.7–77 d in various locations in the Netherlands in case a first order reduction process may be assumed (Zoeteman et al. 1980)

Ground water:

Sediment:

Soil: $t_{½}$ = 8.2 and 7.1 yr for control and sludge-amended Luddington soils, respectively (Meijer et al. 2001).

Biota: $t_{½}$ = 19.2 h (mussels, Ernst 1977).

TABLE 18.1.1.47.1

Reported vapor pressures, octanol-water partition coefficients and octanol-air partition coefficients of α-HCH at various temperatures

Vapor pressure				log K_{OW}		log K_{OA}	
Slade 1945		Balson 1947		Paschke & Schüürmann 1998		Shoeib & Harner 2002	
static method		effusion-manometer		shake flask/GC		generator column-GC/MS	
t/°C	P/Pa	t/°C	P/Pa	t/°C	log K_{OW}	t/°C	log K_{OA}
20	2.67	0	2.0×10^{-4}	5	3.92	5	8.4086
40	8.0	10	8.67×10^{-4}	25	3.79	10	8.1770
60	44.0	20	3.33×10^{-3}	45	3.75	15	7.9681
		30	0.01187			20	7.8100
		40	0.03866	enthalpy of phase transfer:		25	7.6178
		50	0.1160	$\Delta H_{OW}/(kJ\ mol^{-1}) = -9.80$		25	7.611
		60	0.3266	entropy of phase transfer:			
		70	0.8666	$\Delta S_{OW}/(J\ K^{-1}\ mol^{-1}) = 55.4$		log K_{OA} = A + B/(T/K)	
						A	–3.231
		log P = A – B/(T/K)				B	3231
			P/mmHg				
		A	11.950			enthalpy of phase change	
		B	4850			$\Delta H_{OA}/(kJ\ mol^{-1}) = 61.9$	
		temp range: 51–71°C					

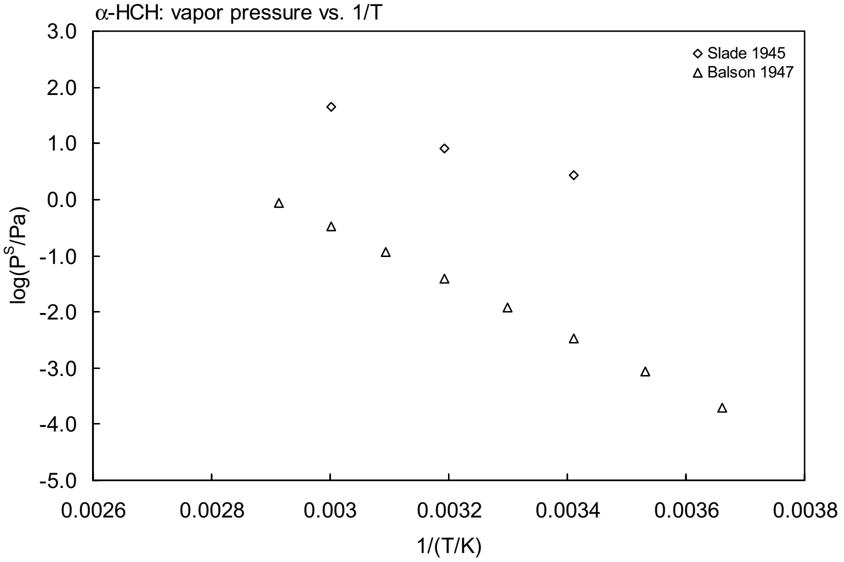


FIGURE 18.1.1.47.1 Logarithm of vapor pressure versus reciprocal temperature for α-HCH.

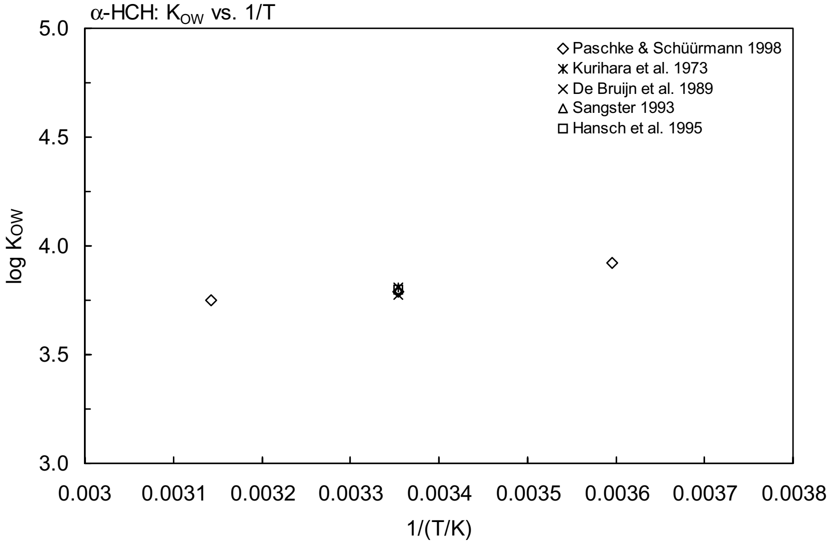


FIGURE 18.1.1.47.2 Logarithm of K_{OW} versus reciprocal temperature for α-HCH.

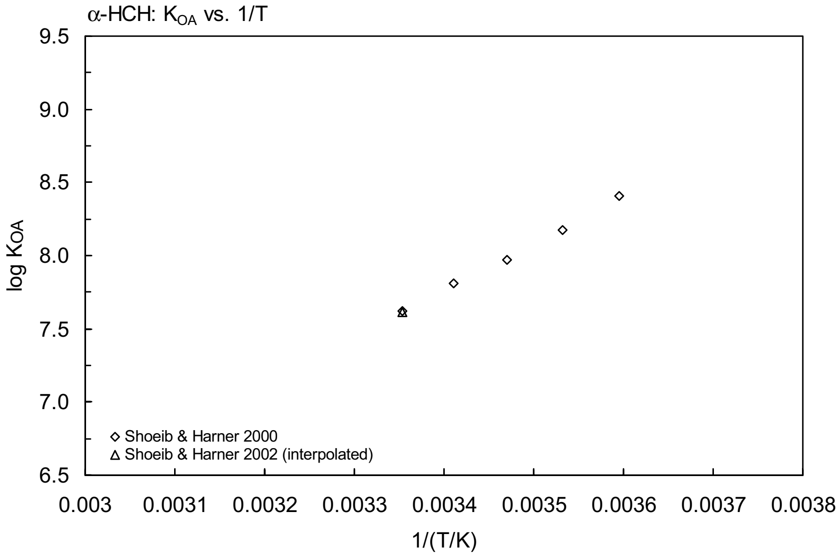


FIGURE 18.1.1.47.3 Logarithm of K_{OA} versus treciprocal temperature for α-HCH.

TABLE 18.1.1.47.2
Reported Henry's law constants of α-HCH at various temperatures and temperature dependence equations

$\ln K_{AW} = A - B/(T/K)$	(1)	$\log K_{AW} = A - B/(T/K)$	(1a)
$\ln (1/K_{AW}) = A - B/(T/K)$	(2)	$\log (1/K_{AW}) = A - B/(T/K)$	(2a)
$\ln (k_H/atm) = A - B/(T/K)$	(3)		
$\ln H = A - B/(T/K)$	(4)	$\log H = A - B/(T/K)$	(4a)
$K_{AW} = A - B\cdot(T/K) + C\cdot(T/K)^2$	(5)		

Kucklick et al. 1991		**McConnell et al. 1993**		**Jantunen et al. 2000**		**Sahsuvar et al. 2003**	
gas stripping-GC		**concentration ratio**		**air stripping-GC**		**air stripping/dynamic HS**	
t/°C	**H/(Pa m^3/mol)**	**t/°C**	**H/(Pa m^3/mol)**	**t/°C**	**H/(Pa m^3/mol)**	**t/°C**	**H/(Pa m^3/mol)**
			Green Bay			dynamic headspace (DHS)	
0.5	0.104	8.0	0.215	10	0.17	5	0.094
10	0.255		Lake Michigan	20	0.43	10	0.15
23	0.677	18.9	0.491	30	0.92	20	0.38
35	1.34		Lake Huron	35	1.52	30	0.79
45	3.27	18.5	0.373	40	2.21	35	1.32
			Lake Erie				
eq. 4a	H/(Pa m^3/mol)	22.3	0.630	eq. 4a	H/(Pa m^3/mol)	gas stripping-GC	
A	9.31		Lake Ontario	A	10.88 ± 0.50	5	0.098
B	2810	22.3	0.630	B	3298 ± 149	10	0.13
seawater					20	0.42	
0.5	0.104					30	0.92
10	0.257					35	1.24
23	0.710						
35	2.10					combined - both methods	
45	5.99					5	0.095
						10	0.15
eq.4a	H/(Pa m^3/mol)					20	0.39
A	9.88					30	0.85
B	2969					35	1.30
						eq. 4a	H/(Pa m^3/mol)
						A	10.13 ± 0.29
						B	3088 ± 84
						enthalpy of transfer air-water	
						ΔH_{WA}/(kJ mol^{-1}) = 59.3	

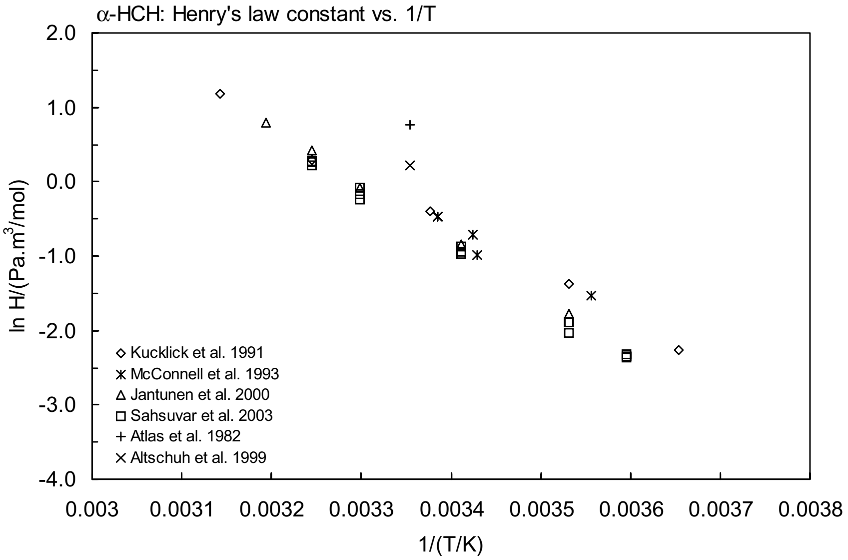
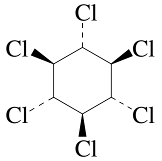


FIGURE 18.1.1.47.4 Logarithm of Henry's law constant versus reciprocal temperature for α-HCH.

18.1.1.48 β-HCH



Common Name: β-HCH
Synonym: β-BHC, β-Hexachlorocyclohexane, 1α,2β,3α,4β,5α,6β-1,2,3,4,5,6-hexachloro-cyclohexane
Chemical Name: β-1,2,3,4,5,6-hexachlorocyclohexane
CAS Registry No: 319-85-7
Molecular Formula: $C_6H_6Cl_6$
Molecular Weight: 290.830
Melting Point (°C):
  309 (Slade 1945; Ballschmiter & Wittlinger 1991)
Boiling Point (°C):
Density (g/cm^3 at 20°C):
Molar Volume (cm^3/mol):
  243.6 (calculated-Le Bas method at normal boiling point)
Enthalpy of fusion, ΔH_{fus} (kJ/mol):
Entropy of fusion, ΔS_{fus} (J/mol K):
Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F: 0.00164 (mp at 309°C)

Water Solubility (g/m^3 or mg/L at 25°C or as indicated and reported temperature dependence equations):
  5.0 (20°C, Slade 1945; Gunther et al. 1968; Horvath 1982)
  0.70 (20°C, shake flask-GC, Kanazawa et al. 1971)
  0.20, 0.13 (28°C, shake flask-centrifuge, membrane filter-GC, max. 0.1 μm particle size, Kurihara et al. 1973)
  0.70 (20°C, Brooks 1974)
  0.24 (generator column-GC/ECD, Weil et al. 1974)
  0.13–0.70 (Callahan et al. 1979)
  2.04 (20°C, Deutsche Forschungsgemeinschaft 1983; Ballschmiter & Wittlinger 1991; Fischer et al. 1991)
  7.0 (Worthing & Walker 1983)
  69.5 (supercooled liquid value, Majewski & Capel 1995)
  344, 418.8 (supercooled liquid: derivation of literature-derived value, final-adjusted value, Xiao et al. 2004)
  $\log [S_L/(\text{mol m}^{-3})] = -110.1/(T/K) - 0.211$ (supercooled liquid, final adjusted eq., Xiao et al. 2004)

Vapor Pressure (Pa at 25°C or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):
  0.67* (20°C, static method, measured range 20–60°C, Slade 1945)
  3.73×10^{-5}* (20°C, effusion-manometer, measured range 0–110°C, Balson 1947)
  4.90×10^{-5} (20°C, Deutsche Forschungsgemeinschaft 1983; Ballschmiter & Wittlinger 1991; Fischer et al. 1991)
  0.266 (GC-RT correlation, Watanabe & Tatsukawa 1989)
  0.0272 (supercooled liquid value, Majewski & Capel 1995)
  0.062, 0.0525 (supercooled liquid P_L LDV literature derived value, FAV final adjusted value, Xiao et al. 2004)
  $\log (P_L/Pa) = -3563/(T/K) + 10.74$ (supercooled liquid, linear regression of literature data, Xiao et al. 2004)
  $\log (P_L/Pa) = -3563/(T/K) + 10.67$ (supercooled liquid, final adjusted eq., Xiao et al. 2004)

Henry's Law Constant ($Pa \cdot m^3/mol$ at 25°C or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):
  0.055 (20–25°C, Mabey et al. 1982)
  0.120 (calculated-P/C, Suntio et al. 1988)
  0.070 (calculated-P/C, Ballschmiter & Wittlinger 1991; Fischer et al. 1991)
  0.0446 (wetted-wall column-GC, Altschuh et al. 1999)

0.022* (dynamic headspace-GC, measured range 5–35°C, Sahsuvar et al. 2003)
$\log [H/(Pa\ m^3/mol)] = 9.96 - 3400/(T/K)$; temp range 5–35°C (dynamic headspace-GC, Sahsuvar et al. 2003)
0.037, 0.037 (LDV literature-derived value, FAV final adjusted value, Xiao et al. 2004)
$\log [H/(Pa\ m^3/mol)] = -3454/(T/K) + 10.16$ (LDV linear regression of literature data, Xiao et al. 2004)
$\log [H/(Pa\ m^3/mol)] = -3673/(T/K) + 10.89$ (FAV final adjusted eq., Xiao et al. 2004)

Octanol/Water Partition Coefficient, log K_{OW} at 25°C or as indicated. Additional data at other temperatures designated * are compiled at the end of this section:

3.80 (shake flask-GC, Kurihara et al. 1973)
4.15 (HPLC-RT correlation, Sugiura et al. 1979)
3.842 ± 0.036; 3.78 (shake flask/slow stirring-GC, De Bruijn et al. 1989)
3.81 (recommended, Sangster 1993)
3.78 (recommended, Hansch et al. 1995)
3.88* ± 0.01 (shake flask/slow stirring-GC, measured range 5–25°C, Paschke & Schüürmann 1998)
3.84, 3.92 (LDV literature-derived value, FAV final-adjusted value, Xiao et al. 2004)
$\log K_{OW} = 847.5/(T/K) + 1.07$ (LDV linear regression of literature data, Xiao et al. 2004)

Octanol/Air Partition Coefficient, log K_{OA} at 25°C and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section:

8.965*, 8.875 (gas saturation-GC/MS, calculated, measured range 5–35°C, Shoeib & Harner 2002)
$\log K_{OA} = -7.69 + 4937/(T/K)$, temp range 5–35°C, (gas saturation-GC, Shoeib & Harner 2002)
8.87, 8.74 (LDV literature-derived value, FAV final adjusted value, Xiao et al. 2004)
$\log K_{OA} = 4937/(T/K) - 7.69$ (LDV linear regression of literature data, Xiao et al. 2004)
$\log K_{OA} = 4391/(T/K) - 5.98$ (FAV final adjusted eq., Xiao et al. 2004)

Bioconcentration Factor, log BCF:

2.99, 2.44, 2.82, 3.17 (golden orfe, carp, brown trout, guppy, Sugiura et al. 1979)
3.08, 2.26, 2.62 (activated sludge, algae, golden ide, reported as log BF, Freitag et al. 1985)
2.66 (calculated, Isnard & Lambert 1988)
3.16, 3.18 (*Brachydanio rerio*, flow-through conditions, Butte et al. 1991; quoted, Devillers et al. 1996)
2.86; 2.606, 2.712 (fish, steady-state, quoted lit.; calculated-MCI χ, calculated-K_{OW}, Lu et al.1999)
2.50; 2.44 (*Oncorhynchus mykiss*, wet wt. basis: quoted exptl.; calculated-QSAR model based on quantum chemical parameters, Wei et al. 2001)

Sorption Partition Coefficient, log K_{OC}:

3.36 (av. lit. value, Gerstl 1991)
3.98 (soil, calculated-S as per Kenaga 1980, this work)
3.50 (derived from exptl., Meylan et al. 1992)
3.53 (calculated-MCI χ, Meylan et al. 1992)
3.36 (soil, calculated-MCI $^1\chi$, Sabljic et al. 1995)
5.50; 3.50 (soil, calculated-universal solvation model; quoted exptl., Winget et al. 2000)

Environmental Fate Rate Constants, k, or Half-Lives, $t_{½}$:

Volatilization:
Photolysis:
Hydrolysis:
Oxidation:
Biodegradation: calculated $t_{½}$ = 178 h in sewage sludge from experiments S1–S3 (Buser & Müller 1995).
Biotransformation:
Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants:
$k_1 = 0.46\ d^{-1}$, $0.33\ d^{-1}$, $0.53\ d^{-1}$, and $0.18\ d^{-1}$ (golden orfe, carp, brown trout, and guppy at steady state, Sugiura et al. 1979)

Half-Lives in the Environment:

TABLE 18.1.1.48.1
Reported vapor pressures and Henry's law constants of β-HCH at various temperatures

Vapor pressure				Henry's law constant	
Slade 1945		Balson 1947		Sahsuvar et al. 2003	
static method		effusion manometer		dynamic headspace-GC	
t/°C	P/Pa	t/°C	P/Pa	t/°C	H/(Pa m^3/mol)
20	0.667	0	1.733×10^{-6}	5	0.0054
40	22.7	10	8.399×10^{-6}	10	0.0092
60	77.3	20	3.733×10^{-5}	20	0.022
		30	1.533×10^{-4}	30	0.053
		40	5.60×10^{-4}	35	0.088
		50	1.907×10^{-3}		
		60	6.00×10^{-3}		
		70	0.01760	ln H = A – B/(t/K)	
		80	0.04933		H/(Pa m^3/mol)
		90	0.1293	A	9.96 ± 0.23
		100	0.3200	B	3400 ± 68
		110	0.7653		
				enthalpy of transfer air-water	
		log P = A – B/(T/K)		ΔH_{WA}/(kJ mol^{-1}) = 65.1	
			P/mmHg		
		A	11.790		
		B	5375		
		temp range: 95–117°C			

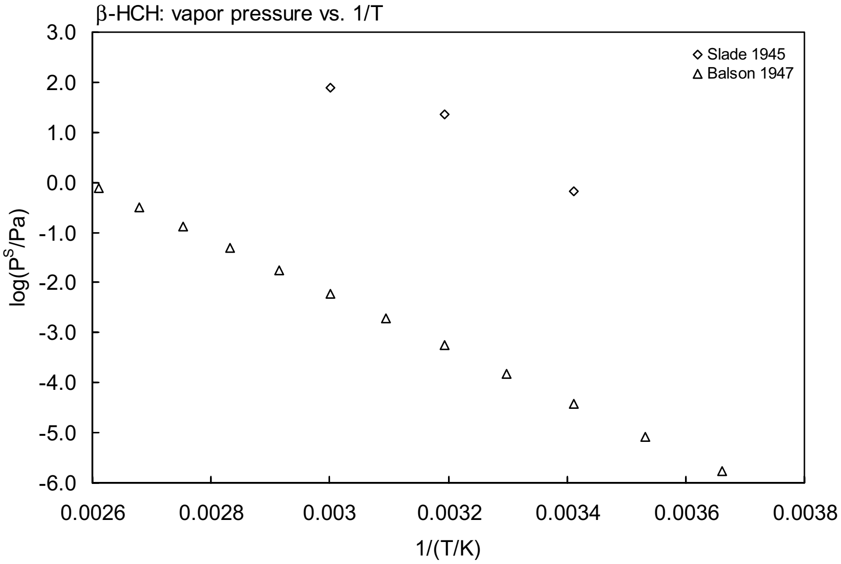


FIGURE 18.1.1.48.1 Logarithm of vapor pressure versus reciprocal temperature for β-HCH.

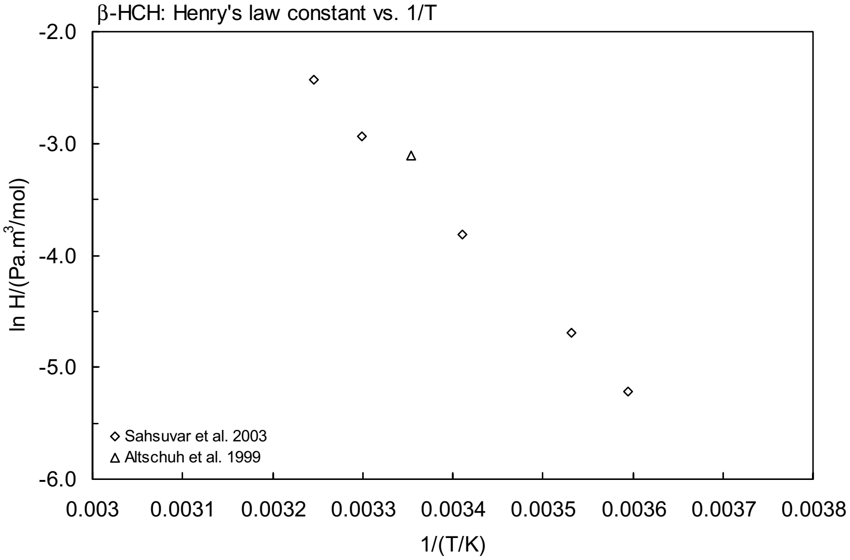


FIGURE 18.1.1.48.2 Logarithm of Henry's law constant versus reciprocal temperature for β-HCH.

TABLE 18.1.1.48.2
Reported octanol-water and octanol-air partition coefficients of β-HCH at various temperatures

log K_{OW}		log K_{OA}	
Paschke & Schüürmann 1998		**Shoeib & Harner 2002**	
shake flask-GC		**generator column-GC/MS**	
t/°C	**log K_{OW}**	**t/°C**	**log K_{OA}**
5	3.99	5	10.0686
25	3.88	15	9.4375
45	3.87	20	8.9875
		25	8.9651
enthalpy of phase transfer:		35	8.3682
$\Delta H_{OW}/(kJ\ mol^{-1}) = -8.20$		25	8.875
entropy of phase transfer:			
$\Delta S_{OW}/(J\ K^{-1}\ mol^{-1}) = 62.7$		$\log K_{OA} = A + B/(T/K)$	
		A	–7.692
		B	4937
		enthalpy of phase change	
		$\Delta H_{OA}/(kJ\ mol^{-1}) = 94.5$	

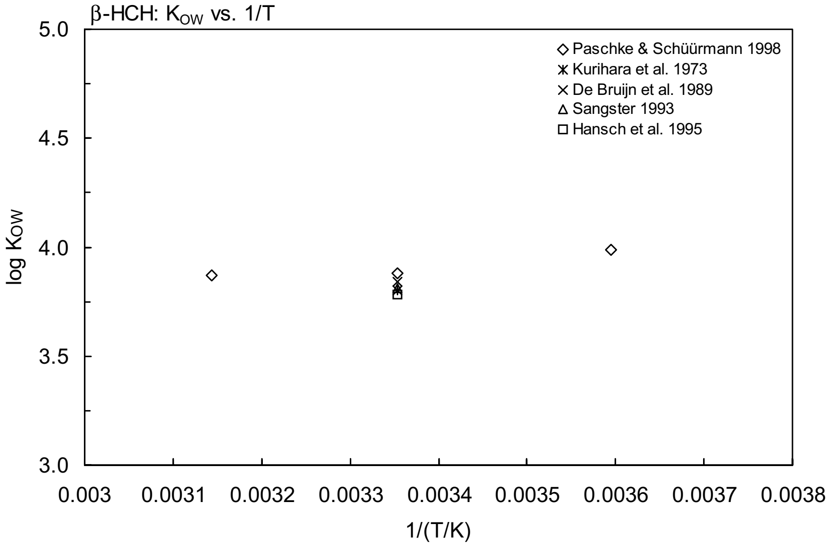


FIGURE 18.1.1.48.3 Logarithm of K_{OW} versus reciprocal temperature for β-HCH.

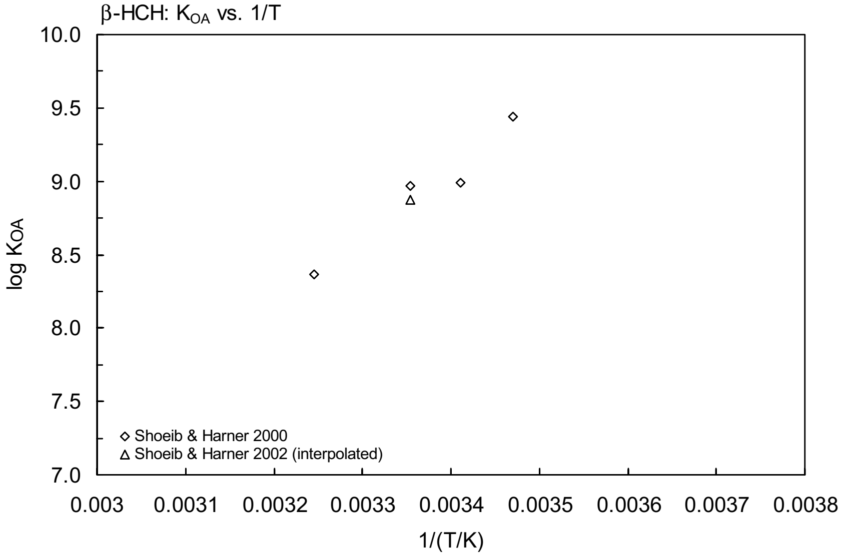
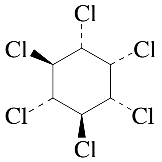


FIGURE 18.1.1.48.4 Logarithm of K_{OA} versus reciprocal temperature for β-HCH.

18.1.1.49 δ-HCH



Common Name: δ-HCH
Synonym: δ-BHC, δ-Hexachlorocyclohexane, 1α,2α,3α,4β,5α,6β-1,2,3,4,5,6-hexachloro-cyclohexane
Chemical Name: δ-1,2,3,4,5,6-hexachlorocyclohexane
CAS Registry No: 319-86-8
Molecular Formula: $C_6H_6Cl_6$
Molecular Weight: 290.830
Melting Point (°C):

141.5	(Lide 2003)

Boiling Point (°C):
Density (g/cm^3 at 20°C):
Molar Volume (cm^3/mol):

243.6	(calculated-Le Bas method at normal boiling point)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

21.34	(DSC method, Plato 1972)
21.50	(Ruelle & Kesselring 1997)

Entropy of fusion, ΔS_{fus} (J/mol K):
Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F: 0.0719 (mp at 141.5°C)

Water Solubility (g/m^3 or mg/L at 25°C or as indicated):

10	(20°C, Slade 1945)
15.7, 10.7	(28°C, shake flask-centrifuge, membrane filter-GC, max. 0.1 μm particle size, Kurihara et al. 1973)
11.6, 8.64	(28°C, shake flask-centrifuge, sonic and centrifuge-GC, max. 0.05 μm particle size, Kurihara et al. 1973)
8.64–31.4	(shake flask-GC, Kurihara et al. 1973)
10	(20°C, quoted, Günther et al. 1968)
21.3	(20°C, shake flask-GC, Kanazawa et al. 1971)
31.4	(generator column-GC/ECD, Weil et al. 1974)
9.01	(20°C, Deutsche Forschungsgemeinschaft 1983; Ballschmiter & Wittlinger 1991; Fischer et al. 1991)

Vapor Pressure (Pa at 25°C or as indicated. Additional data at other temperatures designated * are compiled at the end of this section):

2.67*	(20°C, static method, measured range 20–60°C, Slade 1945)
2.27×10^{-3}*	(20°C, effusion manometer, Balson 1947)
0.150	(GC-RT correlation, Watanabe & Tatsukawa 1989)
0.0309	(supercooled liquid value, Majewski & Capel 1995)

Henry's Law Constant (Pa·m^3/mol at 25°C or as indicated):

0.018	(20–25°C, Mabey et al. 1982)
0.073	(calculated-P/C, Suntio et al. 1988)
0.0825	(calculated-P_L/C_L, Majewski & Capel 1995)

Octanol/Water Partition Coefficient, log K_{OW} at 25°C or as indicated. Additional data at other temperatures designated * are compiled at the end of this section:

4.14	(shake flask-GC, Kurihara et al. 1973)
4.14	(recommended, Sangster 1993)

4.14 (recommended, Hansch et al. 1995)
4.17* ± 0.01 (shake flask-slow stirring-GC, measured range 5–45°C, Paschke & Schüürmann 1998)

Octanol/Air Partition Coefficient, log K_{OA} at 25°C and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section:

8.80*, 8.848 (gas saturation-GC/MS, calculated, measured range 5–35°C, Shoeib & Harner 2002)
log K_{OA} = –7.45 + 4856/(T/K), temp range 5–35°C (gas saturation-GC, Shoeib & Harner 2002)

Bioconcentration Factor, log BCF:

1.95	(calculated-S as per Kenaga 1980, this work)
3.21, 3.25	(*Brachydanio rerio*, flow-through conditions, Butte et al. 1991; quoted, Devillers et al. 1996)
2.45	(rainbow trout, flow-through conditions, Vigano et al. 1992; quoted, Devillers et al. 1996)
2.34; 2.44	(*Oncorhynchus mykiss*, wet wt. basis: quoted exptl.; calculated-QSAR model based on quantum chemical parameters, Wei et al. 2001)

Sorption Partition Coefficient, log K_{OC}:

2.82 (soil, calculated-S as per Kenaga 1980, this work)

Environmental Fate Rate Constants, k, or Half-Lives, $t_{½}$:

Biodegradation: calculated $t_{½}$ = 126 h in sewage sludge from experiments S1–S3 (Buser & Müller 1995).

Half-Lives in the Environment:

TABLE 18.1.1.49.1
Reported vapor pressures, octanol-water partition coefficients and octanol-water partition coefficients of δ-HCH at various temperatures

Vapor pressure				log K_{OW}		log K_{OA}	
Slade 1945		Balson 1947		Paschke & Schüürmann 1998		Shoeib & Harner 2002	
static method		effusion manometer		shake flask-GC		generator column-GC/MS	
t/°C	P/Pa	t/°C	P/Pa	t/°C	log K_{OW}	t/°C	log K_{OA}
20	2.67	0	1.213×10^{-4}	5	4.27	5	10.0436
40	12.0	10	5.466×10^{-4}	25	4.17	15	9.4587
60	45.33	20	2.266×10^{-3}	45	4.15	20	8.9251
		30	8.533×10^{-3}			25	8.7995
		40	0.02946	enthalpy of phase transfer:		35	8.4420
		50	0.09466	$\Delta H_{OW}/(kJ\ mol^{-1}) = -7.60$		25	8.848
		60	0.2780	entropy of phase transfer:			
		70	0.7866	$\Delta S_{OW}/(J\ K^{-1}\ mol^{-1}) = 69.9$		log K_{OA} = A + B/(T/K)	
						A	–7.447
		log P = A – B/(T/K)				B	4856
		eq. 1	P/mmHg				
		A	12.635			enthalpy of phase change	
		B	5100			$\Delta H_{OA}/(kJ\ mol^{-1}) = 93.0$	
		temp range: 55–75°C					

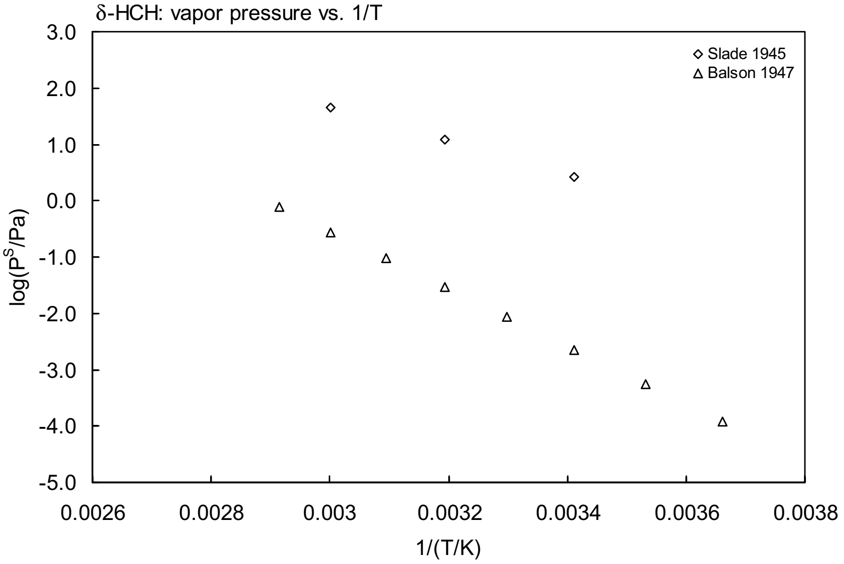


FIGURE 18.1.1.49.1 Logarithm of vapor pressure versus reciprocal temperature for δ-HCH.

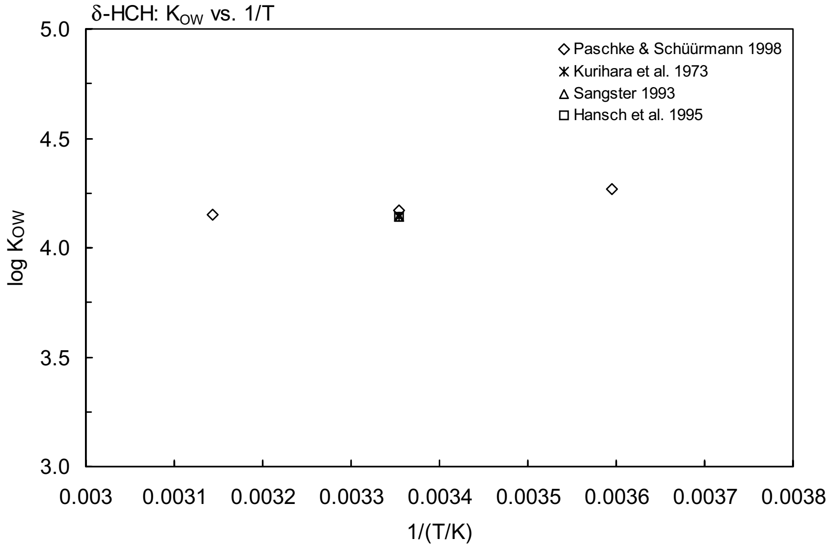


FIGURE 18.1.1.49.2 Logarithm of K_{OW} versus reciprocal temperature for δ-HCH.

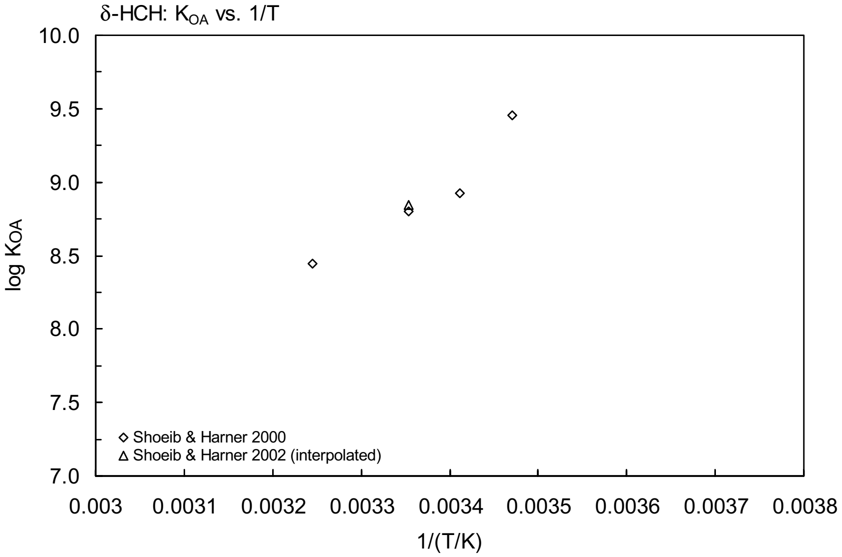
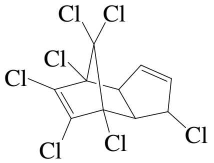


FIGURE 18.1.1.49.3 Logarithm of K_{OA} versus reciprocal temperature for δ-HCH.

18.1.1.50 Heptachlor



Common Name: Heptachlor

Synonym: Aahepta, Aathepta, Agroceres, Basaklor, 3-Chlorochlordene, Drinox, ENT 15152, Hepta, Heptachlorane, Heptagran, Heptagranox, Heptamak, Heptamul, Heptasol, Heptox, methanoindene, NA 2761, NCI-C00180, Rhodiachlor, Soleptax, Velsicol

Chemical Name: 1, 4, 5, 6, 7, 8, 8-heptachloro-3a, 4, 7, 7a-tetrahydro-4, 7-methanoindene; 3–4, 5, 6, 7, 8, 8a-heptachlorodicyclopentadiene

Uses: non-systemic insecticide with contact, stomach, and some respiratory action to control termites, ants, and soil insects in cultivated and uncultivated soils; also used to control household insects

CAS Registry No: 76-44-8

Molecular Formula: $C_{10}H_5Cl_7$

Molecular Weight: 373.318

Melting Point (°C):
95.5 (Lide 2003)

Boiling Point (°C):
135–145 (at 1–1.5 mmHg, Montgomery 1993; Tomlin 1994)

Density (g/cm^3 at 20°C):
1.65–1.67 (25°C, Hartley & Kidd 1987; Tomlin 1994)
1.66 (Montgomery 1993)

Molar Volume (cm^3/mol):
308.2 (calculated-Le Bas method at normal boiling point)

Dissociation Constant, pK_a:

Enthalpy of Vaporization, ΔH_V (kJ/mol):
73.06 (Rordorf 1989)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
22 (Rordorf 1989)
22.97 (Ruelle & Kesselring 1997)

Entropy of Fusion, ΔS_{fus} (J/mol K):

Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F: 0.203 (mp at 95.5°C)

Water Solubility (g/m^3 or mg/L at 25°C or as indicated. Additional data at other temperatures designated * are compiled at the end of this section):
0.056 (25–29°C, shake flask-GC, Park & Bruce 1968)
0.03, 0.125, 0.180* (particle size: 0.01, 0.05 & 5.0μ, shake flask-GC, measured range 15–45°C, Biggar & Riggs 1974)
0.03 (Martin & Worthing 1977; Kenaga 1980a, b; Kenaga & Goring 1980)
<1.0 (Wauchope 1978)
0.056 (Hartley & Graham-Bryce 1980; Worthing & Walker 1987; Hartley & Kidd 1987)
0.05 (Khan 1980)
0.30 (Herbicide Handbook 1983)
0.056 (25–29°C, Worthing & Hance 1991; Tomlin 1994)
0.18 (Montgomery 1993)
0.056 (20–25°C, selected, Augustijn-Beckers et al. 1994; Hornsby et al. 1996)
1.307, 1.307 (supercooled liquid: LDV derivation of literature-derived value, FAV final-adjusted value, Shen & Wania 2005)
$\log [C_L/(\text{mol m}^{-3})] = -770/(T/K) + 0.13$ (supercooled liquid, linear regression of literature data, Shen & Wania 2005)

Vapor Pressure (Pa at 25°C or as indicated or reported temperature dependence equations):
0.025 (Bowery 1964)
0.040 (Eichler 1965; Martin 1972; Quellette & King 1977)
0.021 (20°C, Hartley & Graham-Bryce 1980)
0.053 (Spencer 1982; Worthing 1983, Hartley & Kidd 1987; Worthing & Hance 1991; Tomlin 1994)
0.0213 (20°C, selected exptl. value, Kim 1985)
0.021, 0.410, 5.10, 46, 320 (25, 50, 70, 100, 125°C, gas saturation-GC, Rordorf 1989)
$\log (P_S/Pa) = 14.977 - 4966.6/(T/K)$; measured range 36.4–95.6°C (solid, gas saturation-GC, Rordorf 1989)
$\log (P_L/Pa) = 11.811 - 3816.5/(T/K)$; measured range 96.6–151°C (liquid, gas saturation-GC, Rordorf 1989)
0.031 (supercooled liquid P_L value, GC-RT correlation, Hinckley et al. 1990)
$\log (P_L/Pa) = 11.88 - 3995/(T/K)$ (supercooled liquid, GC-RT correlation, Hinckley et al. 1990)
0.022 (20°C, selected, Taylor & Spencer 1990)
0.040 (20°C, Montgomery 1993)
0.0533 (20–25°C, selected, Augustijn-Beckers et al. 1994; Hornsby et al. 1996)
0.13, 0.13 (supercooled liquid P_L: LDV literature derived value, FAV final adjusted value, Shen & Wania 2005)
$\log (P_L/Pa) = -3870/(T/K) + 12.11$ (supercooled liquid, linear regression of literature data, Shen & Wania 2005)

Henry's Law Constant (Pa·m^3/mol at 25°C or as indicated):
150 (gas stripping-GC, Warner et al. 1987)
154 (WERL Treatability Database, Ryan et al. 1988)
112 (20°C, calculated-P/C, Suntio et al. 1988)
845.4 (calculated-P/C, Jury et al. 1990)
17.8 (calculated-bond contribution method LWAPC, Meylan & Howard 1991)
233 (Montgomery 1993)
29.75 (wetted wall column-GC, Altschuh et al. 1999)
30, 38 (LDV literature-derived value, FAV final adjusted value, Shen & Wania 2005)

Octanol/Water Partition Coefficient, log K_{OW}:
5.44 (HPLC-RT correlation, Veith et al. 1979, 1980; Veith & Kosian 1983)
3.87 (quoted, Rao & Davidson 1980)
5.27 (HPLC-RT correlation, McDuffie 1981)
4.40–5.50 (Montgomery 1993)
5.27, 5.58 (quoted, Hansch et al. 1995)
6.02 (shake flask/slow stirring-GC, Simpson et al. 1995)
5.24 (RP-HPLC-RT correlation, Finizio et al. 1997)
6.10, 5.94 (LDV literature-derived value, FAV final-adjusted value, Shen & Wania 2005)

Octanol/Air Partition Coefficient, log K_{OA} at 25°C and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section:
7.705*, 7.643 (gas saturation-GC/MS, calculated, measured range 5–25°C, Shoeib & Harner 2002)
$\log K_{OA} = -3.95 + 3455/(T/K)$, temp range 5–25°C (gas saturation-GC, Shoeib & Harner 2002)
7.64, 7.76 (LDV literature-derived value, FAV final adjusted value, Shen & Wania 2005)

Bioconcentration Factor, log BCF:
–1.81 (beef biotransfer factor log B_b, correlated-K_{OW}, Kenaga 1980)
–1.48 (vegetation, correlated-K_{OW}, Lichtenstein 1960; Nash 1974)
–2.49 (milk biotransfer factor log B_m, correlated-K_{OW}, Saha 1969)
4.26 (oysters, wet wt. basis, Wilson 1963)
3.26 (bluegill, field tests, Andrews et al. 1966)
3.41 (soft clam, Butler 1971)
3.45–4.33 (estuarine fish for 96-h exposure, Schimmel et al. 1976)
3.76–3.92 (spot fish, whole body 24-d exposure, Schimmel et al. 1976)
3.67 (spot fish, edible tissue 24-d exposure, Schimmel et al. 1976)
3.58 (mosquito fish, Callahan et al. 1979)
3.56, 3.87 (spot fish for 72-h test, 96-h test. Callahan et al. 1979)

4.57, 4.32 (snails, algae, Callahan et al. 1979)
3.98, 4.30 (fathead minnow, 32-d exposure, 276-d exposure, Veith et al. 1979, 1980)
4.30 (sheepshead minnow, Veith et al. 1979)
4.24, 3.33 (fish: flowing water, static water; Kenaga 1980; Kenaga & Goring 1980)
3.65, 3.90 (estimated-S, K_{OW}, Bysshe 1982)
3.11–3.56 (earthworm, Gish & Hughes 1982)
3.98, 4.30 (fathead minnow, Veith & Kosian 1983)
4.03 (clam fat, 60-d expt., Hartley & Johnson 1983)
4.26 (oysters, Biddinger & Gloss 1984)
3.90, 3.90, 3.90 (oyster, pinfish, sheepshead minnow, Zaroogian et al. 1985)
4.30, 4.33 (measured for fathead minnow, sheepshead minnow, Zaroogian et al. 1985)
3.93 (oyster, Zaroogian et al. 1985)
3.98 (calculated, Isnard & Lambert 1988)
4.11 (selected, Chessells et al. 1992)
4.14; 4.406, 4.112 (fish, steady-state, quoted lit.; calculated-MCI χ, calculated-K_{OW}, Lu et al.1999)
4.23, 6.15 (oyster, uptake 6 months: wet wt basis, lipid wt basis, Geyer et al. 2000)
4.30, 5.85 (fathead minnow, uptake 276-d: wet wt basis, lipid wt basis, Geyer et al. 2000)
3.98; 3.67 (*Oncorhynchus mykiss*, wet wt. basis: quoted exptl.; calculated-QSAR model based on quantum chemical parameters, Wei et al. 2001)

Sorption Partition Coefficient, log K_{OC} at 25°C or as indicated:
4.48 (soil, calculated-S as per Kenaga & Goring 1978, Kenaga 1980a)
4.38 (screening model calculations, Jury et al. 1987b)
4.34 (calculated-K_{OW} as per Kenaga & Goring 1980, Chapman 1989)
3.81 (Jury et al. 1990)
5.21 (estimated-QSAR and SPARC, Kollig 1993)
4.38 (Montgomery 1993)
4.38 (20–25°C, selected, Augustijn-Beckers et al. 1994; Hornsby et al. 1996)
4.76 (soil, estimated-general model using molecular descriptors, Gramatica et al. 2000)

Environmental Fate Rate Constants, k, or Half-Lives, $t_{1/2}$:
Volatilization: measured rate constant $k = 3.0\ d^{-1}$ (Glotfelty et al. 1984; quoted, Glotfelty et al. 1989); calculated rate constant $k = 5.0\ d^{-1}$ (Glotfelty et al. 1989).
Photolysis:
Oxidation: $t_{1/2}$ = 5.2–51.7 h in air, based on estimated rate constant for the vapor-phase reaction with hydroxyl radical in air (Atkinson 1987; quoted, Howard et al. 1991).
Hydrolysis: first-order $t_{1/2}$ = 23.1 h, based on rate constant $k = 2.97 \times 10^{-2}\ h^{-1}$ at pH 7.0 and 25°C (Demayo 1972; quoted, Callahan et al. 1979; Kollig et al. 1987; Howard et al. 1991);
rate constant $k = 61\ yr^{-1}$ at pH 7.0 and 25°C (Kollig 1993)
$t_{1/2}$ = 5.4 d at pH 2, $t_{1/2}$ = 0.96 d at pH 7 in natural waters (Capel & Larson 1995)
Biodegradation: aqueous aerobic $t_{1/2}$ = 360–1567 h, based on unacclimated aerobic soil grab sample test data (Castro & Yoshida 1971; quoted, Howard et al. 1991);
rate constant $k = 0.011\ d^{-1}$ by die-away test in soil (Rao & Davidson 1980; quoted, Scow 1982);
estimated $t_{1/2}$ = 220 d in soil (Jury et al. 1990);
aqueous anaerobic $t_{1/2}$ = 1440–6268 h, based on unacclimated aerobic biodegradation half-life (Howard et al. 1991)
$t_{1/2}$(aerobic) = 15 d, $t_{1/2}$(anaerobic) = 60 d in natural waters (Capel & Larson 1995)
Biotransformation:
Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants:

Half-Lives in the Environment:
Air: $t_{1/2}$ = 9.8–59.0 h, based on estimated photooxidation half-life in air (Atkinson 1987; quoted, Howard et al. 1991);
atmospheric transformation lifetime was estimated to be <1 d (Kelly et al. 1994).

Surface water: persistence up to 2 wk in river water (Eichelberger & Lichtenberg 1971);
- $t_{½}$ = 38 d in surface waters in the Netherlands in case a first order reduction process may be assumed (Zoeteman et al. 1980)
- $t_{½}$ = 23.1–129.4 h, based on hydrolysis half-lives (Kollig et al. 1987 and Chapman & Cole 1982; quoted, Howard et al. 1991)
- Biodegradation $t_{½}$(aerobic) = 15 d, $t_{½}$(anaerobic) = 60 d, hydrolysis $t_{½}$ = 5.4 d at pH 2, $t_{½}$ = 0.96 d at pH 7 in natural waters (Capel & Larson 1995).

Ground water: $t_{½}$ = 23.1–129.4 h, based on hydrolysis half-lives (Kollig et al. 1987 and Chapman & Cole 1982; quoted, Howard et al. 1991).

Sediment:

Soil: $t_{½}$ ~ 2–5 yr persistence in soil (Nash & Woolson 1967);
- estimated persistence of 2 yr in soil (Kearney et al. 1969; Edwards 1973; quoted, Morrill et al. 1982; Jury et al. 1987a);
- Best estimated $t_{½}$ = 0.91 yr, true value is between 0.86–0.97 yr when heptachlor was incorporated to 7.5 cm depth in an experimental field (Freeman et al. 1975)
- persistence of >24 months (Wauchope 1978);
- $t_{½}$ < 10 d and subject to plant uptake via volatilization (Callahan et al. 1979; quoted, Ryan et al. 1988);
- first-order $t_{½}$ = 63 d from biodegradation rate constant k = 0.011 d^{-1} by die-away test in soil (Rao & Davidson 1980; quoted, Scow 1982);
- field $t_{½}$ = 0.3 d in moist fallow soil (Glotfelty 1981; quoted, Nash 1983);
- microagroecosystem $t_{½}$ = 3 d in moist fallow soil (Nash 1983);
- measured dissipation rate k = 0.28 d^{-1} (Nash 1983; quoted, Nash 1988);
- estimated dissipation rate k = 1.0 and 0.20 d^{-1} (Nash 1988);
- reported $t_{½}$ = 9–10 months in soil (Hartley & Kidd 1987; quoted, Montgomery 1993);
- $t_{½}$ = 23.1–129.4 h, based on hydrolysis half-lives (Kollig et al. 1987 and Chapman & Cole 1982; quoted, Howard et al. 1991);
- estimated biodegradation $t_{½}$ = 220 d in soil (Jury et al. 1990);
- selected field $t_{½}$ = 250 d (Augustijn-Beckers et al. 1994; Hornsby et al. 1996);
- $t_{½}$ = 9–10 months when used at agricultural rates (Tomlin 1994)
- $t_{½}$ = 7–14 yr in soil (Geyer et al. 2000)

Biota: biochemical $t_{½}$ = 2000 d from screening model calculations (Jury et al. 1987b).

TABLE 18.1.1.50.1
Reported aqueous solubilities and octanol-air partition coefficients of heptachlor at various temperatures

Aqueous solubility				**log K_{OA}**	
Biggar & Riggs 1974				**Shoeib & Harner 2002**	
shake flask-GC				**generator column-GC/MS**	
t/°C	**S/g·m^{-3}**	**S/g·m^{-3}**	**S/g·m^{-3}**	**t/°C**	**log K_{OA}**
particle size	0.01μ	0.05μ	5.0μ		
15			0.100	5	8.5093
25	0.030	0.125	0.180	10	8.2625
35			0.315	15	7.9873
45			0.490	20	7.7934
				25	7.7046
				25	7.643
				log K_{OA} = A + B/(T/K)	
				A	−3.951
				B	3455
				enthalpy of phase change	
				ΔH_{OA}/(kJ mol^{-1}) = 66.2	

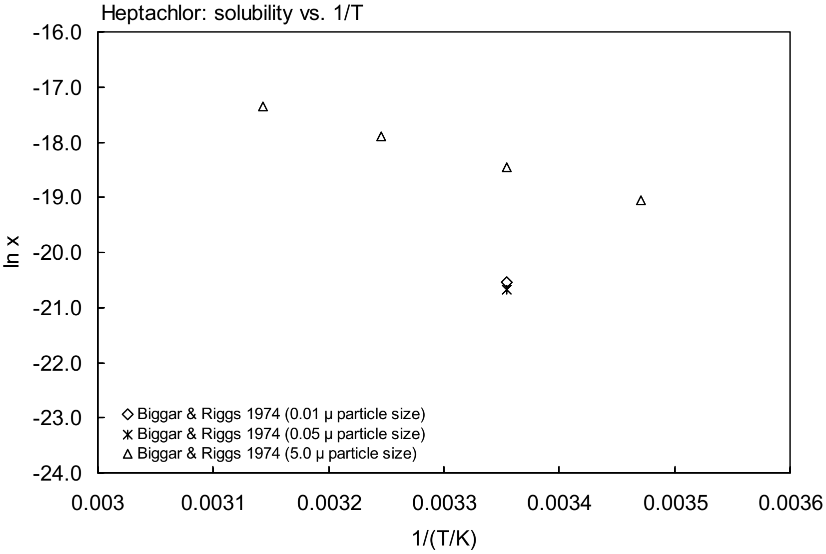


FIGURE 18.1.1.50.1 Logarithm of mole fraction solubility (ln *x*) versus reciprocal temperature for heptachlor.

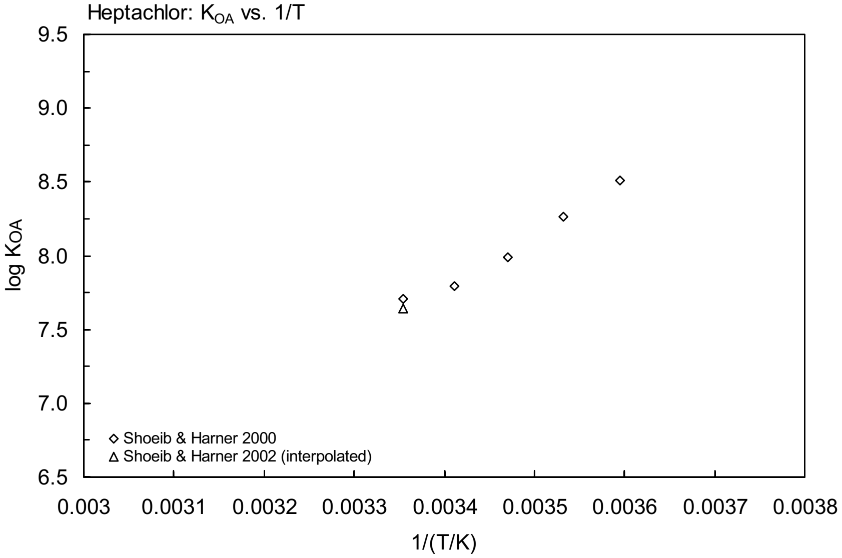
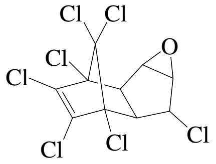


FIGURE 18.1.1.50.2 Logarithm of K_{OA} versus reciprocal temperature for heptachlor.

18.1.1.51 Heptachlor epoxide



Common Name: Heptachlor epoxide
Synonym: β-Heptachlorepoxide, Epoxyheptachlor, HCE, Velsicol 53-CS-17
Chemical Name: 1,4,5,6,7,8,8-heptachloro-2,3-epoxy-3a,4,7,7*a*-tetrahydro-4,7-methanoindan; 2,3,4,5,7,8-hexa-hydro-2, 5-methano-2*H*-indeno(1,2*b*)oxirene
Uses: a degradation product of heptachlor
CAS Registry No: 1024-57-3
Molecular Formula: $C_{10}H_5Cl_7O$
Molecular Weight: 389.317
Melting Point (°C):
160 (Lide 2003)
Boiling Point (°C):
Density (g/cm^3 at 20°C):
Molar Volume (cm^3/mol):
317.2 (calculated-Le Bas method at normal boiling point)
Dissociation Constant, pK_a:
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
21.506 (Ruelle & Kesselring 1997)
Entropy of Fusion, ΔS_{fus} (J/mol K):
61.56 (Plato 1972)
Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F: 0.0474 (mp at 160°C)

Water Solubility (g/m^3 or mg/L at 25°C or as indicated. Additional data at other temperatures designated * are compiled at the end of this section):
0.035 (25–29°C, shake flask-GC, Park & Bruce 1968)
0.025, 0.120, 0.20* (shake flask-GC, particle size: 0.01, 0.05 and 5.0μ, measured range 15–45°C, Biggar & Riggs 1974)
0.35 (generator column-GC/ECD, Weil et al. 1974)
0.20–0.35 (Mills et al. 1982; Mabey et al. 1982)
0.90 (Zaroogian et al. 1985)
0.275 (Montgomery 1993)
5.91 (supercooled liquid value, 20–25°C, Majewski & Capel 1995)
0.60, 0.0004 (predicted-molar volume, mp and mobile order thermodynamics, Ruelle & Kesselring 1997)
7.0, 5.06 (supercooled liquid: LDV derivation of literature-derived value, FAV final-adjusted value, Shen & Wania 2005)

Vapor Pressure (Pa at 25°C or as indicated):
0.045 (estimated, Mabey et al. 1982)
0.00256 (estimated, Howard 1991)
3.47×10^{-4} (20°C, Montgomery 1993)
0.0997 (supercooled liquid value, 20–25°C, Majewski & Capel 1995)
0.013, 0.022 (supercooled liquid P_L: LDV literature derived value, FAV final adjusted value, Shen & Wania 2005)

Henry's Law Constant (Pa m^3/mol at 25°C or as indicated):
395 (calculated-P/C, Mabey et al. 1982)
3.42 (gas-stripping, Warner et al. 1987)
3.25 (Montgomery 1993)
65.5 (20–25°C, Majewski & Capel 1995)

2.13 (wetted-wall column-GC, Altschuh et al. 1999)
2.1, 1.7 (LDV literature-derived value, FAV final adjusted value, Shen & Wania 2005)

Octanol/Water Partition Coefficient, log K_{OW}:
4.43 (Briggs 1981)
5.40 (HPLC-RT correlation, Veith et al. 1979)
4.56 ± 0.05 (shake flask, Noegrohati & Hammers 1992)
3.65 (Montgomery 1993)
5.40, 5.42 (LDV literature-derived value, FAV final-adjusted value, Shen & Wania 2005)

Octanol/Air Partition Coefficient, log K_{OA}:
8.62, 8.59 (LDV literature-derived value, FAV final-adjusted value, Shen & Wania 2005)

Bioconcentration Factor, log BCF:
3.30, 4.90, 3.78 (algae, snail, mosquito-microcosm expt., Lu & Metcalf 1975)
3.23 (mussel, Ernst 1977)
4.16 (fathead minnows, 32-d flow-through aquarium, Veith et al. 1979)
2.03 (microorganism, calculated-K_{OW}, Mabey et al. 1982)
3.37 (clam fat, 60-d expt., Hartley & Johnson 1983)
2.93 (oyster, Zaroogian et al. 1985)
3.87, 3.89 (sheepshead minnow, pinfish, mussel and oyster, Zaroogian et al. 1985)
–1.45 (beef biotransfer factor log B_b, correlated-K_{OW}, Travis & Arms 1988)
3.88 (calculated-K_{OW}, Howard 1991)
>4.16, >5.14(fathead minnow, uptake 32-d: wet wt basis, lipid wt basis, Geyer et al. 2000)
4.16; 4.10 (*Oncorhynchus mykiss*, wet wt. basis: quoted exptl.; calculated-QSAR model based on quantum chemical parameters, Wei et al. 2001)

Sorption Partition Coefficient, log K_{OC}:
2.34 (sediment, calculated-K_{OW}, Mabey et al. 1982)
2.00 (bentonite clay, Hill & McCarty 1967)
4.0–4.3 (suspended solids in river, Frank 1981)
3.89 (calculated-S, Howard 1991)
4.32 (calculated, Montgomery 1993)
3.98 (activated carbon-water, Blum et al. 1994)

Environmental Fate Rate Constants, k, or Half-Lives, $t_{1/2}$:
Volatilization: $t_{1/2}$ = 60 h from a model river (Howard 1991).
Photolysis:
Oxidation: oxidation rate Constants, $k < 3600\ M^{-1}\ h^{-1}$ for reaction with singlet oxygen, and $k = 20\ M^{-1}\ h^{-1}$ for reaction with peroxy radical (Mabey et al. 1982)
$t_{1/2}$ = 6–60 h, based on estimated photooxidation half-life in air (Howard et al. 1991)
Hydrolysis: not expected to be important (Howard et al. 1991)
Biodegradation: $t_{1/2}$ ~ 25 d under anaerobic conditions when incubated with thick digester sludge at 35°C (Howard 1991)
$t_{1/2}$(aerobic) = 792–13248 h, based on aerobic soil grab sample data; $t_{1/2}$(anaerobic) = 24–168 h, based on soil and freshwater mud grab sample data (Howard et al. 1991)
$t_{1/2}$(aerobic) = 33 d, $t_{1/2}$(anaerobic) = 1 d in natural waters (Capel & Larson 1995)
Biotransformation: rate constant for bacterial transformation in water $k = 3 \times 10^{-12}$ mL cell^{-1} h^{-1} (Mabey et al. 1982).
Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants:

Half-Lives in the Environment:
Air: estimated $t_{1/2}$ = 1.5 d for vapor-phase reaction with photochemically produced hydroxyl radical (Howard 1991)
$t_{1/2}$ = 6–60 h, based on estimated photooxidation half-life in air (Howard et al. 1991)
Surface water: $t_{1/2}$ = 35 d in lower Rhine River in case a first order reduction process may be assumed (Zoeteman 1980)

$t_{½}$ = 792–13248 h, based on estimated unacclimated aqueous aerobic biodegradation half-life (Howard et al. 1991)

biodegradation $t_{½}$(aerobic) = 33 d, $t_{½}$(anaerobic) = 1 d in natural waters (Capel & Larson 1995)

Ground water: $t_{½}$ = 24–26496 h, based on estimated unacclimated aqueous aerobic and anaerobic biodegradation half-lives (Howard et al. 1991)

Sediment:

Soil: $t_{½}$ = 792–13248 h, based on aerobic soil grab sample data (Howard et al. 1991)

$t_{½}$ ~ 3 yr in soil (Geyer et al. 2000)

Biota:

TABLE 18.1.1.51.1
Reported aqueous solubilities of heptachlor epoxide at various temperatures

	Biggar & Riggs 1974		
	shake flask-GC		
t/°C	S/g·m^{-3}	S/g·m^{-3}	S/g·m^{-3}
particle size	0.01µ	0.05µ	5.0µ
15			0.110
25	0.025	0.120	0.200
35			0.350
45			0.600

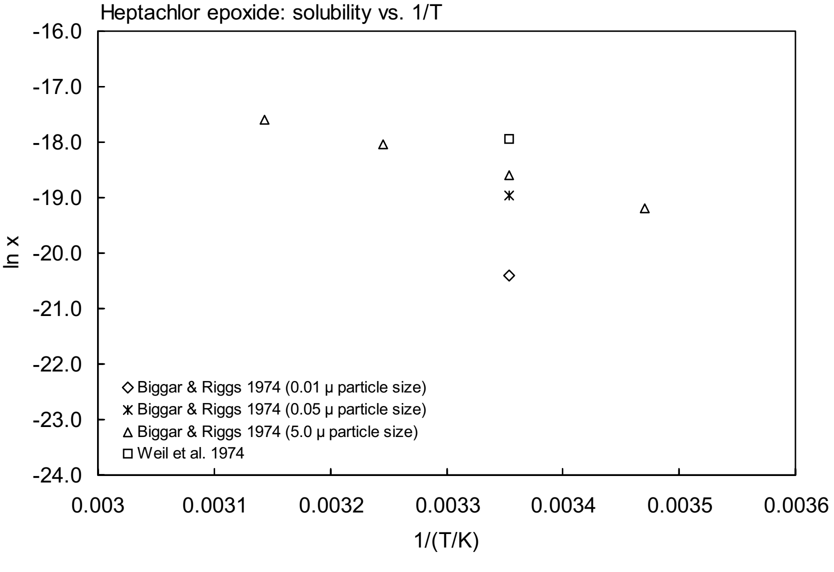
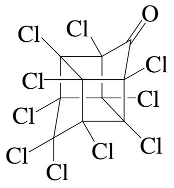


FIGURE 18.1.1.51.1 Logarithm of mole fraction solubility (ln *x*) versus reciprocal temperature for heptachlor epoxide.

18.1.1.52 Kepone



Common Name: Kepone
Synonym: Chlordecone, CIBA 8514
Chemical Name: 1,2,3,4,5,5,6,7,9,10,10-dodecachlorooctahydro-1,3,4-metheno-2-cyclobuta-[*c,d*]-pentalone
CAS Registry No: 143-50-0
Uses: Insecticide/Fungicide
Molecular Formula: $C_{10}Cl_{10}O$
Molecular Weight: 490.636
Melting Point (°C):
  350 (dec. Howard 1991; Montgomery 1993; Lide 2003)
Boiling Point (°C):
Density (g/cm^3 at 20°C):
Molar Volume (cm^3/mol):
  369.9 (calculated-Le Bas method at normal boiling point)
Dissociation Constant, pK_a:
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
Entropy of Fusion, ΔS_{fus} (J/mol K):
Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F: 6.5×10^{-4} (mp at 350°C)

Water Solubility (g/m^3 or mg/L at 25°C or as indicated):
  4.0 (100°C, Günther et al. 1968)
  2.7 (quoted Weil 1978 unpublished result, Kilzer et al. 1979)
  3.0 (20°C, Kenaga & Goring 1978, Kenaga 1980)
  7.6 (24°C, shake flask-nephelometry/fluo., Hollifield 1979; quoted, Howard 1991; Montgomery 1993)

Vapor Pressure (Pa at 25°C):
  3.0×10^{-5} (Kilzer et al. 1979; quoted, Howard 1991; Montgomery 1993)

Henry's Law Constant (Pa·m^3/mol):
  0.00153 (calculated-P/C, Howard 1991)
  0.00311 (calculated-P/C, Montgomery 1993)
  0.00140 (calculated-P/C, this work)

Octanol/Water Partition Coefficient, log K_{OW}:
  5.50 (Di Toro 1985)
  5.41 (shake flask, log P database, Hansch & Leo 1987)
  4.07 (calculated, Montgomery 1993)
  5.41 (recommended, Sangster 1993)
  5.44 (selected, Hansch et al. 1995)

Bioconcentration Factor, log BCF:
  4.04 (shrimp, 10–20 d exposure, Bahner et al. 1979)
  3.92 (Kenaga & Goring 1980)
  4.0, 2.65, 2.76 (sludge, algae, golden ide, Freitag et al. 1985)
  3.84 (oyster, Zaroogian et al. 1985)
  4.39, 4.46 (oyster, calculated-K_{OW} & models, Zaroogian et al. 1985)

4.39, 4.47 (sheephead minnow, calculated-K_{OW} & models, Zaroogian et al. 1985)
3.85 (Spot *Leiostomus xanthurus*, 19-d uptake and 28-d clearance studies, Fisher et al. 1986)
4.11 (grass shrimp *Palaemonetes pugio*, 16-d uptake and 21-d clearance studies, Fisher & Clark 1990)
3.04–3.34 (fathead minnow, quoted, Howard 1991)
3.19, 3.09, 2.84, 0.91 (*Cyprinodon variegatus, Leiostomus xanthrus, Palaemonetes pugio, Callinetes sapidus*, quoted, Howard 1991)
3.36–3.99 (Atlantic menhaden, Howard 1991)
4.34–4.78 (Atlantic silversides, Howard 1991)

Sorption Partition Coefficient, log K_{OC}:
3.38–3.41 (calculated, Howard 1991)
4.74 (calculated, Montgomery 1993)

Environmental Fate Rate Constants, k, or Half-Lives, $t_{½}$:

Volatilization: $t_{½}$ = 3.8–46 yr predicted for evaporation from a river 1 m deep, flowing at 1 m/s with a wind velocity of 3 m/s (Howard 1991).

Photolysis: indefinite in air (Howard et al. 1991).

Oxidation:

Hydrolysis: no hydrolyzable group (Howard et al. 1991).

Biodegradation: aerobic aqueous $t_{½}$ = 7488 to 17,280 h (312 d to 2 yr), based on aerobic aquatic microcosm study, anaerobic $t_{½}$ = 29,952–69,120 h (1248 d to 8 yr) based on unacclimated aerobic biodegradation half-life (Howard et al. 1991).

Biotransformation:

Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants:

Kinetic data of spot *Leiostomus xanthurus* in 19-d uptake and 28-d clearance studies (Fisher et al. 1986)
k_1 = 0.273 d^{-1}; k_2 = 0.037 d^{-1} with $t_{½}$ = 18.7 d, uncontaminated water + 4% ration contaminated food,
k_1 = 217.3 d^{-1}; k_2 = 0.03 d^{-1} with $t_{½}$ = 23.5 d, contaminated water + 4% ration uncontaminated food,
k_1 = 0.265 d^{-1}; k_2 = 0.037 d^{-1} with $t_{½}$ = 18.7 d, uncontaminated water + 8% ration contaminated food,
k_1 = 185.5 d^{-1}; k_2 = 0.027 d^{-1} with $t_{½}$ = 25.5 d, contaminated water + 8% ration uncontaminated food,
k_1 = 0.262 d^{-1}; k_2 = 0.032 d^{-1} with $t_{½}$ = 21.5 d, contaminated food (4% ration) then water,
k_1 = 214 d^{-1}; k_2 = 0.023 d^{-1} with $t_{½}$ = 29.9 d, contaminated water then food (a 4% ration)
k_1 = 0.292 d^{-1}; k_2 = 0.043 d^{-1} with $t_{½}$ = 16.2 d, contaminated food (a 8% ration) then water,
k_1 = 154 d^{-1}; k_2 = 0.020 d^{-1} with $t_{½}$ = 35.4 d, contaminated water then food (a 8% ration)

Kinetic data of grass shrimps in 16-d uptake and 21-d clearance studies (Fisher & Clark 1990)
k_1 = 0.475 d^{-1}; k_2 = 0.017 d^{-1} with $t_{½}$ = 28 d, uncontaminated water + 4% ration contaminated food,
k_1 = 175 d^{-1}; k_2 = 0.014 d^{-1} with $t_{½}$ = 47.8 d, contaminated water + 4% ration uncontaminated food,
k_1 = 0.499 d^{-1}; k_2 = 0.019 d^{-1} with $t_{½}$ = 36.3 d, contaminated food (4% ration) then water,
k_1 = 182 d^{-1}; k_2 = 0.013 d^{-1} with $t_{½}$ = 51.5 d, contaminated water then food (a 4% ration)
k_1 = 0.399 d^{-1}; k_2 = 0.021 d^{-1} with $t_{½}$ = 32.3 d, contaminated food (a 8% ration) then water,
k_1 = 170 d^{-1}; k_2 = 0.011 d^{-1} with $t_{½}$ = 63.7 d, contaminated water then food (a 4% ration)

Half-Lives in the Environment:

Air: estimated $t_{½}$ = 438,000 to 4.2 × 10^7 h or 50–200 yr (Howard et al. 1991).

Surface water: $t_{½}$ = 7488 to 17,280 h or 312 d to 2 yr, based on aerobic aquatic microcosm study of soil and water grab samples (Howard et al. 1991).

Ground water: estimated $t_{½}$ = 14,976 to 34,560 h (624 d to 4 yr) based on aqueous aerobic biodegradation (Howard et al. 1991).

Sediment:

Soil: estimated $t_{½}$ = 7488 to 17,280 h (312 d to 2 yr) based on aerobic aquatic microcosm study (Howard et al. 1991).

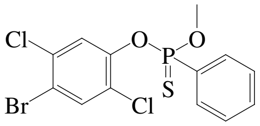
Biota: clearance $t_{½}$ = 28 d (shrimp, 10–20 d exposure, Bahner 1977

Clearance $t_{½}$ = 16.2–35.4 d for spot *Leiostomus xanthurus* (Fisher et al. 1986):
$t_{½}$(4W) = 18.7 d for kepone contaminated water + uncontaminated food at 4% ration
$t_{½}$(4F) = 23.5 d for uncontaminated water + kepone contaminated food at 4% ration

$t_{½}$(8W) = 18.7 d for kepone contaminated water + uncontaminated food at 8% ration,
$t_{½}$(8F) = 25.5 d for uncontaminated water + kepone contaminated food at 8% ration
$t_{½}$(4FW-food) = 21.5 d for dietary accumulation in combined exposure (food-water) at 4% ration
$t_{½}$(4FW-water) = 29.9 d for dietary accumulation in combined exposure (water-food) at 4% ration
$t_{½}$(8FW-food) = 16.2 d for dietary accumulation in combined exposure (food-water) at 8% ration
$t_{½}$(8FW-water) = 35.4 d for dietary accumulation in combined exposure (water-food) at 8% ration

Clearance $t_{½}$ = 32.3–63.7 d for grass shrimps *Palaemonetes pugio* (Fisher & Clark 1990):
$t_{½}$(4W) = 47.8 d for kepone contaminated water + uncontaminated food at 4% ration
$t_{½}$(4F) = 40.6 d for uncontaminated water + kepone contaminated food at 4% ration
$t_{½}$(4FW-food) = 36.3 d for dietary accumulation in combined exposure (food-water) at 4% ration
$t_{½}$(4FW-water) = 51.5 d for dietary accumulation in combined exposure (water-food) at 4% ration
$t_{½}$(8FW-food) = 32.3 d for dietary accumulation in combined exposure (food-water) at 8% ration
$t_{½}$(8FW-water) = 63.7 d for dietary accumulation in combined exposure (water-food) at 8% ration

18.1.1.53 Leptophos



Common Name: Leptophos
Synonym: Abar, Phosvel, VCS-506
Chemical Name: *O*-(4-bromo-2,5-dichlorophenyl) *O*-methyl phenylphosphorothioate
Uses: insecticide
CAS Registry No: 21609-90-5
Molecular Formula: $C_{13}H_{10}BrCl_2O_2PS$
Molecular Weight: 412.066
Melting Point (°C):

71	(Lide 2003)

Boiling Point (°C):
Density (g/cm^3 at 20°C):

1.53	(25°C, Merck Index 1989)

Molar Volume (cm^3/mol):

317.8	(calculated-Le Bas method at normal boiling point)
269.3	(calculated-density)

Dissociation Constant, pK_a:
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
Entropy of Fusion, ΔS_{fus} (J/mol K):
Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F: 0.354 (mp at 71°C)

Water Solubility (g/m^3 or mg/L at 25°C or as indicated):

0.03	(shake flask-UV, Carringer et al. 1975)
0.03	(20°C, GC, Freed 1976)
0.0047	(20°C, shake flask-GC, Chiou et al. 1977)
2.4	(Martin & Worthing 1977; Kenaga 1980; Kenaga & Goring 1980; Khan 1980)
0.07	(20°C, shake flask-GC, Bowman & Sans 1979)
0.0047	(20–25°C, shake flask-GC, Freed et al. 1979)
0.005	(20–25°C, shake flask-GC, Kanazawa 1981)
0.021	(20°C, shake flask-GC, Bowman & Sans 1983a, b)
0.03	(Budavari 1989)

Vapor Pressure (Pa at 25°C or as indicated):

3.07×10^{-6}	(20°C, NIEHS 1975; quoted, Freed et al. 1977)
2.27×10^{-5}	(30°C, NIEHS 1975; quoted, Freed et al. 1977)
3.07×10^{-6}	(20–25°C, Freed et al. 1979)
3.00×10^{-6}	(20°C, selected, Suntio et al. 1988)
0.0002	(Merck Index 1989)

Henry's Law Constant ($Pa{\cdot}m^3/mol$ at 25°C or as indicated):

0.27	(20°C, calculated-P/C, Mackay & Shiu 1981)
0.25	(20°C, calculated-P/C, Suntio et al. 1988)

Octanol/Water Partition Coefficient, log K_{OW}:

6.30	(NIEHS 1975; quoted, Freed et al. 1977)
6.31	(20°C, shake flask-GC, Chiou et al. 1977)
6.31	(Hansch & Leo 1979)
4.32	(20°C, shake flask-GC, Kanazawa 1981)

5.88	(22°C, shake flask-GC, Bowman & Sans 1983b)
6.31	(recommended, Hansch et al. 1995)

Bioconcentration Factor, log BCF:

2.81	(*Daphnia magna*, wet wt. basis, Macek et al. 1979)
2.88, 3.16	(fish: flowing water, static water; Kenaga 1980; Kenaga & Goring 1980)
2.58, 2.86	(calculated-S, calculated-K_{OC}, Kenaga 1980)
3.78	(*Pseudorasbora parva*, Kanazawa 1981)
3.16	(mosquito fish, wet wt. basis, De Bruijn & Hermens 1991)
3.78	(topmouth gudgeon, wet wt. basis, De Bruijn & Hermens 1991)
2.88	(fish, reported as log BAF_W, LeBlanc 1995)

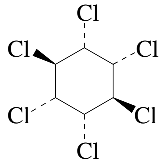
Sorption Partition Coefficient, log K_{OC}:

3.97	(soil, Carringer et al. 1975)
3.43	(soil, calculated-S as per Kenaga & Goring 1978, Kenaga 1980)
3.97, 4.45	(reported as log K_{OM}, estimated as log K_{OM}, Magee 1991)
4.50	(soil, calculated-MCI $^1\chi$, Sabljic et al. 1995)
3.88, 4.74	(soil, estimated-class-specific model, estimated-general model, Gramatica et al. 2000)

Environmental Fate Rate Constants, k, or Half-Lives, $t_{1/2}$:

Half-Lives in the Environment:

18.1.1.54 Lindane (γ-HCH)



Common Name: Lindane (γ-HCH)

Synonym: Aalindan, Aficide, Agrisol G-20, Agrocide, Agronexit, Ambocide, Ameisenatod, Ameisenmittelmerck, Aparacin, Aparasin, Aphtiria, Aplidal, Arbitex, BBX, Ben-hex, Bentox 10, Benzenehexachloride, Benzex, Bexol, BHC, γ-BHC, Celanex, Chloran, Chloresene, Codechine, DBH, Detmol-extrakt, Detox 25, Devoran, Dolmix, ENT 7796, Entomoxan, Exagama, Forlin, Gallogama, Gamacid, Gamaphex, Gamene, Gamiso, Gamahexa, Gamalin, Gammexane, Gammopaz, Gexane, HCCH, Gyben, HCCH, HCH, γ-HCH, Heclotox, Hexa, Hexachlor, γ-Hexachlor, Hexachloran, γ-Hexachloran, Hexachlorane, γ-Hexachlorane, γ-Hexachlorobenzene, Hexamul, Hexapurdre, Hexatox, Hexaverm, Hexdow, Hexicide, Hexyclan, HGI, Hortex, Inexit, Isaton, Isotox, Jacutin, Kokotine, Kotol, Kwell, Lendine, Lentox, Lidenal, Lindafor, Lindagam, Lindagrain, Lindagranox, γ-Lindine, Lindapoudre, Lindatox, Lindosep, Lintox, Lorexane, Milbol 49, Mszycol, NA 2761, NCI-C00204, Neo-scabicidol, Nexen FB, Nexit, Nexit-stark, Nexol-E, Nicochloran, Novigam, Omnitox, Ovadziak, Owadziak, Pedraczak, Pflanzol, Quellada, Silvanol, Soprocide, Spritz-rapidin, Spruehpflanzol, Streunex, Tap 85, TBH, Tri-6, Viton

Chemical Name: 1,2,3,4,5,6-hexachlorocyclohexane; γ-hexachlorocyclohexane; γ-1,2,3,4,5,6-hexachloro-cyclohexane; 1α,2α,3β,4α,5α,6β-1,2,3,4,5,6-hexachloro-cyclohexane

Uses: insecticide and pesticide with contact, stomach, and respiratory action to control a broad spectrum of phytophagous and soil inhibiting insects, public health pests, and animal ectoparasites.

CAS Registry No: 58-89-9

Molecular Formula: $C_6H_6Cl_6$

Molecular Weight: 290.830

Melting Point (°C):

112.5	(Slade 1945; Howard 1991; Montgomery 1993; Milne 1995; Lide 2003)

Boiling Point (°C):

323.4	(Howard 1991; Montgomery 1993; Lide 2003)

Density (g/cm^3 at 20°C):

1.87	(Montgomery 1993)

Molar Volume (cm^3/mol):

243.6	(calculated-Le Bas method at normal boiling point)

Enthalpy of Vaporization, ΔH_V (kJ/mol):

101.13	(Spencer & Cliath 1970)
76	(Rordorf 1989)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

22.4	(Rordorf 1989)
22.13	(Ruelle & Kesselring 1997)

Entropy of Fusion, ΔS_{fus} (J/mol K):

41.4	(Plato & Glasgow 1969)
58.0	(Rordorf 1989)
61.1	(Hinckley et al. 1990; Passivirta et al. 1999)

Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F:

0.12	(20°C, Suntio et al. 1988)
0.138	(Mackay et al. 1986)

Water Solubility (g/m^3 or mg/L at 25°C or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):

10	(20°C, Slade 1945; Günther et al. 1968; Spencer 1973, 1982)
7.3*	(shake flask-UV spectrophotometry, measured range 25–45°C, Richardson & Miller 1960)
0.50–6.60	(particle size of 0.04–5μ, shake flask-GC, room temp., Robeck et al. 1965)
5.7	(partition coefficient, Atkins & Eggleton 1971)

7.52 ± 0.041 (shake flask-centrifuge/GC, Masterton & Lee 1972)
7.40, 5.75 (28°C, shake flask-centrifuge, membrane filter-GC, maximum 0.1 µm particle size, Kurihara et al. 1973)
6.61, 6.24 (28°C, shake flask-centrifuge, sonic and centrifuge-GC, max. 0.05 µm particle size, Kurihara et al. 1973)
12 (26.5°C, Bhavnagary & Jayaram 1974)
0.15*, 0.60*, 6.80* (shake flask-GC, for different particle sizes: 0.01µ, 0.05µ, 5.0µ, measured range 15–45°C, Biggar & Riggs 1974)
7.8 (generator column-GC/ECD, Weil et al. 1974)
0.15 (Martin & Worthing 1977; Hartley & Kidd 1987; Tomlin 1994; Milne 1995)
2.0 (shake flask-nephelometry, Hollifield 1979)
7.88 (20–25°C, shake flask-GC, Kanazawa 1981)
6.50, 9.20 (15, 25°C, shake flask method, average values of 6–7 laboratories, OECD 1981)
10 (20–25°C, shake flask-GC, Platford 1981)
10.3 (shake flask-GC/ECD, Malaiyandi et al. 1982)
9.50, 7.9–8.2 (shake flask-GC/ECD: Milli-Q water, environmental surface waters, Saleh et al. 1982)
6.11 (20°C, Deutsche Forschungsgemeinschaft 1983; Ballschmiter & Wittlinger 1991; Fischer et al. 1991; 1993)
7.87 (24°C, shake flask-GC, Chiou et al. 1986)
7.0 (20–25°C, selected, Wauchope et al. 1992; Hornsby et al. 1996)
$\log [S_L/(\text{mol/L})] = 2.220 - 1237/(T/K)$ (liquid, Passivirta et al. 1999)
67.77, 71.84 (supercooled liquid S_L: derivation of literature-derived value, final-adjusted value, Xiao et al. 2004)
$\log [S_L/(\text{mol m}^{-3})] = -749.8/(T/K) + 2.78$ (supercooled liquid, linear regression of literature data, Xiao et al. 2004)
$\log [S_L/(\text{mol m}^{-3})] = -788.4/(T/K) + 2.04$ (supercooled liquid, final adjusted eq., Xiao et al. 2004)

Vapor Pressure (Pa at 25°C or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):

4.0, 18.7, 64 (20, 40, 60°C static method, Slade 1945)
0.001253* (20°C, effusion manometer, measured range 0–90°C, Balson 1947)
$\log (P/\text{mmHg}) = 15.515 - 6020/(T/K)$; temp range 50–90°C, (effusion manometer, Balson 1947)
0.00435* (20°C, gas-saturation-GC, measured range 20–40°C, Spencer & Cliath 1970)
$\log (P/\text{mmHg}) = 13.544 - 5288/(T/K)$, temp range 20–40°C (gas saturation-GC, Spencer & Cliath 1970)
0.00413 (20°C, Partition coefficient, Atkins & Eggleton 1971)
0.0213 (20°C, Demozay & Marechal 1972)
0.00125 (20°C, Martin 1972, Melnikov 1971, Spencer 1973; Montgomery 1993)
0.0028 (20°C, estimated from diffusion rate, Zimmerli & Marek 1974)
0.0026 (20°C, estimated-relative loss rate, Dobbs & Grant 1980)
0.00426 (20°C, volatilization rate, Burkhard & Guth 1981)
$\log (P/\text{mmHg}) = 15.515 - 6020/(T/K)$ (Gückel et al. 1982)
0.166 (GC-RT correlation, Watanabe & Tatsukawa 1989)
0.0056 (20°C, Hartley & Kidd 1987; Worthing & Walker 1987, Worthing & Hance 1991; Tomlin 1994)
0.107, 0.0654 (P_{GC} by GC-RT correlation, different stationary phases, Bidleman 1984)
0.0552 (supercooled liquid P_L, converted from literature P_S with ΔS_{fus} Bidleman 1984)
0.00321; 0.00368 (20°C, gas saturation-GC, gas saturation-mixed bed-GC, Kim 1985)
0.00435 (20°C, GC-RT correlation, Kim 1985)
6.70×10^{-3}* (gas saturation-GC, measured range 25–125°C, Rordorf 1989)
$\log (P_S/\text{Pa}) = 15.096 - 5148.9/(T/K)$; measured range 45–113°C (solid, gas saturation-GC, Rordorf 1989)
$\log (P_L/\text{Pa}) = 12.05 - 3970.1/(T/K)$; measured range 115–171°C (liquid, gas saturation-GC, Rordorf 1989)
0.0552, 0.0649 (supercooled P_L, converted from literature P_S with different ΔS_{fus} values, Hinckley et al. 1990)
0.107, 0.0706 (P_{GC} by GC-RT correlation with different reference standards, Hinckley et al. 1990)
$\log (P_L/\text{Pa}) = 11.15 - 3680/(T/K)$ (GC-RT correlation, supercooled liquid P_L, Hinckley et al. 1990; quoted, Boehncke et al. 1996))
7.426×10^{-4} (Howard 1991)
0.0044 (20–25°C, selected, Wauchope et al. 1992; Hornsby et al. 1996)

0.0145, 0.0398, 0.1035 (supercooled liquid values at 10°C, 20°C, 30°C, calculated from Hinckley et al. 1990; Cotham & Bildeman 1992)
0.0094* (20°C, gas saturation-GC/ECD, measured range –30 to 30°C, Wania et al. 1994; quoted, Boehncke et al. 1996)
log (P_S/Pa) = 16.99 – 5566/(T/K), temp range –30 to + 30°C (solid, gas saturation-GC, Wania et al. 1994)
0.00737* (Knudsen effusion method, measured range 19.63–53.07°C, Boehncke et al. 1996)
0.00383 (20°C, interpolated from vapor pressure eq. ln (P/Pa) = (34.53 ± 0.21) – (11754 ± 72)/(T/K), temp range 20–50°C, Boehncke et al. 1996)
0.0104* (torsion and Knudsen-effusion methods, measured range 310–384 K, Giustini et al. 1998)
log (P/kPa) = (11.23 ± 0.50) – (4832 ± 150)/(T/K); temp range 310–384 K (torsion and Knudsen-effusion methods, Giustini et al. 1998)
0.189, 0.131; 0.0167 (quoted supercooled liquid P_L: calculated, GC-RT correlation; converted to solid P_S with fugacity ratio F, Passivirta et al. 1999)
log (P_L/Pa) = 13.80 – 4330/(T/K), (supercooled liquid, Passivirta et al. 1999)
0.0776, 0.0759 (supercooled liquid P_L: LDV literature derived value, FAV final adjusted value, Xiao et al. 2004)
log (P_L/Pa) = –3890/(T/K) + 11.94 (supercooled liquid, linear regression of literature data, Xiao et al. 2004)
log (P_L/Pa) = –3905/(T/K) + 11.98 (supercooled liquid, final adjusted eq., Xiao et al. 2004)

Henry's Law Constant (Pa·m^3/mol or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):

0.005 (calculated-P/C, Mackay & Leinonen 1975)
0.22 (gas stripping, Atkins & Eggleton 1971)
0.32 (24°C, calculated-P/C, Chiou et al. 1980)
0.018–0.55 (calculated-P/C, Mabey et al. 1982)
0.124 (20°C, volatilization rate, Burkhard & Guth 1981)
0.27–0.32 (calculated-P/C, Mackay & Shiu 1981)
0.05 (calculated-P/C, Lyman et al. 1982; quoted, Suntio et al. 1988)
0.0486 (calculated-P/C, Thomas 1982)
0.322 (calculated-P/C, Jury et al. 1984, 1987a; Jury & Ghodrati 1989)
0.158 (calculated-P/C, Mackay et al. 1986)
0.202, 0.234 (23°C, wetted-wall column-GC/ECD, Fendinger & Glotfelty 1988)
1.49 (WERL Treatability Database, Ryan et al. 1988)
0.129 (20°C, calculated-P/C, Suntio et al. 1988)
0.322 (calculated-P/C, Taylor & Glotfelty 1988)
0.199, 0.209 (22–24°, fog chamber-concentration ratio-GC/ECD, Fendinger et al. 1989)
0.0486 (20°C, Lyman et al. 1990; quoted, Hemond & Fechner 1994)
0.10 (calculated-P/C, Ballshmiter & Wittlinger 1991; Fischer et al. 1991)
0.296 (calculated-P/C, Howard 1991)
0.353* (distilled water, gas stripping-GC/ECD, measured range 0.5–45°C, Kucklick et al. 1991)
log [H/(Pa·m^3 mol^{-1})] = –2382/(T/K) + 7.54, temp range: 0.5–45°C (gas stripping-GC/ECD, Kucklick et al. 1991, McConnell et al. 1993)
0.0627, 0.137, 0.363, 0.996, 2.57 (0.5, 10, 23, 35, 45°C, gas stripping-GC/ECD, artificial seawater, Kucklick et al. 1991)
log [H/(Pa·m^3 mol^{-1})] = –2703/(T/K) + 8.68; temp range 0.5–45°C (gas stripping-GC/ECD, artificial seawater, Kucklick et al. 1991)
0.17 (calculated-P/C, Calamari et al. 1991)
0.10, 1.50 (calculated-P/C, Fischer et al. 1991)
25.9 (calculated-bond contribution method, Meylan & Howard 1991)
0.13 (20°C), 0.20, 0.339, 0.363 (23°C), 0.158 (Iwata et al. 1993)
0.121 at 8°C in Green Bay, 0.242 at 18.9°C in Lake Michigan, 0.236 at 18.5°C in Lake Huron, 0.301 at 22.3°C in Lake Erie and 0.301 at 22.3°C in Lake Ontario (concn ratio-GC, McConnell et al. 1993)
0.0246 (20°C, Montgomery 1993)
0.520 (wetted wall column-GC, Altschuh et al. 1999)
log [H/(Pa m^3/mol)] = 11.58 – 3049/(T/K) (Passivirta et al. 1999)
0.18* (20°C, air stripping-GC, measured range 10–40°C, Jantunen et al. 2000)

log [H/(Pa m^3/mol)] = 9.51 – 3005/(T/K); temp range 10–40°C (gas stripping, Jantunen et al. 2000)
0.258 (20°C, selected from literature experimentally measured data, Staudinger & Roberts 1996, 2001)
log K_{AW} = 3.715 – 2254/(T/K) (van't Hoff eq. derived from literature data, Staudinger & Roberts 2001)
0.14* (20°C, dynamic headspace-GC, DHS method, measured range 5–35°C, Sahsuvar et al. 2003)
0.15* (20°C, gas stripping-GC, BS method, measured range 5–35°C, Sahsuvar et al. 2003)
0.14* (20°C, mean value of DHS and BS methods, temp range 5–35°C, Sahsuvar et al. 2003)
log [H/(Pa m^3/mol)] = 10.14 – 3208/(T/K); temp range 5–35°C (Sahsuvar et al. 2003)
0.159, 0.193 (20, 23°C, dynamic equilibrium system-GC/MS, measured range 278–293 K, Feigenbrugel et al. 2004)
0.269, 0.309 (LDV literature-derived value, FAV final adjusted value, Xiao et al. 2004)
log [H/(Pa m^3/mol)] = –2940/(T/K) + 9.29 (LDV linear regression of literature data, Xiao et al. 2004)
log [H/(Pa m^3/mol)] = –3117/(T/K) + 9.94 (FAV final adjusted eq., Xiao et al. 2004)
0.165* (seawater, dynamic equilibrium system-GC/MS, measured range 278–293 K, Xiao et al. 2004)

Octanol/Water Partition Coefficient, log K_{OW} at 25°C or as indicated. Additional data at other temperatures designated * are compiled at the end of this section:

3.72 (shake flask-GC, Kurihara et al. 1973)
3.65 (HPLC-RT correlation, Sugiura et al. 1979)
3.85 (HPLC-RT correlation, Veith et al. 1979)
2.81 (Rao & Davidson 1980)
3.66 (shake flask-GC, concn. ratio, Kanazawa 1981)
3.62 (HPLC-k′ correlation, McDuffie 1981)
3.25 (shake flask-GC, Platford 1982)
3.53 (shake flask-GC/FID, Hermens & Leeuwangh 1982)
3.90 (Elgar 1983)
3.61 (Hansch & Leo 1985)
3.67 (HPLC-RT correlation, Eadsforth 1986)
3.00 (HPLC-RT correlation, De Kock & Lord 1987)
3.57 (shake flask-GC, Kishi & Hashimoto 1989)
3.688 ± 0.021 (shake flask/slow stirring-GC, De Bruijn et al. 1989)
3.51 (shake flask-GC, Noegrohati & Hammers 1992)
3.20–3.89 (Montgomery 1993)
5.32 (RP-HPLC-RT correlation, Sicbaldi & Finizio 1993)
3.55 (recommended, Sangster 1993)
3.52 (RP-HPLC-RT correlation, Finizio et al. 1997)
3.72* ± 0.01 (shake flask-slow stirring-GC, measured range 5–35°C, Paschke & Schüürmann 1998)
3.80; 3.71 (quoted lit.; calculated, Passivirta et al. 1999)
3.70, 3.83 (LDV literature-derived value, FAV final-adjusted value, Xiao et al. 2004)
log K_{OW} = 282.2/(T/K) + 2.78 (LDV linear regression of literature data, Xiao et al. 2004)
log K_{OW} = 533.2/(T/K) + 2.04 (LDV linear regression of literature data, Xiao et al. 2004)

Octanol/Air Partition Coefficient, log K_{OA} at 25°C and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section:

7.70 (calculated-K_{OW}/K_{AW}, Wania & Mackay 1996)
8.08 (calculated, Finizio et al. 1997)
7.847*, 7.849 (gas saturation-GC/MS, calculated, measured range 5–25°C, Shoeib & Harner 2002)
log K_{OA} = –3.61 + 3415/(T/K), temp range: 5–25°C (gas saturation-GC, Shoeib & Harner 2002)
7.84, 7.74 (LDV literature derived value, FAV final adjusted value, Xiao et al. 2004)
log K_{OA} = 3415/(T/K) – 3.61 (LDV linear regression of literature data, Xiao et al. 2004)
log K_{OA} = 3521/(T/K) – 4.07 (FAV final adjusted eq., Xiao et al. 2004)

Bioconcentration Factor, log BCF:

–1.78 (beef biotransfer factor log B_b, correlated-K_{OW}, Radeleff et al. 1952; Kenaga 1980;)
–0.41 (vegetation, correlated-K_{OW}, Lichtenstein 1959; Voerman & Besemer 1975)
–2.60 (milk biotransfer factor log B_m, correlated-K_{OW}, Saha 1969)

2.15, 2.34 (Voerman & Tammes 1969)
1.83, 3.24 (brine shrimp, silverside fish, Matsumura & Benezet 1973)
1.98, 2.26 (brine shrimp in water, brine shrimp in sand, Matsumura & Benezet 1973)
3.21 (northern brook silverside fish to lindane residues on sand, Matsumura & Benezet 1973)
2.75, 2.66 (fish, snail, Metcalf et al. 1973)
2.26 (fathead minnow, Canton et al. 1975)
2.23, 2.65 (zooplankton, Hamelink & Waybrant 1976)
2.00 (mussels, steady state, Ernst 1977)
1.92, 2.34, 1.80, 2.69 (pink shrimp, pinfish, grass shrimp, sheepshead minnow, Schimmel et al. 1977; quoted, Howard 1991)
2.88, 2.45, 2.65, 2.97 (golden orfe, carp, brown trout, guppy, Sugiura et al. 1979)
2.68 (fathead minnow, Veith et al. 1979)
2.26 (fathead minnow, 32-d exposure, Veith et al. 1979; Veith & Kosian 1983)
2.51, 2.75 (fish: flowing water, static water; Kenaga 1980b; Kenaga & Goring 1980)
3.26, 1.73 (calculated-S, K_{OC}, Kenaga 1980)
–0.26 (average beef fat diet, Kenaga 1980b)
2.67, 2.25 (fathead minnow, 30-d exposure, 32-d exposure, Veith et al. 1980)
3.10 (topmouth gudgeon, Kanazawa 1981)
2.19 (mussel, quoted average, Geyer et al. 1982)
3.10 (topmouth gudgeon, Kanazawa 1983)
3.42 (clam fat, 60-d exptl., Hartley & Johnson 1983)
2.38, 2.46 (algae: exptl., calculated, Geyer et al. 1984)
2.26 (fathead minnow, Davies & Dobbs 1984)
2.38, 2.88, 2.91 (algae, fish, activated sludge, Klein et al. 1984)
2.38, 2.57, 2.91 (algae, golden ide, activated sludge, Freitag et al. 1985)
2.89–3.32 mean 3.08; 2.94–5.46 mean 3.30 (*p,p′*-DDE, rainbow trout, 15°C, steady-state BCF on 7- to 96-d laboratory study in 2 tanks with different water concn, Oliver & Niimi 1985)
3.32, 3.20; 3.00 (rainbow trout: kinetic BCF, steady-state BCF; Lake Ontario field BCF, Oliver & Niimi 1985)
2.50 (*Salmo gairdneri* Richardson fry, Ramamoorthy 1985)
2.78, 2.73, 2.78; 2.61 (mussel, pinfish, sheepshead minnow; calculated-K_{OW} and models, Zaroogian et al. 1985)
2.38, 2.67 (quoted values: mussel, sheepshead minnow, Zaroogian et al. 1985)
2.76; 2.43 (salmon fry in humic water April 1982; Oct. 1983, at steady state, Carlberg et al. 1986)
2.42, 2.84; 2.45–3.18 (salmon fry in lake water, quoted lit. values, Carlberg et al. 1986)
2.33 (*Daphnia magna*, wet wt. basis, Korte & Freitag 1986)
3.53 (azalea leaves, Bacci & Gaggi 1987)
2.38 (paddy field fish, Soon & Hock 1987)
4.30 (zooplankton, chum salmon, Kawano et al. 1988)
3.53, 5.88 (dry leaf, wet leaf, Bacci et al. 1990)
2.33 (*Daphnia magna*, Geyer et al. 1991)
2.09, 2.70, 2.29, 2.34 (zebrafish: egg, embryo, yolk sac fry, juvenile, Görge & Nagel 1990)
1.96 (calculated, Banerjee & Baughman 1991)
2.93, 2.96 (*Brachydanio rerio*, Butte et al. 1991)
2.67 (selected, Chessells et al. 1992)
1.58 (*Hydrilla*, Hinman & Klaine 1992)
2.16–2.57 (rainbow trout in early life stages on wet wt. basis, Vigano et al. 1992; quoted, Devillers et al. 1996)
3.77–3.85 (rainbow trout in early life stages on lipid basis, Vigano et al. 1992)
2.65 ± 2.23; 1.63–3.63 (aquatic organisms, wet wt basis, average value; range, Geyer et al. 1997)
4.04 (aquatic organisms, lipid basis, Geyer et al. 1997)
2.65; 2.606, 2.676 (fish, steady-state, quoted lit.; calculated-MCI χ, calculated-K_{OW}, Lu et al.1999)

Sorption Partition Coefficient, log K_{OC}:

2.96 (soil, Hamaker & Thompson 1972;, Kenaga 1980a, b; Kenaga & Goring 1980)
4.09 (soil, calculated-S as per Kenaga & Goring 1978, Kenaga 1980)
3.40 (soil, Kenaga 1980)
2.87 (average of 3 soils, HPLC-RT, McCall et al. 1980)

4.64 (calculated-S, Mill et al. 1980)
3.03 (av. for 3 soils, Rao & Davidson 1982)
2.88, 2.95, 2.74; 2.87 (Commerce soil, Tracy soil, Catlin soil; average soil, McCall et al. 1980)
4.07, 2.90 (estimated-S, K_{OW}, Lyman 1982)
3.11 (soil, screening model simulations, Jury et al. 1984, 1987a, b; Jury & Ghodrati)
4.30, 3.50 (field data of river sediment, calculated-K_{OW}, Oliver & Charlton 1984)
3.03 (Rao & Davidson 1982, Howard 1991)
2.63–3.18 (reported as log K_{OM}, Mingelgrin & Gerstl 1983)
3.04 (Caron et al. 1985)
1.63 (log K_P with first-order adsorption rate 0.088 h^{-1}, Miller & Weber 1986)
3.11, 2.82 (quoted, calculated-MCI χ, Gerstl & Helling 1987)
0.114 (screening model calculations, Jury et al. 1987b)
4.02 (RP-HPLC-k′ correlation, cyanopropyl column, Hodson & Williams 1988)
3.47 (calculated-K_{OW} as per Kenaga & Goring 1980, Chapman 1989)
2.38 (average of 2 soils, Kanazawa 1989)
2.84, 3.11, 3.08, 2.98, 2.88 (5 soils: clay loam/kaolinite, light clay/montmorillonite, light clay/montmorillite, sandy loam/allophane, clay loam/allophane, batch equilibrium-sorption isotherm, Kishi et al. 1990)
3.11 (soil, Mackay & Stiver 1991)
3.04 (soil, 20–25°C, selected, Wauchope et al. 1992; Hornsby et al. 1996)
2.38–3.52 (quoted lit. range, Montgomery 1993)
3.00 (calculated-MCI $^1\chi$, Sabljic et al. 1995)
3.00; 4.57 (soil, quoted exptl.; estimated-general model, Gramatica et al. 2000)
5.40; 3.30 (soil, calculated-universal solvation model; quoted exptl., Winget et al. 2000)
3.02, 3.00, 3.08 (soils: organic carbon OC $\geq$ 0.1%, OC $\geq$ 0.5%, 0.1 $\leq$ OC < 0.5%, average, Delle Site 2001)
3.49 (sediment: organic carbon OC $\geq$ 0.5%, average, Delle Site 2001)

Environmental Fate Rate Constants, k, or Half-Lives, $t_{1/2}$:

Volatilization: $t_{1/2}$ = 191 d was estimated from water (Mackay & Leinonen 1975, quoted, Howard 1991)
estimated $t_{1/2}$ > 200 d (Callahan et al. 1979);
$t_{1/2}$(exptl.) = 3.2 d in nonstirred water and $t_{1/2}$(exptl) = 1.5 d in stirred water from 4.5 cm deep distilled water at 24°C (Chiou et al. 1980; quoted, Howard 1991);
estimated half-lives: 3.4 d in nonstirred water and 2.3 d in stirred water (Chiou et al. 1980);
$t_{1/2}$ = 22 d, estimated from a model river of 1 m deep flowing 1 m/s with a wind speed of 3 m/s (Lyman et al. 1982; quoted, Howard 1991);
initial k = 4.4×10^{-2} h^{-1} and predicted k = 1.4×10^{-2} h^{-1} from soil with $t_{1/2}$ = 49.5 h (Thomas 1982);
$t_{1/2}$(calc) = 2760 h from water (Thomas 1982);
measured rate constant k(exptl) = 3.0 d^{-1} (Glotfelty et al. 1984; quoted, Glotfelty et al. 1989);
calculated rate constant k = 0.01 d^{-1} (Glotfelty et al. 1989);
$t_{1/2}$ = 266 d from lab. and field experiments (Jury et al. 1984; quoted, Spencer & Cliath 1990);
half-lives in soil surfaces at 20 ± 1°C: $t_{1/2}$ = 5.5 to 15.9 d in peat soil and $t_{1/2}$ = 2.7 to 6.7 d in sandy soil; half-lives in plant surfaces at 20 ± 1°C: $t_{1/2}$ = 0.56 d in bean, $t_{1/2}$ = 0.40 d in turnips and $t_{1/2}$ = 0.31 d in oats (Dörfler et al. 1991).

Photolysis: k_P(aq.) = 1.429×10^{-2} d^{-1} for photolysis in natural waters (Malaiyandi et al. 1982)
k_P(aq.) = 8.9×10^{-4} h^{-1} for Milli-Q water, k_P = 4.1×10^{-3} h^{-1} for natural surface water samples from eutrophic pond, k_P = 3.9×10^{-4} h^{-1} from eutrophic pond, k_P = 4.5×10^{-4} h^{-1} from oligotrophic rock quarry and the half-lives were 779, 169, 1791, and 1540 h, respectively, under direct sunlight (Saleh et al. 1982; quoted, Howard 1991)

Oxidation: rate constant k, for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO3} with NO_3 radical and k_{O3} with O_3 or as indicated, *data at other temperatures see reference:
k_{OH} = 6.94×10^{-12} cm^3 $molecule^{-1}$ s^{-1} with a $t_{1/2}$ ~ 2.3 d (Atkinson 1987; quoted, Howard 1991)
k(aq.) = 4.2×10^8 M^{-1} s^{-1} for the reaction (Fenton with reference to DBCP) with hydroxyl radical in aqueous solutions at pH 2.9 and at 24 ± 1°C (Buxton et al. 1988; quoted, Faust & Hoigné 1990; Haag & Yao 1992)
k(aq.) $\leq$ 0.04 M^{-1} s^{-1} for direct reaction with ozone in water at pH 2.7–6.3 and 23°C, with a $t_{1/2}$ $\geq$ 10 d at pH 7 (Yao & Haag 1991).

calculated tropospheric lifetimes due to gas-phase reaction with OH radical was estimated to be about 7 d (Atkinson et al. 1992)

k_{OH} (aq.) = $(5.8 \pm 1.9) \times 10^8$ M^{-1} s^{-1} (Fenton with reference to DBCP); and k = $(5.2 \pm 0.9) \times 10^8$ M^{-1} s^{-1} (photo-Fenton with reference to DBCP) for the reaction with hydroxyl radicals in aqueous solutions at pH 2.9 and at 24 ± 1°C (Haag & Yao 1992)

Hydrolysis: k(neutral) = 1.6×10^{-4} h^{-1} indicating that neutral hydrolysis is unimportant, rate constants of 7.5×10^{-3}, 8.99×10^{-4}, and 1.07×10^{-3} h^{-1} corresponded to half-lives of 92, 771 and 648 h in natural surface water samples from eutrophic pond, dystrophic reservoir and oligotrophic rock quarry, respectively (Saleh et al. 1982; quoted, Howard 1991)

k(neutral) = $(1.2 \pm 0.2) \times 10^{-4}$ h^{-1} with a calculated $t_{1/2}$ = 206 d at pH 7 (Ellington et al. 1987, 1988; quoted, Montgomery 1993)

$t_{1/2}$ = 42 yr at pH 8 and 5°C (Ngabe et al. 1993)

$t_{1/2}$ = 191 d at pH 7, and $t_{1/2}$ = 11 h at pH 9 at 22°C (Tomlin 1994)

$t_{1/2}$ = 240 d at pH 2, $t_{1/2}$ = 210 d at pH 7 and $t_{1/2}$ = 0.015 d at pH 12 in natural waters (Capel & Larson 1995)

Biodegradation: k = 0.0026 d^{-1} by die-away test in soil (Rao & Davidson 1980; quoted, Scow 1982);

$t_{1/2}$ = half-life of 266 d (soil, Jury et al. 1987);

$t_{1/2}$ = 3 to 30, 30 to 300 d and >300 d for river, lake and ground water, respectively (Zoeteman et al. 1980; quoted, Howard 1991);

$t_{1/2}$ = 266 d for 100-d leaching screening test in 0–10 cm depth of soil (Jury et al. 1984, 1987a, b; Jury & Ghodrati 1989)

$t_{1/2}$(aerobic) = 31 d, $t_{1/2}$(anaerobic) = 5.9 d in natural waters (Capel & Larson 1995)

$t_{1/2}$(calc) = (20.4 ± 0.1) h in sewage sludge from experiments S1–S3 (Buser & Müller 1995)

Biotransformation:

Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants:

k_1 = 3.13 h^{-1}; k_2 = 0.0313 h^{-1} (mussels, Ernst 1977)

k_1 = 130 d^{-1}; k_2 = 0.063 d^{-1} (rainbow trout, Oliver & Niimi 1985)

k_1 = 14, 179, 196 h^{-1} (zebrafish: egg, yolk sac fry, juvenile, Görge & Nagel 1990)

k_2 = 0.06 h^{-1} (*Chironomus riparius*-water only system, Lydy et al. 1992)

k_2 = 0.0661 h^{-1} (*Chironomus riparius*-screened system, Lydy et al. 1992)

k_2 = 0.08 h^{-1} (*Chironomus riparius*-3% organic carbon system, Lydy et al. 1992)

k_2 = 0.0661 h^{-1} (*Chironomus riparius*-15% organic carbon system, Lydy et al. 1992)

k_1 = 9.0–26.4 h^{-1}; k_2 = 0.04–0.18 h^{-1} (rainbow trout in early life stages on wet wt. basis, Vigano et al. 1992)

k_1 = 180–939 h^{-1}; k_2 = 0.031–0.13 h^{-1} (rainbow trout in early life stages on lipid basis, Vigano et al. 1992)

Half-Lives in the Environment:

Air: $t_{1/2}$ ~ 2.3 d was estimated, based on rate constant 6.94×10^{-12} cm^3 $molecule^{-1} \cdot s^{-1}$ for the vapor-phase reaction with hydroxyl radical in air (Howard 1991);

calculated tropospheric lifetimes due to gas-phase reaction with OH radical was estimated to be about 7 d (Atkinson et al. 1992);

atmospheric transformation lifetime was estimated to be <1 d (Kelly et al. 1994)

Lifetime of 13 d was estimated for atmospheric reaction with OH radical in the tropics (Schreitmüller and Ballschmiter 1995);

half-lives in the Great Lake's atmosphere. $t_{1/2}$ = 7.9 ± 1.2 yr at Eagle Harbor, $t_{1/2}$ = 4.3 ± 0.5 yr at Sleeping Bear Dunes and $t_{1/2}$ = 4.9 ± 0.5 yr at Sturgeon Point, when accounting the agricultural application effects, half-lives are, $t_{1/2}$ = 9.1 ± 1.3 yr at Eagle Harbor, $t_{1/2}$ = 4.6 ± 0.4 yr at Sleeping Bear Dunes and $t_{1/2}$ = 5.4 ± 0.4 yr at Sturgeon Point (Buehler et al. 2004)

Surface water: $t_{1/2}$ = 10–138 d in various locations in the Netherlands in case a first order reduction process may be assumed; and $t_{1/2}$ = 3–30 d in rivers and $t_{1/2}$ = 30–300 d in lakes (Zoeteman et al. 1980);

hydrolysis $t_{1/2}$(exptl) = 92 h, $t_{1/2}$(calc) = 89 h for Roselawn Cemetery Pond at pH 9.3; $t_{1/2}$(exptl) = 771 h, $t_{1/2}$(calc) = 578 h for Cross Lake at pH 7.3; $t_{1/2}$(exptl) = 648 h, $t_{1/2}$(calc) = 231 h for Indiana Quarry at pH 7.8; photolysis half-lives for direct sunlight during July and adjusted for mid-winter: $t_{1/2}$ = 779 h, 1560 h for Milli-Q water at pH 6.98, $t_{1/2}$ = 169 h, 339 h for Roselawn Pond at pH 9.3, $t_{1/2}$ = 1791 h, 3590 h for Cross Lake and $t_{1/2}$ = 1540 h, 3090 h for Indiana Quarry (Saleh et al. 1982);

$t_{1/2}$ > 10 d for direction reaction with ozone in water at 23°C and pH 7 (Yao & Haag 1991);

hydrolysis $t_{1/2}$ = 191 d at pH 7, and $t_{1/2}$ = 11 h at pH 9 at 22°C (Tomlin 1994).

Biodegradation $t_{1/2}$(aerobic) = 31 d, $t_{1/2}$(anaerobic) = 5.9 d, hydrolysis $t_{1/2}$ = 240 d at pH 2, $t_{1/2}$ = 210 d at pH 7 and $t_{1/2}$ = 0.015 d at pH 12 in natural waters (Capel & Larson 1995)

Ground water: $t_{1/2}$ –300 d (Zoeteman et al. 1980).

Sediment:

Soil: $t_{1/2}$ ~ 2 yr persistence in soil (Nash & Woolson 1967; quoted, Kaufman 1976);

persistence of 3 yr in soil (Edwards 1973; quoted, Morrill et al. 1982);

$t_{1/2}$ > 50 d and subject to plant uptake via volatilization (Callahan et al. 1979; quoted, Ryan et al. 1988)

First-order $t_{1/2}$ = 266 d in soil from biodegradation rate constant k = 0.0026 d^{-1} by die-away test in soil (Rao & Davidson 1980; quoted, Scow 1982);

field $t_{1/2}$ = 0.3 d in moist fallow soil (Glotfelty 1981; quoted, Nash 1983);

microagroecosystem $t_{1/2}$ = 1–4 d in moist fallow soil (Nash 1983); measured dissipation rate of 0.16 d^{-1} (Nash 1983; quoted, Nash 1988);

estimated dissipation rate of 0.20, 0.10 d^{-1} (Nash 1988);

biodegradation $t_{1/2}$ = 266 d (soil, Jury et al. 1984, 1987);

first-order adsorption rate 0.088 h^{-1} (Miller & Weber 1986; quoted, Brusseau & Rao 1989);

half-lives in soil surfaces at 20 ± 1°C: $t_{1/2}$ = 5.5 to 15.9 d in peat soil and $t_{1/2}$ = 2.7 to 6.7 d in sandy soil (Dörfler et al. 1991); reported $t_{1/2}$ = 266 d in soil (Jury et al. 1987a, b; Jury & Ghodrati 1989; quoted, Montgomery 1993);

reaction $t_{1/2}$= 266 d (Mackay & Stiver 1991);

selected field $t_{1/2}$ = 400 d (Wauchope et al. 1992; Dowd et al. 1993; Hornsby et al. 1996);

$t_{1/2}$ = 14 d for soil depth < 5 cm, $t_{1/2}$ = 90 d for 5–20 cm and $t_{1/2}$ = 180 d for >20 cm (Dowd et al. 1993)

$t_{1/2}$ = 14.5 and 16.0 yr for control and sludge-amended Luddington soils, respectively (Meijer et al. 2001)

Biota: $t_{1/2}$ = 22.1 h (mussels, Ernst 1977);

$t_{1/2}$ = 46 d (rainbow trout, Oliver & Niimi 1985);

biological half-lives for fishes: $t_{1/2}$ = 11 d for trout muscle, $t_{1/2}$ = 1 d for goldfish, $t_{1/2}$ < 1 d for sunfish and $t_{1/2}$ = 4 d for guppy (Niimi 1987);

$t_{1/2}$ = 678 h (azalea leaves, Bacci & Gaggi 1987);

biochemical $t_{1/2}$ = 266 d from screening model calculations (Jury et al. 1987b);

half-lives in plant surfaces at 20 ± 1°C: $t_{1/2}$ = 0.56 d in bean, $t_{1/2}$ = 0.40 d in turnips and $t_{1/2}$ = 0.31 d in oats (Dörfler et al. 1991);

elimination half-lives in the midge (*Chironomus riparius)* under varying sediment conditions: $t_{1/2}$ = 11 h for water only system, $t_{1/2}$ = 10 h for screened system, $t_{1/2}$ = 9 h for 3% organic carbon system and $t_{1/2}$ = 6 h for 15% organic carbon system (Lydy et al. 1992);

half-lives $t_{1/2}$ (in h) = 12.09 × L(% lipid) – 10.09, in different aquatic organisms (Geyer et al. 1997).

Average $t_{1/2}$ = 90 d (for pesticides used in conjunction with forest management, Neary et al. 1993).

TABLE 18.1.1.54.1
Reported aqueous solubilities of lindane at various temperatures

Richardson & Miller 1960		**Biggar & Riggs 1974**				**OECD 1981**	
shake flask-UV spectro.		**shake flask-GC**				**shake flask method**	
t/°C	**S/g·m^{-3}**	**t/°C**	**S/g·m^{-3}**	**S/g·m^{-3}**	**S/g·m^{-3}**	**t/°C**	**S/g·m^{-3}**
		particle size	0.01µ	0.05µ	5.0µ		
25	7.30	15	0.075	0.330	2.150	15	6.50
35	12.0	25	0.150	0.600	6.80	25	9.20
45	14.0	35	0.315	0.950	11.40		
		45	0.575	1.450	15.20		

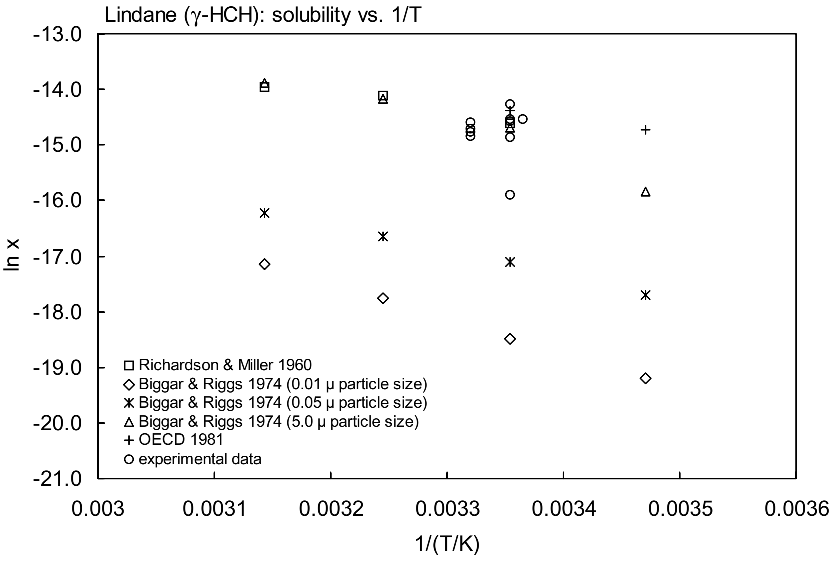


FIGURE 18.1.1.54.1 Logarithm of mole fraction solubility (ln *x*) versus reciprocal temperature for lindane (γ-HCH).

TABLE 18.1.1.54.2
Reported vapor pressures of lindane at various temperatures and the coefficients for the vapor pressure equations

$\log P = A - B/(T/K)$ (1) $\ln P = A - B/(T/K)$ (1a)
$\log P = A - B/(C + t/°C)$ (2) $P = A - B/(C + t/°C)$ (2a)
$\log P = A - B/(C + T/K)$ (3)
$\log P = A - B/(T/K) - C \cdot \log (T/K)$ (4)

1.

Balson 1947		**Spencer & Cliath 1970**		**Wania et al. 1994**		**Boehncke et al. 1996**	
effusion manometer		**gas saturation-GC**		**gas saturation-GC**		**Knudsen effusion**	
t/°C	**P/Pa**	**t/°C**	**P/Pa**	**t/°C**	**P/Pa**	**t/°C**	**P/Pa**
0	3.87×10^{-5}	20	0.004346	–30	1.701×10^{-6}	19.63	0.00374
10	2.40×10^{-4}	30	0.0171	–20	7.353×10^{-6}	24.95	0.00737
20	1.253×10^{-3}	40	0.0608	–10	8.435×10^{-5}	28.42	0.0116
30	6.00×10^{-3}	30 wet	0.0167	0	4.489×10^{-4}	33.58	0.0225
40	0.0257	30 dry	0.0173	10	2.209×10^{-3}	37.82	0.0281
50	0.1027			20	9.395×10^{-3}	37.86	0.0386
60	0.3706	eq. 1	P/mmHg	30	4.192×10^{-2}	43.26	0.0718
70	1.233	A	13.544			48.06	0.123
80	3.853	B	5288			53.07	0.217
90	11.479			eq. 1	P/Pa	20	3.83×10^{-3}
		$\Delta H_V = 101.13$ kJ/mol		A	16.99		
eq. 1	P/mmHg			B	5566	eq. 1a	P/Pa
A	15.515					A	34.53
B	6020			enthalpy of sublimation:		B	11754
temp range: 60–92°C		**Rordorf 1989**		$\Delta H_{sub} = 106.6$ kJ/mol		temp range: 293–323 K	
$\Delta H_V = 115.06$ kJ/mol		**gas saturation-GC**				enthalpy of sublimation:	
		25	0.067			$\Delta H_{sub} = 97.7$ kJ/mol	
		50	0.15				
		75	2.0				

TABLE 18.1.1.54.2 (*Continued*)

Balson 1947		**Spencer & Cliath 1970**		**Wania et al. 1994**		**Boehncke et al. 1996**	
effusion manometer		**gas saturation-GC**		**gas saturation-GC**		**Knudsen effusion**	
t/°C	**P/Pa**	**t/°C**	**P/Pa**	**t/°C**	**P/Pa**	**t/°C**	**P/Pa**
		100	20.0				
		125	150				
		eq. 1	P/Pa				
		A	15.096				
		B	5148.9				
		eq. 1	P/Pa				
		A	12.05				
		B	3970.1				

2.

Giustini et al. 1998

torsion		**torsion**		**Knudsen effusion**		**Knudsen effusion**	
t/°C	**P/Pa**	**t/°C**	**P/Pa**	**t/°C**	**P/Pa**	**t/°C**	**P/Pa**
run 1–4		run 5–8		cell K.1		cell K.2	
50	0.162	73	1.9498	37.5	0.0562	70	1.5849
54	0.245	76	2.4547	39.5	0.0776	71.5	1.9055
59	0.407	79	3.3113	44.5	0.1023	72	1.7783
65	0.646	83	4.6774	45.0	0.1175	73.5	2.2387
69	1.148	88	7.2444	48.5	0.1622	74.5	2.3988
74	1.778	93	11.482	49.5	0.1995	75	3.0903
80	2.754	98	17.378	53.5	0.2951	80.5	4.0738
88	5.370	66	0.9550	55.0	0.3311	81	4.2658
97	11.220	69	1.5136	55.5	0.3631	84	7.0795
59	0.4074	76	2.3442	56.5	0.3981	87.5	7.0795
64	0.7244	79	3.0200	63.0	0.8318	89	9.3325
69	1.047	83	4.6774	63.5	0.8128	94	12.303
74	1.622	88	7.2444	65.5	0.9772	99.5	23.442
82	3.311	93	11.482	66.5	1.0471		
88	5.495	99	19.953				
92	8.710	68	1.2303	eq. 1	kPa	eq. 1	kPa
60	0.4074	72	1.7783	A	10.89	A	11.46
66	0.8128	77	2.7542	B	4706	B	4889
71	1.2303	82	4.3652	for temp 310.5–339.5 K		for temp 343–377 K	
76	1.8621	88	7.0795				
82	2.9512	94	13.490				
89	5.0119	101	24.547				
98	13.183	104	30.903				
66	0.8128	80	4.3652				
71	1.2303	83	5.6234				
76	2.0417	88	9.1201				
81	2.8184	93	15.136				
87	4.6774	97	20.417				
92	7.7625	102	30.903				
96	11.482	106	48.978				
		111	66.069				

Combining the above 4 equations, the final equation

log (P/kPa) = 11.23 ± 0.5 – (4832 ± 150)/(T/K)

for temperature range 310 to 384 K

ΔH_{sub} = 92.5 kJ/mol at 350 K

at 25°C P = 0.0104 Pa

(*Continued*)

TABLE 18.1.1.54.2 (*Continued*)

Giustini et al. 1998							
torsion		torsion		Knudsen effusion		Knudsen effusion	
t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa
eq. 1	kPa						
A	10.78	eq. 1	kPa				
B	4709	A	11.79				
		B	5025				
for temp 323–370 K		for temp 339–384 K					

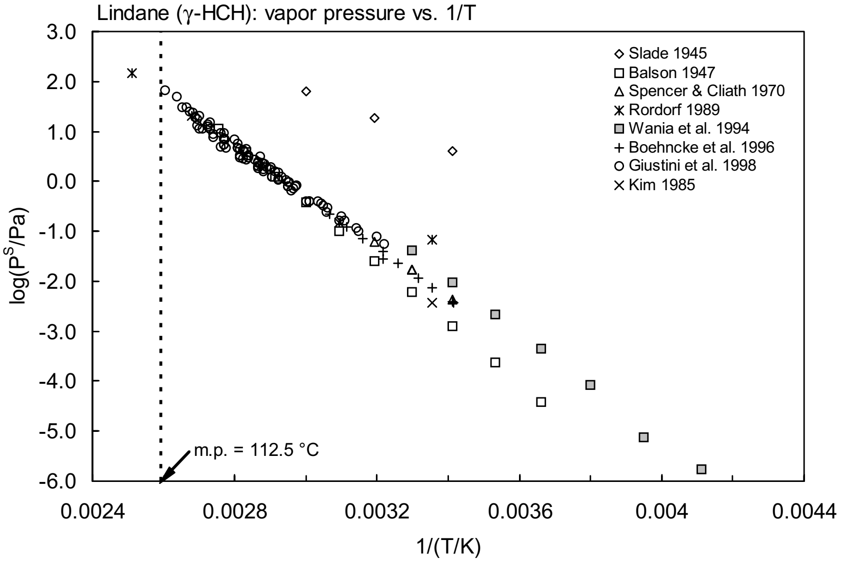


FIGURE 18.1.1.54.2 Logarithm of vapor pressure versus reciprocal temperature for lindane (γ-HCH).

TABLE 18.1.1.54.3
Reported Henry's law constants of lindane (-HCH) at various temperatures and temperature dependence equations

$\ln K_{AW} = A - B/(T/K)$	(1)	$\log K_{AW} = A - B/(T/K)$	(1a)
$\ln (1/K_{AW}) = A - B/(T/K)$	(2)	$\log (1/K_{AW}) = A - B/(T/K)$	(2a)
$\ln (k_H/atm) = A - B/(T/K)$	(3)		
$\ln H = A - B/(T/K)$	(4)	$\log H = A - B/(T/K)$	(4a)
$K_{AW} = A - B\cdot(T/K) + C\cdot(T/K)^2$	(5)		

Kucklick et al. 1991		McConnell et al. 1993		Jantunen et al. 2000		Sahsuvar et al. 2003	
gas stripping-GC		concentration ratio		air stripping-GC		air stripping/dynamic HS	
t/°C	H/(Pa m³/mol)	t/°C	H/(Pa m³/mol)	t/°C	H/(Pa m³/mol)	t/°C	H/(Pa m³/mol)
distilled water		Green Bay				dynamic headspace (DHS)	
0.5	0.0721	8.0	0.121	10	0.073	5	0.039
10	0.126	Lake Michigan		20	0.18	10	0.062
15	0.187	18.9	0.242	30	0.39	20	0.14
20	0.258	Lake Huron		35	0.58	30	0.33
23	0.339	18.5	0.236	40	0.80	35	0.60

TABLE 18.1.1.54.3 (*Continued*)

Kucklick et al. 1991		McConnell et al. 1993		Jantunen et al. 2000		Sahsuvar et al. 2003	
gas stripping-GC		concentration ratio		air stripping-GC		air stripping/dynamic HS	
t/°C	H/(Pa m³/mol)	t/°C	H/(Pa m³/mol)	t/°C	H/(Pa m³/mol)	t/°C	H/(Pa m³/mol)
25	0.353		Lake Erie				
35	0.624	22.3	0.310	eq. 4a	H/(Pa m³/mol)	gas stripping-GC	
45	1.170			A	9.51 ± 0.49	5	0.044
	22.3	0.301		B	3005 ± 145	10	0.054
eq.4a	H/(Pa m³/mol)					20	0.15
A	7.54 ± 0.54					30	0.34
B	2392 ± 160					35	0.55
seawater						combined - both methods	
0.5	0.0627					5	0.040
10	0.137					10	0.061
23	0.363					20	0.14
35	0.996					30	0.33
45	2.57					35	0.59
eq. 4a	H/(Pa m³/mol)					eq. 4a	H/(Pa m³/mol)
A	8.68 ± 0.96					A	10.14 ± 0.55
B	2703 ± 276					B	3208 ± 161
for temp range 0.5–23°C							
						enthalpy of transfer, air-water	
						$\Delta H_{WA}/(\text{kJ mol}^{-1}) = 61.4$	

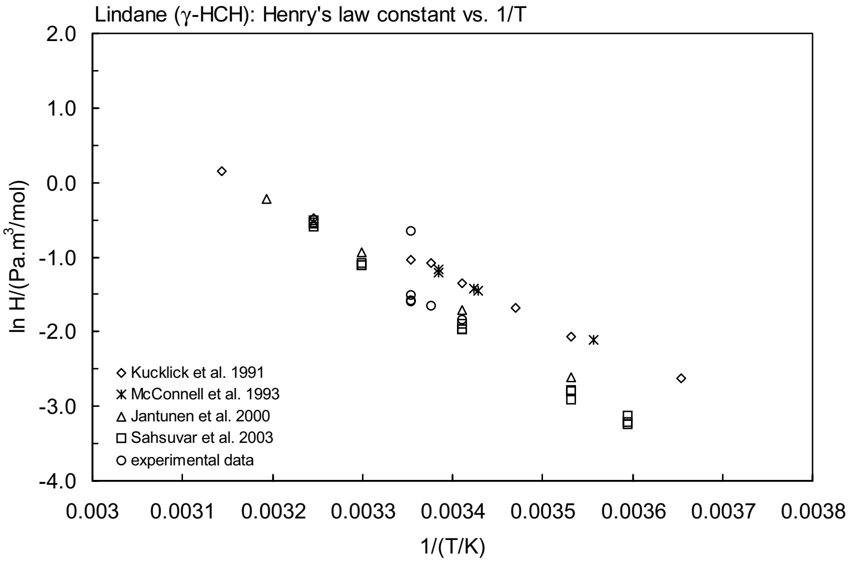


FIGURE 18.1.1.54.3 Logarithm of Henry's law constant versus reciprocal temperature for lindane (γ-HCH).

TABLE 18.1.1.54.4
Reported octanol-water and octanol-air partition coefficients of lindane (γ-HCH) at various temperatures

log K_{OW}		log K_{OA}	
Paschke & Schüürmann 1998		Shoeib & Harner 2002	
shake flask-GC		generator column-GC/MS	
t/°C	log K_{OW}	t/°C	log K_{OA}
5	3.85	5	8.6845
25	3.72	10	8.4493
45	3.73	15	8.2181
		20	8.0643
enthalpy of phase transfer:		25	7.8473
$\Delta H_{OW}/(kJ\ mol^{-1}) = -10.40$		25	7.849
entropy of phase transfer:			
$\Delta S_{OW}/(J\ K^{-1}\ mol^{-1}) = 52.2$		log K_{OA} = A + B/(T/K)	
		A	–3.611
		B	3415
		enthalpy of phase change	
		$\Delta H_{OA}/(kJ\ mol^{-1}) = 65.4$	

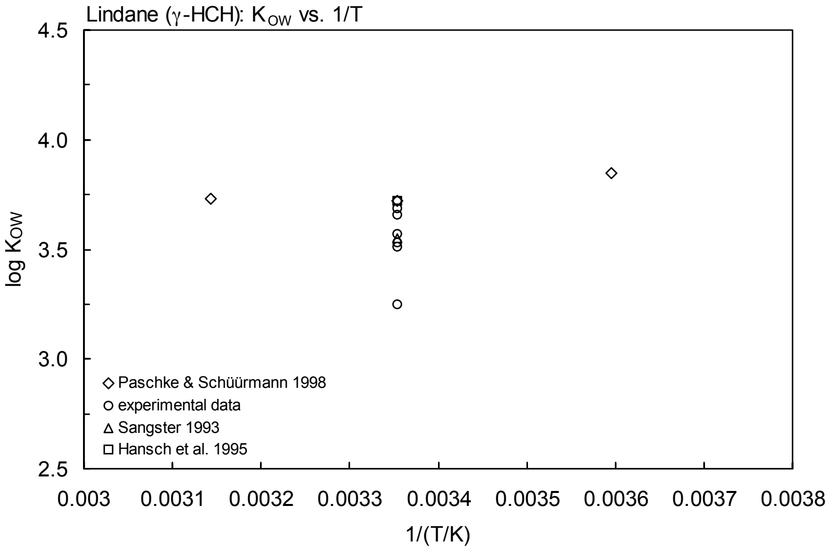


FIGURE 18.1.1.54.4 Logarithm of K_{OW} versus reciprocal temperature for lindane (γ-HCH).

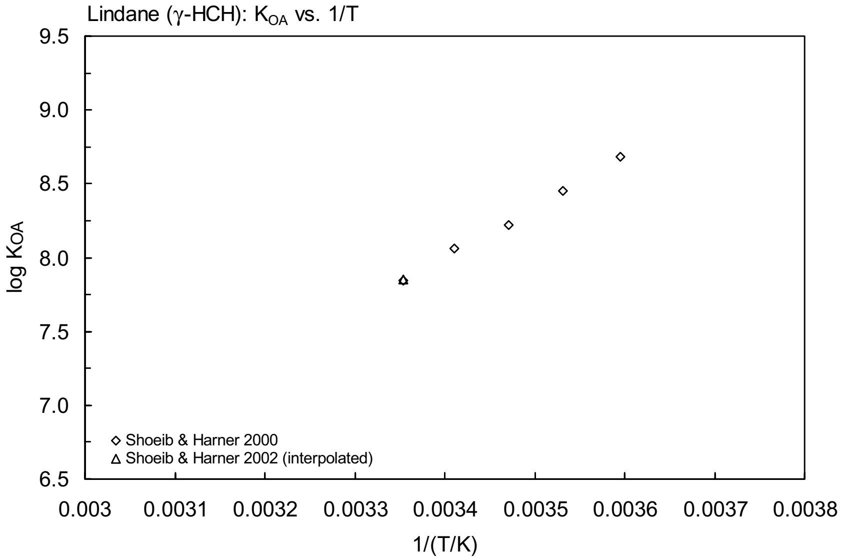
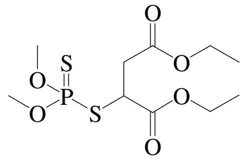


FIGURE 18.1.1.54.5 Logarithm of K_{OA} versus reciprocal temperature for lindane (γ-HCH).

18.1.1.55 Malathion



Common Name: Malathion

Synonym: American Cyanamid 4049, Calmathion, Carbethoxy malathion, Carbetovur, Carbetox, Carbofos, Carbophos, Celthion, Chemathion, Cimexan, Cythion, Detmol MA, EL 4049, Emmatos, Emmatos extra, ENT 17034, Ethiolacar, Etio, Fog 3, Formal, Forthion, Fosfothion, Fyfanon, Hithion, Karbofos, Kop-thion, Kypfos, Malacide, Malafor, Malakill, Malagran, Malamar, Malaphele, Malaphos, Malasol, Malaspray, Malatol, Malatox, Maldison, Malmed, Malphos, Maltox, Mercaptothion, MLT, Moscardia, NA 2783, NCI-C00215, Oleophosphothion, Orthomalathion, Phosphothion, Prioderm, Sadofos, Sadophos, SF 60, Siptox I, Sumitox, Tak, TM-4049, Vegfru malatox, Vetiol, Zithiol

Chemical Name: *S*-[1,2-bis(ethoxycarbonyl)ethyl] *O,O*-dimethyl phosphorodithioate

Uses: as insecticide to control sucking and chewing insects and spider mites on vegetables, fruits, ornamentals, field crops in greenhouses, gardens and forestry; also used as acaricide.

CAS Registry No: 121-75-5

Molecular Formula: $C_{10}H_{19}O_6PS_2$

Molecular Weight: 330.358

Melting Point (°C):

1.4	(Lide 2003)

Boiling Point (°C):

120	(at 0.2 mmHg, Melnikov 1971; Freed et al. 1977)
156–157	(at 0.7 mmHg, Hartley & Kidd 1987; Worthing & Hance 1991; Montgomery 1993; Tomlin 1994)

Density (g/cm^3 at 20°C):

1.23	(25°C, Spencer 1982; Hartley & Kidd 1987; Worthing & Hance 1991; Montgomery 1993)

Molar Volume (cm^3/mol):

319.1	(calculated-Le Bas method at normal boiling point)

Dissociation Constant, pK_a:

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

Entropy of Fusion, ΔS_{fus} (J/mol K):

Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F: 1.0

Water Solubility (g/m^3 or mg/L at 25°C or as indicated):

145	(20°C, Macy 1948; Melnikov 1971; Spencer 1973)
145	(Spiller 1961; Willis & McDowell 1982)
145	(room temp., Spencer 1973; Martin & Worthing 1977; Worthing & Walker 1987, Worthing & Hance 1991; Hartley & Kidd 1987; Tomlin 1994)
150	(Hartley & Graham-Bryce 1980; Beste & Humburg 1983)
145	(22°C, Khan 1980)
143	(20°C, shake flask-GC, Bowman & Sans 1983a, b)
130	(20–25°C, selected, Wauchope et al. 1992; Hornsby et al. 1996)
145, 164	(20°C, 30°C, Montgomery 1993)

Vapor Pressure (Pa at 2 5°C or as indicated):

1.67×10^{-4}	(20°C, Wolfdietrich 1965; Melnikov 1971; Montgomery 1993)
7.33×10^{-4}	(20°C, evaporation rate-gravimetric method, Gückel et al. 1973)
2.90×10^{-3}	(Woolford 1975)
1.30×10^{-3}	(20°C, Hartley & Graham-Bryce 1980)
5.30×10^{-3}	(30°C, Khan 1980)
9.20×10^{-4}	(20°C, GC, Seiber et al. 1981)
1.05×10^{-3}	(gas saturation-GC, Kim et al. 1984; Kim 1985)
0.60×10^{-3}	(20°C, extrapolated-Clausius-Clapeyron eq., Kim et al. 1984, Kim 1985)

0.67×10^{-3} (20°C, GC-RT correlation, Kim et al. 1984; Kim 1985)
5.30×10^{-3} (30°C, Hartley & Kidd 1987; Tomlin 1994)
4.70×10^{-3} (GC-RT correlation, supercooled liquid value, Hinckley et al. 1990)
1.07×10^{-3} (20–25°C, selected, Wauchope et al. 1992; Hornsby et al. 1996)
0.0063 (liquid P_L, GC-RT correlation; Donovan 1996)
1.07×10^{-3} (selected, Halfon et al. 1996)
0.00174 (gradient GC method; Tsuzuki 2000)
1.78×10^{-3}; 1.35×10^{-3}, 2.51×10^{-3} (gradient GC method; estimation using modified Watson method: Sugden's parachor, McGowan's parachor, Tsuzuki 2000)

Henry's Law Constant (Pa·m^3/mol at 25°C or as indicated):
0.038 (calculated-P/C, Mackay & Shiu 1981)
2.30×10^{-3} (20°C, calculated-P/C, Suntio et al. 1988)
3.22×10^{-3} (calculated-P/C, Taylor & Glotfelty 1988)
2.03×10^{-3} (calculated-P/C, Howard 1991)
4.96×10^{-4} (calculated-bond contribution method, Meylan & Howard 1991)
4.9×10^{-4} (23°C, quoted, Schomburg et al. 1991)
4.9×10^{-4} (Montgomery 1993)

Octanol/Water Partition Coefficient, log K_{OW}:
2.89 (20°C, shake flask-GC, Chiou et al. 1977)
2.89 (shake flask-GC, Freed et al. 1979; Yoshioka et al. 1986)
2.36 (Hansch & Leo 1979, 1985)
2.36 (Rao & Davidson 1980)
2.82 (shake flask-GC/FID, Hermens & Leeuwangh 1982)
2.94 (shake flask/slow-stirring method-GC, De Bruijn et al. 1991)
2.75 (Worthing & Hance 1991; Tomlin 1994)
2.36–2.89 (Montgomery 1993)
2.68 (RP-HPLC-RT correlation, Saito et al. 1993)
2.18 (RP-HPLC-RT correlation, Sicbaldi & Finizio 1993)
2.36 (recommended, Sangster 1993)
2.36 (selected, Hansch et al. 1995)
2.18 (RP-HPLC-RT correlation, Finizio et al. 1997)
3.57 (RP-HPLC-RT correlation, Nakamura et al. 2001)
3.38 (RP-HPLC-RT correlation using short ODP column, Donovan & Pescatore 2002)

Bioconcentration Factor, log BCF:
1.11 (carp, calculated. from k_1 of Bender 1969, McLeese et al. 1976)
–4.74 (beef biotransfer factor logB_b, correlated-K_{OW}, Pasarela et al. 1962)
0.867, 1.47 (lake trout, coho salmon, Howard 1991)
2.94, 2.98 (white shrimp, brown shrimp, Conte & Parker 1975)
1.57 (calculated-S, Kenaga 1980a; quoted, Howard 1991)
0.40 (*Triaenodes tardus*, Belluck & Felsot 1981)
1.54 (willow shiner, Tsuda et al. 1989)
0.85 (carp, wet wt. basis, De Bruijn & Hermens 1991)
2.00 (topmouth gudgeon, wet wt. basis, De Bruijn & Hermens 1991)
1.57 (Pait et al. 1992)

Sorption Partition Coefficient, log K_{OC}:
2.45 (soil, calculated-S as per Kenaga & Goring 1978, Kenaga 1980a)
3.26 (av. soils/sediments, Rao & Davidson 1980)
3.25 (Rao & Davidson 1980)
3.25 (Karickhoff 1981)
2.83, 3.29, 2.50 (estimated-S, calculated-S and mp, estimated-K_{OW}, Karickhoff 1981)
2.36 (Bomberger et al. 1983)

3.25 (screening model calculations, Jury et al. 1987b)
0.903 (selected, USDA 1989; Neary et al. 1993)
3.26 (soil, 20–25°C, selected, Wauchope et al. 1992; Hornsby et al. 1996)
2.61 (Montgomery 1993)
3.07 (soil, calculated-MCI $^1\chi$, Sabljic et al. 1995)
3.07; 2.76, 2.29 (soil, quoted exptl.; estimated-class-specific model, estimated-general model, Gramatica et al. 2000)
3.08, 3.05 (soils: organic carbon OC ≥ 0.1%, OC ≥ 0.5%, average, Delle Site 2001)
2.68–2.72 (sediments from San Diego Creek and Bonita Creek, shake flask-GC, Bondarenko & Gan 2004)

Environmental Fate Rate Constants, k, or Half-Lives, $t_{½}$:

Volatilization: $t_{½}$ = 131 d, based on volatilization rate from water with a wind speed of 0–2.5 m/s (Sanders & Seiber 1984; quoted, Howard 1991).

Photolysis: $t_{½}$ = 15 h for direct sunlight photolysis in aqueous media (Wolfe et al. 1976)
$t_{½}$ = 900 h in distilled water at pH 6 with wavelength λ > 290 nm; $t_{½}$ = 16 h by sunlight in a natural water from Suwannee River (Wolfe et al. 1977)
$t_{½}$ = 990–20000 h for both atmospheric and aqueous photolysis, based on experimental photolysis rate constant in aqueous solution at pH 6 exposure to >290 nm under summer sunlight at 40°N (Howard et al. 1991)

Oxidation: rate constant k, for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO3} with NO_3 radical and k_{O3} with O_3 or as indicated, *data at other temperatures see reference:
photooxidation $t_{½}$ = 1.0–9.8 h, based on an estimated rate constant for the vapor-phase reaction with hydroxyl radical in air (Howard et al. 1991)
k_{OH}(calc) = 64 × 10^{-12} cm^3 $molecule^{-1}$ s^{-1} at room temp. (Winer & Atkinson 1990)
calculated lifetime τ = 3 h for reaction with OH radical in the troposphere (Atkinson et al. 1992)

Hydrolysis: $t_{½}$ = 10.5 d at pH 7.4 and 20°C (Freed et al. 1977, 1979; Montgomery 1993)
$t_{½}$ = 120 d at pH 6.1 and $t_{½}$ = 11 d at pH 7.4 in water and soil at 20°C as per Ruzicka et al. 1967 using GC-RT correlation method for hydrolysis rates determination (Freed et al. 1979)
k(acid) = (4.8 ± 0.2) × 10^{-5} M^{-1} s^{-1} with $t_{½}$ > 4 yr for acid degradation at pH 4 at 27°C; k(alkaline) = (5.5 ± 0.3) M^{-1} s^{-1} with a $t_{½}$ = 36 h for alkaline degradation at pH 8 at 27°C, $t_{½}$ = 1 h at 40°C and $t_{½}$ = 40 h at 0°C and pH 8; all for 10^{-4} M in 1% acetonitrile and water at 27°C; $t_{½}$ = 20 h for distilled water and $t_{½}$ = 22 h for natural river water from Withlacoochee River, pH 8.2 (Wolfe et al.1977)
k(acid) = 4.8 × 10^{-5} M^{-1} s^{-1}; k(neutral) = 7.7 × 10^{-9} s^{-1} and k(alkaline) = 5.5 M^{-1} s^{-1} all for 10^{-4} M in 1% acetonitrile and water at 27°C (Wolfe et al. 1977; quoted, Harris 1982)
$t_{½}$ = 8.8 yr, based on reported k = 2.5 × 10^{-2} M^{-1} s^{-1} at pH 7 and 0°C; $t_{½}$(base) = 14 h at pH 9 and 27°C (Howard et al. 1991)
$t_{½}$ = 9 d at pH 6 (Montgomery 1993)
$t_{½}$ = 3200 d at pH 7, $t_{½}$ = 0.0006 d at pH 12 in natural waters (Capel & Larson 1995)

Biodegradation: k = 6.2 × 10^{-8} mL $cell^{-1}$ d^{-1} (Paris et al. 1975; quoted, Scow 1982)
k = 5.0 × 10^{-8} mL $cell^{-1}$ d^{-1} (Baughman & Lassiter 1978; quoted, Scow 1982)
k = 2.6 – 16.1 × 10^{-7} mL $cell^{-1}$ d^{-1} (Paris et al. 1978; quoted, Scow 1982);
k = 1.4 d^{-1} in soil (Rao & Davidson 1980; quoted, Scow 1982)
k = (4.5 ± 0.74) × 10^{-11} L $cell^{-1}$ h^{-1} in North American waters (Paris et al. 1981)
$t_{½}$(aq. aerobic) = 100–1236 h, based on estimated aqueous aerobic biodegradation half-life; $t_{½}$(aq. anaerobic) = 400–4944 h based on unacclaimed aerobic biodegradation (Howard et al. 1991).
$t_{½}$(aerobic) = 4.2 d, $t_{½}$(anaerobic) = 17 d in natural waters (Capel & Larson 1995)

Biotransformation: transformation rate k = 7.8 × 10^{-3} mg (mg fungi)$^{-1}$ h^{-1} by a fungi *Aspergillus orgzae* at 28°C in aqueous solution (Lewis et al. 1975)
k = 1.9 × 10^{-1} mg (mg fungi)$^{-1}$ d^{-1} in aquatic systems (Lewis et al. 1975; quoted, Scow 1982)

Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants:
k_1 = 1.07 d^{-1} (carp, Bender 1969; quoted, McLeese et al. 1976)
k_2 = 0.08 d^{-1} (carp, calculated. from k_1 of Bender 1969, McLeese et al. 1976)
k_2 = 0.49 h^{-1} (willow shiner, Tsuda et al. 1989)

Half-Lives in the Environment:

Air: $t_{1/2}$ = 1.0–9.8 h, based on an estimated rate constant for the vapor-phase reaction with hydroxyl radical in air (Howard et al. 1991);

calculated lifetime of 3 h for the vapor-phase reaction with OH radical in the troposphere (Atkinson et al. 1992).

Surface water: persistence of up to 4 wk in river water (Eichelberger & Lichtenberg 1971);

$t_{1/2}$ = 100–1236 h, based on unacclimated aerobic river die-away test data and estuarine water grab sample data (Howard et al. 1991);

$t_{1/2}$ = 1.65 d in Indian River water, at 24 ppt salinity and pH 8.16 (Wang & Hoffman 1991);

$t_{1/2}$ = 212 d at 6°C, $t_{1/2}$ = 42 d at 22°C in darkness for Milli-Q water, pH 6.1; $t_{1/2}$ = 55 d at 6°C, $t_{1/2}$ = 19 d at 22°C in darkness, 8 d under sunlight conditions for river water at pH 7.3; $t_{1/2}$ = 53 d at 6°C, $t_{1/2}$ = 7 d at 22°C in darkness for filtered river water at pH 7.3; $t_{1/2}$ = 41 d at 6°C, $t_{1/2}$ = 6 d at 22°C in darkness, $t_{1/2}$ = 14 d under sunlight conditions for seawater at pH 8.1 (Lartiges & Garrigues 1995)

Biodegradation $t_{1/2}$(aerobic) = 4.2 d, $t_{1/2}$(anaerobic) = 17 d, hydrolysis $t_{1/2}$ = 3200 d at pH 7 and $t_{1/2}$ = 0.0006 d at pH 12 in natural waters (Capel & Larson 1995)

Ground water: $t_{1/2}$ = 200–2472 h, based on estimated aqueous aerobic biodegradation half-life (Howard et al. 1991).

Sediment: $t_{1/2}$ = 2 d in sediment suspension (Cotham & Bidleman 1989)

first-order degradation k = 0.902 d^{-1} with $t_{1/2}$ = 0.8 d under aerobic conditions, k = 0.302 d^{-1} with $t_{1/2}$ = 2.3 d under anaerobic conditions in sediment from San Diego Creek, Orange County, CA; first-order degradation k = 0.506 d^{-1} with $t_{1/2}$ = 1.4 d under aerobic conditions, k = 0.431 d^{-1} with $t_{1/2}$ = 1.6 d under anaerobic conditions in sediment from Bonita Creek, Orange County, CA (Bondarendo & Gan 2004)

Soil: estimated persistence of one week (Kearney et al. 1969; Edwards 1973; quoted, Morrill et al. 1982; Jury et al. 1987);

$t_{1/2}$ = 72–168 h, based on unacclimated aerobic soil grab sample data (Walker & Stojanovic 1973; quoted, Howard et al. 1991);

biodegradation rate constant of 1.4 d^{-1} in soil (Rao & Davidson 1980; quoted, Scow 1982);

non-persistent in soil with $t_{1/2}$ < 20 d (Willis & McDowell 1982);

$t_{1/2}$ = 1 d in screening model simulations (Jury et al. 1987b);

Degradation $t_{1/2}$ = 8 d in a coarse sandy soil, $t_{1/2}$ = 19 d in sandy loam (Kjeldsen et al. 1990)

selected field $t_{1/2}$ = 1.0 d (Wauchope et al. 1992; Dowd et al. 1993; Halfon et al. 1996; Hornsby et al. 1996);

soil $t_{1/2}$ = 11 d (Pait et al. 1992);

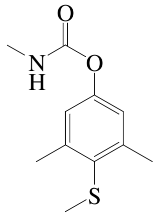
$t_{1/2}$ = 1 d for soil depth < 5 cm, $t_{1/2}$ = 7 d for soil depth 5–20 cm and $t_{1/2}$ = 14 d for soil depth >20 cm (Dowd et al. 1993).

Biota: biochemical $t_{1/2}$ = 1 d from screening model calculations (Jury et al. 1987b);

excretion $t_{1/2}$ = 1.4 h (willow shiner, Tsuda et al. 1989);

average $t_{1/2}$ = 20 d in the forest (USDA 1989; quoted, Neary et al. 1993).

18.1.1.56 Methiocarb



Common Name: Methiocarb
Synonym: Bayer 37344, Draza, Ensurol, Mercaptodimethur, Mesurol, Mesurol Phenol, metmercapturon
Chemical Name: 4-methylthio-3,5-xylyl methylcarbamate; 3,5-dimethyl-4-(methylthio)phenol methylcarbamate
Uses: Insecticide/Acaricide/Molluscicide/Repellent; to control slugs and snails in a wide range of agricultural situations; broad range control of lepidoptera, coleoptera, diptera, and homoptera and spider mites in pome fruit, stone fruit, citrus fruit, strawberries, hops, potatoes, beet, maize, oilseed rape, vegetables and ornamentals; also used as a bird repellent.
CAS Registry No: 2032-65-7
Molecular Formula: $C_{11}H_{15}NO_2S$
Molecular Weight: 225.308
Melting Point (°C):

120	(Lide 2003)

Boiling Point (°C):
Density (g/cm^3 at 20°C):

1.236	(Tomlin 1994)

Molar Volume (cm^3/mol):

261.4	(calculated-Le Bas method at normal boiling point)
182.3	(calculated-density)

Dissociation Constant, pK_a:
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
Entropy of Fusion, ΔS_{fus} (J/mol K):
Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F: 0.117 (mp at 120°C)

Water Solubility (g/m^3 or mg/L at 25°C or as indicated):

30	(20°C, Hartley & Kidd 1987; Worthing & Walker 1987; Milne 1995)
27	(20°C, Tomlin 1994)
24	(20–25°C, selected, Hornsby et al. 1996)

Vapor Pressure (Pa at 25°C or as indicated):

0.015	(60°C, Hartley & Kidd 1987)
1.5×10^{-5}	(20°C, Tomlin 1994)
3.6×10^{-5}	(Tomlin 1994)
0.016	(20–25°C, selected, Hornsby et al. 1996)

Henry's Law Constant (Pa·m^3/mol):

0.120	(calculated-P/C, this work)

Octanol/Water Partition Coefficient, log K_{OW}:

2.92	(shake flask as per Fujita et al. 1964; Briggs 1981)
2.92	(selected, Magee 1991)
3.34	(Tomlin 1994)
2.92	(recommended, Hansch et al. 1995)
2.82	(Pomona-database, Müller & Kördel 1996)
2.95	(RP-HPLC-RT correlation using short ODP column, Donovan & Pescatore 2002)

Bioconcentration Factor, log BCF:

Sorption Partition Coefficient, log K_{OC}:

2.32 (20°C, sorption isotherm, converted from log K_{OM} of 2.08, Briggs 1981)
2.08, 2.33 (reported as log K_{OM}, converted from K_{OM} multiplied by 1.724, Magee 1991)
2.82 (soil, HPLC-screening method, mean value of different stationary and mobile phases, Kördel et al. 1993, 1995)
2.32 (soil, calculated-MCI $^1\chi$, Sabljic et al. 1995)
2.82; 2.26 (HPLC-screening method; calculated-PCKOC fragment method, Müller & Kördel 1996)
2.48 (20–25°C, estimated, Hornsby et al. 1996)
3.12, 2.45, 2.38, 2.88, 2.80 (first generation Eurosoils ES-1, ES-2, ES-3, ES-4, ES-5, shake flask/batch equilibrium-HPLC/UV, Gawlik et al. 1998)
2.25 (sandy loam soil, column equilibrium method-HPLC/UV, 20°C, Xu et al. 1999)
2.741, 2.641, 2.377, 2.493, 2.824 (second generation Eurosoils ES-1, ES-2, ES-3, ES-4, ES-5, shake flask/batch equilibrium-HPLC/UV and HPLC-k′ correlation, Gawlik et al. 2000)
2.32; 2.23, 2.22 (soil, quoted exptl.; estimated-class specific model, estimated-general model, Gramatica et al. 2000)

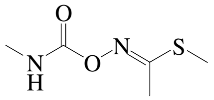
Environmental Fate Rate Constants, k, or Half-Lives, $t_{1/2}$:

Photolysis: photodegradation half-life of 6–16 d (Tomlin 1994).

Half-Lives in the Environment:

Soil: field $t_{1/2}$ = 30 d (20–25°C, estimated, Hornsby et al. 1996).

18.1.1.57 Methomyl



Common Name: Methomyl

Synonym: Du Pont 1179, ENT 27341, Lannate, Mesomile, Nu-bait II, Nudrin, SD 14999, WL 18236

Chemical Name: *S*-methyl-*N*-(methylcarbamoyloxy) thioacetimidate; methyl-*N*-(((methylamino)-carbonyl)oxy) ethan-imidothioate

Uses: insecticide/acaricide; control a wide range of insects and spider mites in fruit, vines, olives, hops, vegetables, ornamentals, field crops, cucurbits, flax, cotton, soya beans, etc.; also used for control of flies in animal and poultry houses and dairies.

CAS Registry No: 16752-77-5

Molecular Formula: $C_5H_{10}N_2O_2S$

Molecular Weight: 162.210

Melting Point (°C):

78–79	(Worthing & Hance 1991; Montgomery 1993; Tomlin 1994; Milne 1995)
78	(Lide 2003)

Boiling Point (°C):

Density (g/cm^3 at 20°C):

1.2946	(25°C, Spencer 1982; Worthing & Hance 1991; Tomlin 1994)
1.2946	(24°C, Milne 1995; Montgomery 1993)

Molar Volume (cm^3/mol):

179.9	(calculated-Le Bas method at normal boiling point)

Dissociation Constant, pK_a:

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

22.267	(DSC method, Plato 1972)

Entropy of Fusion, ΔS_{fus} (J/mol K):

Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F: 0.302 (mp at 78°C)

Water Solubility (g/m^3 or mg/L at 25°C or as indicated):

58000	(Worthing 1979; Khan 1980; Worthing 1983, 1987, Worthing & Hance 1991)
10000	(Kenaga 1980a; Kenaga & Goring 1980)
> 1000	(20°C, shake flask-GC, Bowman & Sans 1983a)
57900	(Hartley & Kidd 1987; Montgomery 1993; Tomlin 1994; Milne 1995)
58000	(20–25°C, selected, Hornsby et al. 1996)

Vapor Pressure (Pa at 25°C or as indicated):

3.47×10^{-3}	(20°C, Hartley & Graham-Bryce 1980)
6.66×10^{-3}	(Khan 1980; Spencer 1982)
0.162	(30°C, GC, Seiber et al. 1981)
6.67×10^{-3}	(Worthing 1983)
3.47×10^{-3}	(20°C, selected exptl. value, Kim 1985)
7.53×10^{-2}, 1.99×10^{-2}	(20°C, GC-RT correlation, GC-RT correlation with mp correction, Kim 1985)
6.65×10^{-3}	(Hartley & Kidd 1987; Worthing & Hance 1991; Montgomery 1993; Tomlin 1994)
6.67×10^{-3}	(20–25°C, selected, Hornsby et al. 1996)

Henry's Law Constant ($Pa \cdot m^3/mol$ at 25°C or as indicated:

1.82×10^{-5}	(calculated, Lyman et al. 1982)
6.50×10^{-5}	(20°C, calculated-P/C, Suntio et al. 1988)
6.48×10^{-5}	(calculated-P/C, Montgomery 1993)

Octanol/Water Partition Coefficient, log K_{OW}:

0.30	(Dow Chemical data, Kenaga & Goring 1980)
1.08	(Rao & Davidson 1980)
0.131	(22°C, shake flask-GC, Bowman & Sans 1983b)
0.60	(shake flask-HPLC, Drabel & Bachmann 1983)
0.60	(Hansch & Leo 1985)
0.13, 1.08	(Montgomery 1993)
0.60	(recommended, Sangster 1993)
0.09	(Tomlin 1994)
0.60	(selected, Hansch et al. 1995)

Bioconcentration Factor, log BCF:

0.477, 0.903	(calculated-S, calculated-K_{OC}, Kenaga 1980)
0.230, 0.110	(calculated-K_{OW}, calculated-S, Howard 1991)

Sorption Partition Coefficient, log K_{OC}:

2.20	(soil, Fung & Uren 1977)
1.45	(soil, calculated-S as per Kenaga & Goring 1978, Kenaga 1980)
1.71; 1.00	(calculated-K_{OW}; calculated-S, Lyman et al. 1982)
2.20	(Worthing 1983)
1.08	(soil, calculated-MCI χ and fragments contribution, Meylan et al. 1992)
1.86, 2.20	(Montgomery 1993)
1.86	(estimated-chemical structure, Lohninger 1994)
1.86	(Tomlin 1994)
1.30	(soil, calculated-MCI $^1\chi$, Sabljic et al. 1995)
1.86	(soil, 20–25°C, selected, Hornsby et al. 1996)
1.16, 1.62	(soil, estimated-class-specific model, estimated-general model, Gramatica et al. 2000)

Environmental Fate Rate Constants, k, Half-Lives, $t_{1/2}$

Volatilization:

Photolysis:

Oxidation: photooxidation $t_{1/2}$ ~ .14 months, based on vapor-phase reaction with hydroxyl radical in air (GEMS 1986; quoted, Howard 1991).

Hydrolysis: experimental $t_{1/2}$ = 262 d from rate constant $k = 8.9 \times 10^{-5}\ h^{-1}$ has been determined in pure water at pH 7 and 25°C (Ellington et al. 1987, 1988; quoted, Howard 1991; Montgomery 1993).

Biodegradation: rate constants $k = -0.000215\ h^{-1}$ in nonsterile sediment, $k = -0.000747\ h^{-1}$ in sterile sediment by shake-tests at Range Point and $k = -0.000175\ h^{-1}$ in nonsterile water and $k = -0.000383\ h^{-1}$ in sterile water by shake-tests at Range Point (Walker et al. 1988).

Biotransformation:

Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants:

Half-Lives in the Environment:

Air: $t_{1/2}$ ~ 1.14 months, based on rate constant $k = 2.919 \times 10^{-13}\ cm^3$/molecules for the vapor-phase reaction with $8 \times 10^5/cm^3$ hydroxyl radical in air (GEMS 1986; quoted, Howard 1991).

Surface water: experimental $t_{1/2}$ = 262 d has been determined in pure water at 25°C (Ellington et al. 1988; quoted, Howard 1991).

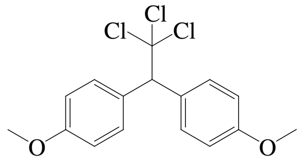
Ground water: $t_{1/2}$ < 0.2 d in ground water samples (Smelt et al. 1983; quoted, Tomlin 1994).

Sediment:

Soil: field $t_{1/2}$ = 30 d (20–25°C, selected, Hornsby et al. 1996).

Biota: $t_{1/2}$ ~ 3–5 d in plants following leaf application (Harvey & Reiser 1973; quoted, Tomlin 1994); $t_{1/2}$ = 0.4–8.5 d on cotton plants, $t_{1/2}$ = 0.8–1.2 d on mint plants and $t_{1/2}$ ~ 2.5 d on Bermuda grass (Willis & McDowell 1987; quoted, Howard 1991).

18.1.1.58 Methoxychlor



Common Name: Methoxychlor
Synonym: Chemform, Dimethoxy-DDT, DMDT, DMTD, ENT 1716, Maralate, Marlate, Methorcide, Methoxo, Metox, Moxie NCI-C00497
Chemical Name: 1,1,1-trichloro-2,2-bis(4-methoxyphenyl)ethane; 1,1′-(2,2,2-trichloroethylidene)bis[4-methoxybenzene]
Uses: insecticide to control mosquito larvae, house flies, and other insect pests in field crops, fruits, and vegetables; also to control ectoparasites on cattle, sheep, and goats.
CAS Registry No: 72-43-5
Molecular Formula: $C_{16}H_{15}Cl_3O_2$
Molecular Weight: 345.648
Melting Point (°C):
87 (Lide 2003)
Boiling Point (°C):
Density (g/cm^3 at 20°C):
1.41 (25°C, Hartley & Kidd 1987; Montgomery 1993; Tomlin 1994; Milne 1995)
Molar Volume (cm^3/mol):
354.3 (calculated-Le Bas method at normal boiling point)
245.1 (calculated-density)
Dissociation Constant, pK_a:
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
27.614 (DSC method, Plato & Glasgow 1969)
23.88 (Ruelle & Kesselring 1997)
Entropy of Fusion, ΔS_{fus} (J/mol K):
Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F: 0.246 (mp at 87°C)

Water Solubility (g/m^3 or mg/L at 25°C or as indicated and reported temperature dependence equations. Additional data at other temperatures designated *, are compiled at the end of this section):
0.10* (shake flask-UV, measured range 25–45°C, Richardson & Miller 1960)
0.62 (Karpoor et al. 1970)
0.003, 0.01, 0.045* (particle size of 0.01, 0.05 and 5.0μ; shake flask-GC, measured range 15–45°C, Biggar & Riggs 1974)
0.10 (generator column-GC/ECD, Weil et al. 1974)
0.12 (shake flask-GC/ECD, Zepp et al. 1976, Karickhoff et al. 1979; Karickhoff 1981)
0.1–0.25 (Wauchope 1978)
0.10 (Weber et al. 1980)
0.10 (Worthing 1983, 1987, Worthing & Hance 1991; Hartley & Kidd 1987; Tomlin 1994; Milne 1995)
0.10 (20–25°C, selected, Wauchope et al. 1992; Hornsby et al. 1996)
0.04 (24°C, Montgomery 1993)

Vapor Pressure (Pa at 25°C or as indicated):
$< 1.33 \times 10^{-4}$ (20–25° C, Weber et al. 1980)
1.910×10^{-4} (estimated, Howard 1991)

Henry's Law Constant (Pa·m^3/mol at 25°C or as indicated):
1.60 (estimated, Hine & Mookerjee 1975; quoted, Howard 1991)
0.999 (calculated-P/C, this work)
0.0206 (wetted wall column-GC, Altschuh et al. 1999)

Octanol/Water Partition Coefficient, log K_{OW}:

4.68 (HPLC-RT correlation, Veith & Morris 1978)
5.08 (shake flask-UV, Karickhoff et al. 1979; Karickhoff 1981)
4.30 (HPLC-RT correlation, Veith et al. 1979, 1980)
4.20 (Mackay et al. 1980)
4.83 (Belluck & Felsot 1981)
4.51 (HPLC-k′ correlation, McDuffie 1981)
4.83 (shake flask-UV, Nishimura & Fujita 1983)
4.68–5.08 (Hansch & Leo 1985)
4.91, 4.26 (shake flask, RP-TLC-RT correlation, Renberg et al. 1985)
3.31, 5.08 (Montgomery 1993)
4.95 (recommended, Sangster 1993)
5.08 (recommended, Hansch et al. 1995)
4.58 (RP-HPLC-RT correlation, Finizio et al. 1997)

Octanol/Air Partition Coefficient, log K_{OA}:

Bioconcentration Factor, log BCF:

–1.70 (bioaccumulation factor logBF, adipose tissue in female Albino rats, Harris et al. 1974)
4.68, 3.08, 3.72, 3.92 (*Bacillus subtilis*, *Flavobacterium harrisonii*, *Aspergillus sp.*, *Chlorella pyrenoidosa*, Paris et al. 1975; Paris & Lewis 1976)
4.40 (bacterial sorption, Paris & Lewis 1976)
2.14 (sheepshead minnow, Parrish et al. 1977)
3.92, 3.72 (algae, fungi, Wolfe et al. 1977)
3.92 (fathead minnows, 32 d exposure, Veith et al. 1979, 1980)
3.70–3.93, 2.54–3.05 (snail, Stonefly, Anderson & Defoe 1980)
2.27, 3.19 (fish: flowing water, static water; Kenaga 1980b; Kenaga & Goring 1980)
4.21, 3.91 (calculated-S, K_{OC}, Kenaga 1980)
1.15 (*Triaendoes tardus*, Belluck & Felsot 1981)
4.20, 3.04, 3.91 (estimated-S, K_{OW}, K_{OC}, Bysshe 1982)
3.92 (fathead minnows, Veith & Kosian 1983)
4.08 (mussel, Renberg et al. 1985)
3.18 (soft clams, Hawker & Connell 1986)
3.92 (calculated, Isnard & Lambert 1988)
5.40 (calculated field bioaccumulation, Thomann 1989)
5.29 (rainbow trout lipid base, estimated, Noegrohati & Hammers 1992)
3.98; 4.05 (*Oncorhynchus mykiss*, wet wt. basis: quoted exptl.; calculated-QSAR model based on quantum chemical parameters, Wei et al. 2001)

Sorption Partition Coefficient, log K_{OC}:

2.79 (water-sediment, Wolfe et al. 1977)
4.90 (av. for isotherms on sediments, Karickhoff et al. 1979)
3.99–4.61, 4.90–5.00, 4.86–4.96 (sand, fine silt, clay Karickhoff et al. 1979)
4.90 (soil, quoted, Kenaga 1980a, b; Kenaga & Goring 1980; Bysshe 1982)
5.03 (soil, calculated-S as per Kenaga & Goring 1978, Kenaga 1980)
6.04 (calculated-S, Mill et al. 1980)
4.90 (av. soils/sediments, Rao & Davidson 1980)
4.67, 4.69, 5.54 (estimated-S, K_{OW}, S and mp, Karickhoff 1981)
4.26 (soil, screening model calculations, Jury et al. 1987b)
4.99 (RP-HPLC-k′ correlation, cyanopropyl column, Hodson & Williams 1988)
4.63 (soil, calculated-MCI χ and fragment contribution, Meylan et al. 1992)
4.90 (soil, 20–25°C, selected, Wauchope et al. 1992; Hornsby et al. 1996)
4.90 (estimated-QSAR and SPARC, Kollig 1993)
4.90, 4.95 (Montgomery 1993)
4.90 (soil, calculated-MCI $^1\chi$, Sabljic et al. 1995)

Environmental Fate Rate Constants, k, or Half-Lives, $t_{½}$:

Volatilization: $t_{½}$ = 4.5 d from water was estimated based on Henry's law constant for a model river 1 m deep with a current of 1 m/s and a wind speed of 3 m/s (Howard 1991).

Photolysis: midsummer direct photolysis $t_{½}$ = 690 h in water, $t_{½}$ = 4100 h in hydrocarbon media; midday $t_{½}$ = 1100 h average over all seasons in water at latitude 40°N, daily average direct photolysis $t_{½}$ = 4.5 months (12-h days) in water in the Central U.S. (Zepp et al. 1976)

photodecomposition $t_{½} > 300$ h in distilled water, $t_{½}$ = 2.2 h in Suwannee River water, $t_{½}$ = 5.4 h in Tombigbee River water, $t_{½}$ = 2.9 h in Alabama River water with methoxychlor at 40 ppb under sunlight (Zepp et al. 1976)

$t_{½}$ = 300–2070 h in both air and natural water, based on measured photolysis rates in distilled water under midday sunlight and adjusted for approximate winter sunlight intensity (Howard et al. 1991).

Oxidation:

photooxidation $t_{½}$ = 2.2–5.4 h in natural water, based on measured photooxidation in river water exposed to midday May sunlight (Zepp et al. 1976; quoted, Howard et al. 1991);

photooxidation $t_{½}$ ~ 1.12–11.2 h in air, based on rate constant for the vapor-phase reaction with hydroxyl radical in air (Atkinson 1987; quoted, Howard et al. 1991)

k(aq.) = (270 ± 80) $M^{-1}\ s^{-1}$ for direct reaction with ozone in water at pH 2 and 24 ± 1°C, with $t_{½}$ = 21 min at pH 7 (Yao & Haag 1991).

k_{OH}(aq.) = $2 \times 10^{10}\ M^{-1}\ s^{-1}$ for the reaction with hydroxyl radicals in aqueous solutions at 24 ± 1°C (Haag & Yao 1992).

Hydrolysis: k(alkaline) = $3.8 \times 10^{-4}\ M^{-1}\ s^{-1}$ with $t_{½}$ = 2100 d at 27°C, k(neutral) = $2.2 \times 10^{-8}\ s^{-1}$ at pH 3–7 corresponds to a $t_{½}$ = 367 d at pH 9 and 27°C (Wolf et al. 1977)

Overall rate constant k = $5.5 \times 10^{-8}\ s^{-1}$ with $t_{½}$ = 147 d; k = $3.0 \times 10^{-8}\ s^{-1}$ with $t_{½}$ = 270 d at 25°C and pH 7 (Mabey & Mill 1978)

k(alkaline) = $3.8 \times 10^{-4}\ M^{-1}\ s^{-1}$, k(neutral) = $2.2 \times 10^{-8}\ s^{-1}$, 1×10^{-8} M in water at 27°C (Harris 1982)

$t_{½}$ = 1.05 yr, based on neutral and base catalyzed hydrolysis rate constants Howard et al. 1991)

k = 0.60 yr^{-1} at pH 7 and 25°C (Kollig 1993)

$t_{½}$ = 370 d at pH 2, $t_{½}$ = 370 d at pH 7 and $t_{½}$ = 270 d at pH 12 in natural waters (Capel & Larson 1995)

Biodegradation: $t_{½}$(aq. aerobic) = 4320–8760 h (6 months to 1 yr), based on very slow biodegradation observed in an aerobic soil die-away test study data (Fogel et al. 1982; quoted, Howard et al. 1991)

$t_{½}$(aq. anaerobic) = 1200–4320 h (50 d to 6 months), based on anaerobic soil die-away test study data (Fogel et al. 1982; quoted, Howard et al. 1991)

k = –0.00236 h^{-1} in nonsterile sediment and k = –0.000639 h^{-1} in sterile sediment by shake-tests at Range Point and k = –0.000139 h^{-1} in nonsterile water and k = –0.00000327 h^{-1} in sterile water by shake-tests at Range Point (Walker et al. 1988)

$t_{½}$(aerobic) = 180 d, $t_{½}$(anaerobic) = 50 d in natural waters (Capel & Larson 1995).

Biotransformation:

Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants:

k_1 = 14.4–37.5 h^{-1} (*Chironomus tentans* larvae in pond sediment-water system, 96-h exposure, calculated by using first-order kinetic and concn factors, Muir et al. 1983)

k_1 = 11.4–82.0 h^{-1} (*Chironomus tentans* larvae in river sediment-water system, 96-h exposure, calculated by using first-order kinetic and concn factors, Muir et al. 1983)

k_1 = 35.8–54.9 h^{-1} (*Chironomus tentans* larvae in sediment (sand)-water system, 96-h exposure, calculated by using first-order kinetic and concn factors, Muir et al. 1983)

k_1 = 35.8–54.9 h^{-1} (*Chironomus tentans* larvae in sediment (sand)-water system, 96-h exposure, calculated by using initial uptake data of 0–12 h, Muir et al. 1983)

k_2 = 45.4–38.6 h^{-1} (*Chironomus tentans* larvae in pond sediment-water system, calculated by concentration decay curve, Muir et al. 1983)

k_2 = 0.030 h^{-1} (*Chironomus tentans* larvae in sediment (sand)-water system, calculated by concentration decay curve, Muir et al. 1983)

Half-Lives in the Environment:

Air: $t_{½}$ ~ 1.12–11.2 h, based on rate constant for the vapor-phase reaction with hydroxyl radicals in air (Atkinson 1987; quoted, Howard et al. 1991);

atmospheric transformation lifetime was estimated to be < 1 d (Kelly et al. 1994).

Surface water: midsummer direct photolysis $t_{1/2}$ = 690 h in water; midday $t_{1/2}$ = 1100 h average over all seasons in water at latitude 40°N, daily average direct photolysis $t_{1/2}$ = 4.5 months (12-h days) in water in the Central U.S. (Zepp et al. 1976)

$t_{1/2}$ = 2.2–5.4 h, based on measured photooxidation in river water exposed to midday May sunlight (Zepp et al. 1976; quoted, Howard et al. 1991);

measured k = (270 ± 80) M^{-1} s^{-1} for direct reaction with ozone in water at pH 2.7–6.4 and 24 ± 1°C, with a $t_{1/2}$ = 2.1 min at pH 7 (Yao & Haag 1991)

biodegradation $t_{1/2}$(aerobic) = 180 d, $t_{1/2}$(anaerobic) = 50 d, hydrolysis $t_{1/2}$ = 370 d at pH 2, $t_{1/2}$ = 370 d at pH 7 and $t_{1/2}$ = 270 d at pH 12 in natural waters (Capel & Larson 1995).

Ground water: $t_{1/2}$ = 1200–8760 h, based on aerobic and anaerobic soil die-away test study data (Fogel et al. 1982; quoted, Howard et al. 1991).

Sediment:

Soil: $t_{1/2}$ = 1.5 wk at pH 4.7 and 6.5 and $t_{1/2}$ = 1.0 wk at pH 7.8 (Carlo et al. 1952; quoted, Kaufman 1976);

$t_{1/2}$ = 4320–8760 h, based on very slow biodegradation observed in an aerobic soil die-away test study data (Fogel et al. 1982; quoted, Howard et al. 1991);

$t_{1/2}$ = 42 d in screening model calculations (Jury et al. 1987b);

selected field $t_{1/2}$ = 120 d (Wauchope et al. 1992; Hornsby et al. 1996).

Biota: elimination $t_{1/2}$ = 9.6 h in pond sediment-water, $t_{1/2}$ = 23.2 h in sand-water system (*Chironomus tentans* larvae, Muir et al. 1983);

$t_{1/2}$ = 0.4–8.5 d on cotton plants, $t_{1/2}$ = 0.8–1.2 d on mint plants and $t_{1/2}$ ~ 2.5 d on Bermuda grass (Willis & McDowell 1987; quoted, Howard 1991).

TABLE 18.1.1.58.1
Reported aqueous solubilities of methoxychlor at various temperatures

Richardson & Miller 1960		Biggar & Riggs 1974			
shake flask-UV spec.		shake flask-GC			
t/°C	S/g·m^{-3}	t/°C	S/g·m^{-3}	S/g·m^{-3}	S/g·m^{-3}
		particle size	0.01μ	0.05μ	5.0μ
25	0.10	15	-	-	0.020
35	0.20	25	0.003	0.010	0.045
45	0.40	35	-	-	0.095
		45	-	-	0.185

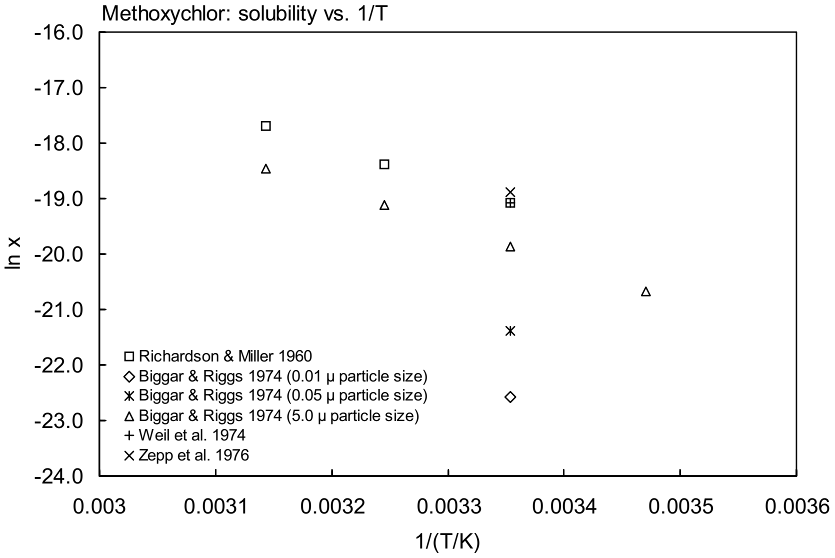
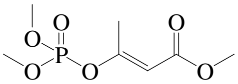


FIGURE 18.1.1.58.1 Logarithm of mole fraction solubility (ln *x*) versus reciprocal temperature for methoxychlor.

18.1.1.59 Mevinphos



Common Name: Mevinphos

Synonym: Apavinfos, CMDP, Compound 2046, Duraphos, ENT 22374, Fosdrin, Gesfid, Gestid, Meniphos, Menite, NA 2783, OS 2046, PD 5, Phosdrin, Phosfene

Chemical Name: 2-carbomethoxy-1-methylvinyl dimethyl phosphate; 1-methoxycarbonyl-1-propen-2-yl dimethyl phosphate; methyl-3-(dimethoxyphosphinoyloxy)but-2-enoate 2-carbomethoxy-1-methylvinyl dimethyl phosphate

Uses: contact insecticide and acaricide to control chewing insects and spider mites in fruits, vegetables, and ornamentals.

CAS Registry No: 7786-34-7 [formerly 298-01-1 for (E) isomer & 338-45-4 for (Z) isomer] for cis-isomer and 338-45-4 for *trans*-isomer]

Molecular Formula: $C_7H_{13}O_6P$

Molecular Weight: 224.1 48

Melting Point (°C):

–56.1	(Montgomery 1993; Lide 2003)
21	((E) isomer, Lide 2003)
6.9	((Z) isomer, Lide 2003)

Boiling Point (°C)

99–103	(at 0.03 mmHg, Martin 1971; Freed et al. 1977; Milne 1995)
76.0	(at 0.2 mmHg, Melnikov 1971; Freed et al. 1979)
110	(at 1.6 mmHg, Hartley & Kidd 1987)
106–107.5	(at 1 mmHg, Montgomery 1993)

Density (g/cm^3 at 20°C):

1.24	(Hartley & Kidd 1987; Tomlin 1994; Milne 1995)
1.25	(Montgomery 1993)
1.235, 1.245	((E) isomer, (Z) isomer, Tomlin 1995)

Molar Volume (cm^3/mol):

180.7	(calculated from density)

Dissociation Constant, pK_a:

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

Entropy of Fusion, ΔS_{fus} (J/mol K):

Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F: 1.0

Water Solubility (g/m^3 or mg/L at 25°C or as indicated):

miscible	(Spencer 1973; Worthing 1979; Freed et al. 1979)
> 2000	(shake flask-GC, Bowman & Sans 1983a)
miscible	(Hartley & Kidd 1987; Tomlin 1994)
miscible	(Worthing & Walker 1987)
600000	(20–25°C, selected, Wauchope 1989; Wauchope et al. 1992; Hornsby et al. 1996)

Vapor Pressure (Pa at 25°C or as indicated):

0.293	(20°C, Eichler 1965)
0.293	(20–25°C, Melnikov 1971)
0.757	(20°C, GC-RT correlation, Kim et al. 1984; Kim 1985)
0.017	(20°C, Hartley & Kidd 1987; Tomlin 1994)
0.0173	(20–25°C, selected, Wauchope et al. 1992; Hornsby et al. 1996)
0.293	(20°C, Montgomery 1993)

Henry's Law Constant (Pa·m^3/mol):

6.35×10^{-6}	(calculated-P/C, this work)

Octanol/Water Partition Coefficient, log K_{OW}:

0.845	(Melnikov 1971)
0.954	(Freed et al. 1977)
0.550	(selected, Dao et al. 1983)
1.20	(shake flask, Log P Database. Hansch & Leo 1987)
0.200	(selected, Boehncke et al. 1990)
0.130	(Tomlin 1994)
1.20	(recommended, Hansch et al. 1995)

Bioconcentration Factor, log BCF:

Sorption Partition Coefficient, log K_{OC}:

1.64	(soil, 20–25°C, selected, Wauchope et al. 1992; Hornsby et al. 1996)
1.64	(estimated-chemical structure, Lohninger 1994)
2.30	(soil, calculated-MCI $^1\chi$, Sabljic et al. 1995)
2.12, 1.56	(soil, *cis*-mevinphos, estimated-class-specific model, estimated-general model, Gramatica et al. 2000)
2.28, 1.67	(soil, *trans*-mevinphos, estimated-class-specific model, estimated-general model, Gramatica et al. 2000)

Environmental Fate Rate Constants, k, or Half-Lives, $t_{1/2}$:

Hydrolysis: $t_{1/2}$ = 1.8 h for *cis*- and $t_{1/2}$ = 3.0 h for *trans*-isomer at pH 11.6 (Casida et al. 1956; quoted, Montgomery 1993);

$t_{1/2}$ = 30–35 d (Melnikov 1971; quoted, Freed et al. 1977);

$t_{1/2}$ = 120 d at pH 6, $t_{1/2}$ = 35 d at pH 7, $t_{1/2}$ = 3 d at pH 9, and $t_{1/2}$ = 1.4 h at pH 11 (Montgomery 1993; Tomlin 1994).

Half-Lives in the Environment:

Air:

Surface water:

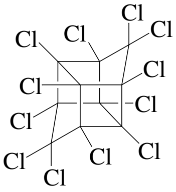
Ground water:

Sediment:

Soil: selected field $t_{1/2}$ = 3 d (Wauchope et al. 1992; Hornsby et al. 1996).

Biota: estimated $t_{1/2}$ = 19 ± 2 and 24 ± 7 h in lettuce in the summer and $t_{1/2}$ = 20 ± 11 h in the fall, $t_{1/2}$ = 50 h in cauliflower in the summer and $t_{1/2}$ = 18 ± 1 h in the fall, $t_{1/2}$ = 25 ± 2 h in celery in the summer and $t_{1/2}$ = 16 h in the fall (Spencer et al. 1992)

18.1.1.60 Mirex



Common Name: Mirex
Synonym: Bichlorendo, Declorane, ENT 25719, Ferriamicide, Paramex, Perclordecone
Chemical Name: 1,1a,2,2,3,3a,4,5,5,5a,5b,6-dodecachloro-octahydro-1,3,4-methano-1H-cyclobuta(cd) pentalene; dodecachloro-pentacyclodecane
Uses: Insecticide.
CAS Registry No: 2385-85-5
Molecular Formula: $C_{10}Cl_{12}$
Molecular Weight: 545.542
Melting Point (°C):
485 (dec., Smith et al. 1978; Spencer 1982; Kühne et al. 1995; Milne 1995; Lide 2003)
Boiling Point (°C):
Molar Volume (cm^3/mol):
403.2 (calculated-Le Bas method at normal boiling point)
Dissociation Constant, pK_a:
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
Entropy of Fusion, ΔS_{fus} (J/mol K):
Fugacity Ratio, at 25°C (assuming ΔS_{fus} = 56 J/mol K), F: 3.1×10^{-5} (mp at 485°C)

Water Solubility (g/m^3 or mg/L at 25°C or as indicated):
0.001 (from D. Dollar of Miss. State Chem. Lab. unpublished results, Alley 1973)
0.085 (shake flask-LSC, Metcalf et al. 1973)
0.60 (Neely 1978; quoted, Kenaga 1980; Kenaga & Goring 1980)
7.0×10^{-5} (22°C, shake flask-GC, Smith et al. 1978)
0.02 (24°C, Verschueren 1983)
7.0×10^{-5} (20–25°C, estimated, Augustijn-Beckers et al. 1994; Hornsby et al. 1996)

Vapor Pressure (Pa at 25°C or indicated and reported temperature dependence equations):
8.0×10^{-4} (50°C, Smith, et al. 1978)
1.3×10^{-4} (20°C, Smith et al. 1978)
1.0×10^{-4} (20°C, selected, Suntio et al. 1988)
9.0×10^{-7} (10°C, estimated, McLachlan et al. 1990)
2.5×10^{-4}, 2.9×10^{-4}, 2.8×10^{-4} (GC-RT correlation, supercooled liquid, Hinckley et al. 1990)
5.2×10^{-5} (12°C, extrapolated supercooled liquid value, Hinckley et al. 1990)
1.1×10^{-4} (20–25°C, selected, Augustijn-Beckers et al. 1994; Hornsby et al. 1996)

Henry's Law Constant (Pa·m^3/mol and reported temperature dependence equations):
1013 (20°C, calculated, Smith et al. 1978)
53.2 (22°C, gas stripping-GC/ECD, Yin & Hassett 1986)
$\log [H/(atm\ m^3/mol)] = 12.709 - 4711/(T/K)$, temp range: 8–24°C (gas stripping-GC, Yin & Hassett 1986)
840 (20°C, calculated-P/C, Suntio et al. 1988)
44.1 (20°C, selected from literature experimentally measured data, Staudinger & Roberts 1996, 2001)
$\log K_{AW} = 13.899 - 4585/(T/K)$, (van't Hoff eq. derived from literature data, Staudinger & Roberts 2001)

Octanol/Water Partition Coefficient, $\log K_{OW}$:
7.50 (Hansch & Leo 1979)
6.89 (HPLC-RT correlation, Veith et al. 1979; Veith & Kosian 1983)

5.28 (shake flask, Log P Database, Hansch & Leo 1987)
5.28 (recommended, Sangster 1993)
5.28 (recommended, Hansch et al. 1995)
7.13–7.24 (shake flask/slow stirring-GC/ECD, both phases, Fisk et al. 1999)

Octanol/Air Partition Coefficient, log K_{OA}:

Bioconcentration Factor, log BCF:
2.34, 3.07 (*Gambusia, Physa*, Metcalf et al. 1973)
2.78 (*Oedogonium sp.*, Metcalf et al. 1973)
2.18 (bioaccumulation factor log BF, adipose tissue in female Albino rats, Ivie et al. 1974)
–2.02 (milk biotransfer factor log B_m, correlated-K_{OW}, Dorough & Ivie 1974)
2.34 (fish in static water, Metcalf 1974)
–1.25 (beef biotransfer factor log B_b, correlated-K_{OW}, Bond et al. 1975)
–1.14 (vegetation, correlated-K_{OW}, De La Cruz & Rajanna 1975)
3.86; 3.51; 3.61; 3.70 (*Chlorococcum sp.*; *Chlamydomonas sp.*; *Dunaliella tertiolecta*; *Thallasidsira pseudomana*, Hollister et al. 1975)
5.60 (bacterial sorption, Smith et al. 1978)
4.26 (fathead minnows, 32-d exposure, Veith et al. 1979, 1980)
2.91 (calculated-S, Kenaga 1980)
4.71 (fathead minnow to ^{14}C mirex, Huckins et al. 1982)
4.34 (fish, correlated, Mackay 1982)
4.26 (fathead minnow, Veith & Kosian 1983)
4.09, 3.41 (algae, fish, Verschueren 1983)
6.50 (fish, selected, Paterson & Mackay 1985)
1.78–2.87 highest value 2.87 but not equilibrated (rainbow trout, 15°C, steady-state BCF on 7- to 96-d laboratory study, Oliver & Niimi 1985)
> 4.08; 2.87 (rainbow trout, kinetic BCF-k_1/k_2; steady-state BCF in laboratory studies, Oliver & Niimi 1985)
6.08; 7.18 (rainbow trout, calculated-K_{OW}, Lake Ontario field data, Oliver & Niimi 1985)
2.87 (fish, Oliver & Niimi 1985; Oliver 1987)
4.34 (worms, Oliver 1987)
6.17 (oligochaetes, Connell et al. 1988)
6.41 (smelt, Oliver & Niimi 1988)
4.31 (*Poecilia reticulata*, Gobas et al. 1989; quoted, Devillers et al. 1996)
6.42, 7.16 (guppy, correlated, Gobas et al. 1989)
6.40 (Markwell et al. 1989)
4.72, 7.07 (dry leaf, wet leaf, Bacci et al. 1990)
7.07 (wet leaf, Bacci et al. 1990)
5.97, 7.16 (guppy 6.5% lipid: wet wt basis, lipid wt basis, Geyer et al. 2000)
3.79–4.26, 3.95–4.40 (human, fat: wet wt basis, lipid wt basis, Geyer et al. 2000)

Bioaccumulation Factor log BAF:
8.27 (calculated field bioaccumulation, Thomann 1989)

Sorption Partition Coefficient, log K_{OC}:
5.56 (natural sediment, Smith et al. 1978)
7.38 (av. soils/sediments, Smith et al. 1978)
3.76 (soil, quoted exptl., Kenaga 1980)
3.08 (soil, calculated-S as per Kenaga & Goring 1978, Kenaga 1980)
6.00, 5.67 (derived from exptl., calculated-MCI χ, Meylan et al. 1992)
6.42 ± 0.39 (suspended particulate matter of the St. Lawrence River, Comba et al. 1993)
6.00 (20–25°C, soil, estimated, Augustijn-Beckers et al. 1994; Hornsby et al. 1996)
6.00 (soil, calculated-MCI $^1\chi$, Sabljic et al. 1995)

Rate Constants, k, and Environmental Half-Lives, $t_{½}$:

Volatilization: $k = 5.37 \times 10^{-2}$ h^{-1} (Hill et al. 1976) with $t_{½}$ = 500 h from river, $t_{½}$ = 700 h from pond, $t_{½}$ = 1980 h from eutrophic lake, and 1 $t_{½}$ = 980 h from oligotrophic lake (Smith et al. 1978).

Photolysis: rate constants $k < 5.0 \times 10^{-8}$ s^{-1} (laboratory data, Smith et al. 1978);

$k = 4.2 \times 10^{-3}$ d^{-1} (field data, Smith et al. 1978);

$t_{½} = 3.9 \times 10^3$ h (aquatic half-life, Haque et al. 1980);

k = 0.123 d^{-1} (sunlight, distilled water containing 2.0 mg DOC/L humic acid, Mudambi & Hasset 1988);

k = 0.033 d^{-1} (sunlight, distilled water, summer, Mudambi & Hassett 1988);

k = 0.102 d^{-1} (sunlight, Lake Ontario water, Mudambi & Hassett 1988);

k = 0.019 d^{-1} (sunlight, distilled water, fall, Mudambi & Hassett 1988).

Oxidation: laboratory data k < 30 M^{-1} s^{-1} (Smith et al. 1978); $t_{½}$ >> 0.7 yr (Smith et al. 1978; quoted, Cheung 1984).

Hydrolysis: laboratory data rate constant $k = 1 \times 10^{-10}$ s^{-1} (Smith et al. 1978); $k = 2 \times 10^{-10}$ s^{-1} with $t_{½}$ = 250 yr (Cheung 1984);

degradation rate constant $k = 1.93 \times 10^{-4}$ h^{-1} (Mackay et al. 1985; quoted, Mackay & Paterson 1991).

Biodegradation: slow process (Cheung 1984).

Biotransformation:

Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants:

$k_1 > 8.50$ d^{-1} (rainbow trout, Oliver & Niimi 1985)

$k_2 < 0.0007$ d^{-1} (rainbow trout, Oliver & Niimi 1985)

$k_2 = 0.017$ d^{-1} with $t_{½}$ = 42 d and $k_2 = 0.009$ d^{-1} with $t_{½}$ = 78 d for food concn of 21 ng/g and 145 ng/g, respectively, in a 30-d uptake followed by 160-d depuration studies for juvenile rainbow trout (Fisk et al. 1998)

Half-Lives in the Environments:

Air:

Surface water: overall $t_{½}$ = 0.83 h in river or stream, $t_{½}$ = 420 h in pond, and $t_{½}$ = 1480 h by sorption in both eutrophic lake and oligotrophic lake; with photolysis $t_{½}$ > 8000 h and oxidation $t_{½}$ > 1000 h in pond, river, eutrophic lake and oligotrophic lake (Smith et al. 1978);

degradation rate constant $k = 1.93 \times 10^{-4}$ h^{-1} (Mackay et al. 1985; quoted, Mackay & Paterson 1991);

$t_{½}$ = 7 d in sunlit, air-equilibrated humic acid solution, or natural water (Mudambi & Hassett 1988; Burns et al. 1996).

Ground water:

Soil: estimated field $t_{½}$ = 3000 d (Augustijn-Beckers et al. 1994; Hornsby et al. 1996)

$t_{½}$ = 8.2 yr, extremely persistent in soil (Geyer et al. 2000)

Biota: $t_{½}$ > 1000 d (Skea et al. 1981; Oliver & Niimi 1985);

$t_{½}$ > 28 d in fathead minnow to ^{14}C mirex (Huckins et al. 1982);

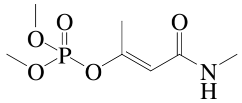
$t_{½}$ > 500 d (4°C, rainbow trout, Niimi & Palazzo 1985);

$t_{½}$ = 114 d as observed and $t_{½}$ = 495 d as adjusted (12°C, rainbow trout, Niimi & Palazzo 1985);

$t_{½}$ = 103 d as observed and $t_{½}$ > 1000 d as adjusted (18°C, rainbow trout, Niimi & Palazzo 1985).

Depuration $t_{½}$ = 42–78 d in 30-d uptake and 160-d depuration studies (juvenile rainbow trout, Fisk et al. 1998)

18.1.1.61 Monocrotophos



Common Name: Monocrotophos
Synonym: Apadrin, Azodrin, Bilobran, Crotos, ENT 27129, Monocron, Nuvacron
Chemical Name: dimethyl (E)-1-methyl-2-(2-methylcarbamoyl)vinyl phosphate
Uses: systemic insecticide and acaricide to control pests in cotton, sugar cane, coffee, tobacco, olives, rice hops, sorghum, maize, deciduous fruits, citrus fruits, potatoes, sugar beet, tomatoes, soya beans, and ornamentals.
CAS Registry No: 6923-22-4
Molecular Formula: $C_7H_{14}NO_5P$
Molecular Weight: 223.164
Melting Point (°C):
55 (Lide 2003)
Boiling Point (°C):
125 (at 0.0005 mmHg, Hartley & Kidd 1987; Worthing & Hance 1991; Montgomery 1993; Tomlin 1994; Milne 1995)
Density (g/cm^3 at 20°C):
1.33 (Hartley & Kidd 1987; Worthing & Hance 1991; Montgomery 1993; Milne 1995)
1.22 (Tomlin 1994)
Molar Volume (cm^3/mol):
Dissociation Constant, pK_a:
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
Entropy of Fusion, ΔS_{fus} (J/mol K):
Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F: 0.508 (mp at 55°C)

Water Solubility (g/m^3 or mg/L at 25°C or as indicated):
miscible (Spencer 1973; Budavari 1989)
miscible (Hartley & Kidd 1987; Montgomery 1993; Tomlin 1994)
1000000 (Worthing & Walker 1987, Worthing & Hance 1991; Milne 1995)
1000000 (20–25°C, selected, Wauchope et al. 1992; Hornsby et al. 1996)

Vapor Pressure (Pa at 25°C or as indicated):
9.33×10^{-3} (20°C, Eichler 1965)
9.33×10^{-3} (20°C, Wolfdietrich 1965; Melnikov 1971; Budavari 1989)
9.33×10^{-4} (20°C, Hartley & Graham-Bryce 1980)
5.09×10^{-3} (20°C, GC-RT correlation without mp correlation, Kim et al. 1984; Kim 1985)
2.30×10^{-3} (20°C, GC-RT correlation with mp correction, Kim 1985)
9.00×10^{-3} (Hartley & Kidd 1987)
2.90×10^{-4} (20°C, Worthing & Hance 1991; Tomlin 1994)
9.33×10^{-3} (20–25°C, selected, Wauchope et al. 1992; Hornsby et al. 1996)
9.00×10^{-3} (20°C, Montgomery 1993)
0.0295; 0.0039, 0.019 (gradient GC method; estimation using modified Watson method: Sugden's parachor, McGowan's parachor, Tsuzuki 2000)

Henry's Law Constant (Pa·m^3/mol at 25°C or as indicated):
2.08×10^{-6} (20–25°C, calculated-P/C, this work)

Octanol/Water Partition Coefficient, log K_{OW}:
–1.97 (calculated, Montgomery 1993)
–0.22 (calculated, Tomlin 1994)
–0.20 (recommended, Hansch et al. 1995)

Octanol/Air Partition Coefficient, log K_{OA}:

Bioconcentration Factor, log BCF

Sorption Partition Coefficient, log K_{OC}:

0.0	(soil, 20–25°C, estimated, Wauchope et al. 1992; Hornsby et al. 1996)
2.29, 1.65	(soil, *trans*-isomer, estimated-class-specific model, estimated-general model using molecular descriptors, Gramatica et al. 2000)

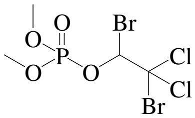
Environmental Fate Rate Constants, k, or Half-Lives, $t_{½}$:

Hydrolysis: calculated $t_{½}$ = 96 d at pH 5, $t_{½}$ = 66 d at pH 7 and $t_{½}$ = 17 d at pH 9 and 20°C (Worthing & Hance 1991; Montgomery 1993; Tomlin 1994).

Half-Lives in the Environment:

Soil: selected field $t_{½}$ = 30 d (Wauchope et al. 1992; Hornsby et al. 1996);
$t_{½}$ = 1–5 d in laboratory soil (Tomlin 1994).

18.1.1.62 Naled



Common Name: Naled
Synonym: Arthodibrom, Dibrom, Bromex, Bromchlophos
Chemical Name: 1,2-dibromo-2,2-dichloroethyl dimethyl phosphate
CAS Registry No: 300-76-5
Uses: insecticide
Molecular Formula: $C_4H_7Br_2Cl_2O_4P$
Molecular Weight: 380.784
Melting Point (°C):
27 (Lide 2003)
Boiling Point (°C):
110/0.5 mmHg (Spencer 1982; Hartley & Kidd 1987; Worthing & Walker 1987; Montgomery 1993; Tomlin 1994)
Density (g/cm^3 at 20°C):
1.96 (20°C, Hartley & Kidd 1987; Montgomery 1993; Tomlin 1994)
1.97 (20°C, Worthing 1987)
Molar Volume (cm^3/mol):
Dissociation Constant, pK_a:
Enthalpy of Vaporization, ΔH_V (kJ/mol):
77.23 (Rordorf 1989)
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
Entropy of Fusion, ΔS_{fus} (J/mol K):
Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F: 0.956 (mp at 27°C)

Water Solubility (g/m^3 or mg/L at 25°C):
practically insoluble in water (Hartley & Kidd 1987; Worthing & Walker 1987)
0.3, 2000 (quoted, Wauchope et al. 1992)
2000 (20–25°C, selected, Wauchope et al. 1992; Hornsby et al. 1996)
10 (Montgomery 1993)

Vapor Pressure (Pa at 25°C or as indicated and reported temperature dependence equations):
0.266 (20°C, Hartley & Kidd 1987; Worthing & Walker 1987; Tomlin 1994)
6.0×10^{-2}, 0.67, 5.20, 31.0, 150 (25, 50, 70, 100, 125°C, gas saturation-GC, Rordorf 1989)
$\log (P_L/Pa) = 12.307 - 4034.2/(T/K)$; measured range 50.5–120°C (liquid, gas saturation-GC, Rordorf 1989)
0.267, 0.00267 (Wauchope et al. 1992)
0.0267 (20–25°C, selected, Wauchope et al. 1992; Hornsby et al. 1996)
0.267 (20°C, Montgomery 1993)

Henry's Law Constant (Pa·m^3/mol at 25°C):

Octanol/Water Partition Coefficient, log K_{OW}:
1.38 (shake flask-GC/UV, Hussain et al. 1974)

Octanol/Air Partition Coefficient, log K_{OA}:

Bioconcentration Factor, log BCF or log K_B:

Sorption Partition Coefficient, log K_{OC}:

133, 2.26; 2.26	(soil, quoted values; selected, Wauchope et al. 1992; Hornsby et al. 1996)
2.14, 3.38	(soil, estimated-class-specific model, estimated-general model using molecular descriptors, Gramatica et al. 2000)

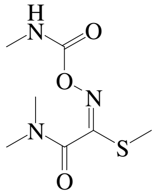
Environmental Fate Rate Constants, k, or Half-Lives, $t_{½}$:

Volatilization:
Photolysis: degraded by sunlight (Tomlin 1994).
Oxidation:
Hydrolysis: completely hydrolyzed in water within 2 d (Windholz 1983; quoted, Montgomery 1993);
rapidly hydrolyzed in water > 90% in 48 h at room temp. (Spencer 1982; Hartley & Kidd 1987; Worthing 1987; Tomlin 1994).
Biodegradation:
Biotransformation:
Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants:

Half-Lives in the Environment:

Air:
Surface water: completely hydrolyzed within 2 d (Windholz 1983; quoted, Montgomery 1993);
rapidly hydrolyzed in water > 90% in 48 h at room temp. (Spencer 1982; Hartley & Kidd 1987; Worthing 1987; Tomlin 1994).
Ground water:
Sediment:
Soil: field $t_{½}$ = 1 d (Wauchope et al. 1992; Hornsby et al. 1996).
Biota:

18.1.1.63 Oxamyl



Common Name: Oxamyl
Synonym: D 1410, Dioxamyl, Dupont 1410, Nematicide 1410, Thioxamyl, Vydate
Chemical Name: *N,N*-dimethylcarbamoyloxyimino-2-(methylthio)acetamide; ethanimidothioic acid, 2-(dimethylamino)-*N*-[[(methylamino)carbonyl]oxy]-2-oxo-methyl ester
Uses: insecticide/acaricide/nematicide
CAS Registry No: 23135-22-0
Molecular Formula: $C_7H_{13}N_3O_3S$
Molecular Weight: 219.261
Melting Point (°C):

109	(Lide 2003)

Boiling Point (°C):

dec	(Lide 2003)

Density (g/cm^3 at 20°C):

0.97	(Montgomery 1993; Tomlin 1994; Milne 1995)

Molar Volume (cm^3/mol):

212.4	(calculated-Le Bas method at normal boiling point)
226.1	(calculated-density)

Dissociation Constant, pK_a:
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
Entropy of Fusion, ΔS_{fus} (J/mol K):
Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F: 0.150 (mp at 109°C)

0.15	(20°C, Suntio et al. 1988)

Water Solubility (g/m^3 or mg/L at 25°C or as indicated):

281000	(Martin & Worthing 1977)
280000	(Khan 1980, Spencer 1982; Montgomery 1993; Tomlin 1994; Milne 1995)
282500	(Briggs 1981, Gerstl & Helling 1987)
282000	(20–25°C, selected, Wauchope et al. 1992; Hornsby et al. 1996)

Vapor Pressure (Pa at 25°C or as indicated):

0.0306	(Khan 1980; Spencer 1982)
0.0306	(20–25°C, selected, Wauchope et al. 1992; Hornsby et al. 1996)
0.0311	(Montgomery 1993)
0.0310	(Tomlin 1994)

Henry's Law Constant (Pa·m^3/mol):

0.00026	(calculated-P/C, Suntio et al. 1988)
0.260	(calculated-P/C, Montgomery 1993)

Octanol/Water Partition Coefficient, log K_{OW}:

–0.432	(Briggs 1973)
–0.47	(20–25°C, shake flask-^{14}C-labeled compound-LSC, Briggs 1981)
–0.432	(shake flask-centrifuge-liquid scintillation counting method, Gerstl 1984; Gerstl & Helling 1987)

–0.40 (Montgomery 1993)
–0.44 (pH 5, Tomlin 1994)
–0.47 (selected, Hansch et al. 1995)

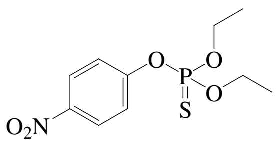
Bioconcentration Factor, log BCF:

Sorption Partition Coefficient, log K_{OC}:
0.707 (soil, sorption isotherm, converted form reported log K_{OM} of 0.47, Briggs 1981)
1.66, 1.07, 1.20, 1.32, 1.84 (5 Israeli soils, organic matter: 0.11% pH 8.5; 0.68% pH 7.9; 0.95% pH 7.8; 1.23% pH 7.2; and 2.03% pH 7.7, reported as K_{OM}, batch equilibrium-adsorption isotherms, Gerstl 1984)
0.176–1.16, –0.886–0.38 (reported as K_{OM}, estimated-S, estimated-K_{OW}, Gerstl 1984)
0.778 (soil, screening model calculations, Jury et al. 1987b)
2.47 (calculated-MCI χ, Gerstl & Helling 1987)
0.70 (soil, Carsel 1989)
1.40 (soil, Wauchope et al. 1992; Hornsby et al. 1996)
–0.70 to 1.40 (Montgomery 1993)
1.00 (soil, calculated-MCI ${}^1\chi$, Sabljic et al. 1995)
1.06, 1.68 (soil, estimated-class-specific model, estimated-general model, Gramatica et al. 2000)
1.43, 1.36 (soils: organic carbon OC ≥ 0.1%, OC ≥ 0.5%, average, Delle Site 2001)
1.08 (sediment: organic carbon OC ≥ 0.5%, average, Delle Site 2001)

Environmental Fate Rate Constants, k, or Half-Lives, $t_{½}$:
Volatilization:
Photolysis: $t_{½}$ = 55.4 h (absorbance wavelength 223 nm) (Montgomery 1993).
Oxidation:
k(aq.) = (620 ± 150) $M^{-1}\,s^{-1}$ for direct reaction with ozone in water at pH 2–7 and 24 ± 1°C, with a $t_{½}$ = 54 s at pH 7 (Yao & Haag 1991).
Hydrolysis: hydrolysis $t_{½}$ > 31 d at pH 5, 8 d at pH 7 and $t_{½}$ = 3 h at pH 9 (Tomlin 1994).
Biodegradation: decomposition rate constants range from k = 0.182 d^{-1} to 0.021 d^{-1} corresponding to v = 4 to 33 d in Bet Dagan soil depending on moisture, and decomposition rate constant ranges from k = 0.23 to 0.11 d^{-1} corresponding to $t_{½}$ = 3.1 to 6.5 d in five Israeli soils (Gerstl 1984);
$t_{½}$ = 6 d in screening model calculations (Jury et al. 1987b); .
Biotransformation:
Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants:

Half-Lives in the Environment:
Air:
Surface water: measured rate constant k = (620 ± 150) $M^{-1}\,s^{-1}$ for direct reaction with ozone in water at pH 2.0–7.0 and 24 ± 1°C, with $t_{½}$ = 54 s at pH 7 (Yao & Haag 1991).
Ground water:
Sediment:
Soil: $t_{½}$ = 9–15 d (Harvey & Han 1978);
$t_{½}$ = 12–68 d for soils from Holland depending on the moisture content (Smelt et al. 1979);
$t_{½}$ = 15 d in several soils at 15°C (Bromilow et al. 1980);
decomposition in soil was as a function of moisture content, and followed first-order kinetics with reported soil $t_{½}$ = 4–13 d at 25°C and, $t_{½}$ = 32.7 d at 15°C, $t_{½}$ = 3.8 d at 35° in Bet Dagan soil; rate constants between k = 0.11–0.23 d^{-1} and with $t_{½}$ ~ 4 d in 5 Israeli soils (Gerstl 1984);
$t_{½}$ = 6 d in screening model calculations (Jury et al. 1987b);
$t_{½}$ = 7 d (Worthing & Hance 1991);
$t_{½}$ = 8–50 d (Ou & Rao 1986) and
$t_{½}$ = 10.2–13.1, 6.2, 7.1 and 17.8 d in Pitstone, Devizes, Sutton, Veany soils, respectively (Montgomery 1993);
field $t_{½}$ = 4 d (selected, Wauchope et al. 1992; Hornsby et al. 1996).
Biota:

18.1.1.64 Parathion



Common Name: Parathion

Synonym: AAT, AATP, AC 3422, Alkron, Alleron, American Cyanamid 3422, Aphamite, Aralo, B 404, Bay E-605, Bladan, Corothion, Corthion, Corthione, Danthion, DDP, Diethyl parathion, DNDP, DPP, E 605, Ecatox, Ekatox, ENT 15108, Ethlon, Ethyl parathion, Etilon, Folidol, Fosfermo, Fosferno, Fosfex, Fosfive, Fosova, Fostern, Fostox, Gearphos, Genithion, Kolphos, Kypthion, Lethalaire G54, Lirothion, Murfos, NA 2783, NCI-C00226, Niran, Nitrostigmine, Orthophos, Pac, Panthion, Paradust, Paraflow, Paramar, Paraphos, Paraspray, Parathene, Parathion-ethyl, Parawet, Penphos, Pestox plus, Pethion, Phoskil, Phosphemol, Phosphenol, Phosphostigmine, RB, Rhodiasol, Rhodiatox, Rhodiatrox, Selephos, SNP, Soprathion, Stathion, Strathion, Sulphos, Super rodiatox, T-47, Thiofos, Tiophos, Tox 47, Vapophos, Vitrex

Chemical Name: *O,O*-diethyl *O*-4-(nitrophenyl) phosphorothioate; diethyl 4-nitrophenyl phosphorothioate; phosphorothioc acid *O,O*-diethyl *O*-(4-nitrophenyl) ester

Uses: insecticide and acaricide to control chewing and sucking insects and mites in fruits, vegetables, ornamentals and field crops.

CAS Registry No: 56-38-2

Molecular Formula: $C_{10}H_{14}NO_5PS$

Molecular Weight: 291.261

Melting Point (°C):

6.1	(Melnikov 1971; Freed et al. 1977; Montgomery 1993; Tomlin 1994; Milne 1995; Lide 2003)

Boiling Point (°C):

115	(at 0.05 mmHg, Melnikov 1971; Freed et al. 1977)
375	(Montgomery 1993; Milne 1995)
105	(at 80 Pa, Tomlin 1994)

Density (g/cm^3 at 20°C):

1.265	(25°C, Spencer 1982; Hartley & Kidd 1987; Milne 1995)
1.26	(25°C, Merck Index 1989; Montgomery 1993)
1.2694	(25°C, Worthing & Hance 1991; Tomlin 1994)

Molar Volume (cm^3/mol):

251.9	(calculated-Le Bas method at normal boiling point)
230.3	(calculated from density)

Dissociation Constant, pK_a:

7.14	(Kortum et al. 1961; Wolfe 1980)

Enthalpy of Vaporization, ΔH_V (kJ/mol):

89.92	(Rordorf 1989)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

19.87	(DSC method, Plato & Glasgow 1969)

Entropy of Fusion, ΔS_{fus} (J/mol K):

Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F: 1.0

Water Solubility (g/m^3 or mg/L at 25°C or as indicated):

24	(Macy 1948; Günther et al. 1968; Melnikov 1971; Spencer 1973)
18–31	(rm temp., > 95% purity with max. particle size 0.07–5.0μ, shake flask-GC, Robeck et al. 1965)
11.9	(20°C, NIEHS 1975; quoted, Freed et al. 1977)
11.9	(20°C, O'Brien 1975)
24	(Martin & Worthing 1977; Worthing & Walker 1987; Hartley & Kidd 1987)
24	(Wauchope 1978; Khan 1980; Lyman 1982; Willis & McDowell 1982)
12.4	(20°C, shake flask-GC, Bowman & Sans 1979, 1983b)
6.54	(shake flask-GC, Felsot & Dahm 1979)

20 (Windholz 1983, Budavari 1989)
14.0 (shake flask-GC or LSC, Gerstl & Mingelgrin 1984)
11 (20°C, Worthing & Hance 1991; Tomlin 1994; Milne 1995)
12.9, 15.2 (20°C, 30°C, Montgomery 1993)
12 (20°C selected, Siebers & Mattusch 1996)
24 (20° C, selected, Hornsby et al. 1996)

Vapor Pressure (Pa at 25°C or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):

5.04×10^{-3}*, 12.3×10^{-3} (20, 30°C, calculated by Spencer et al. 1979-gas saturation, temp range 20–45°C, Bright et al. 1950)
$\log (P/\text{mmHg}) = 7.761 - 3395/(T/K)$; temp range 25.2–65.5°C (gas saturation, Bright et al. 1950)
2.56×10^{-3} (20°C, effusion, measured range 25.2–65.5°C, Williams 1951)
$\log (P/\text{mmHg}) = 10.30 - 4400/(T/K)$; temp range 25.2–65.5°C (effusion, Williams 1951)
0.76×10^{-3} (20°C, Wolfdietrich 1965)
5.07×10^{-3} (20°C, Spencer 1973)
5.85×10^{-4} (20°C, evaporation rate-gravimetric method Gückel et al. 1973, 1974)
0.76×10^{-3} (20°C, Gückel et al. 1973, 1974)
1.29×10^{-3}* (25°C, gas saturation method, measured range 25–45°C, Spencer et al. 1979)
$\log (P/\text{mmHg}) = 12.66 - 5274/(T/K)$; temp range 24.9–45°C (gas saturation Spencer et al. 1979)
6.41×10^{-4}* (20°C, evaporation rate, measured range 20–60°C, Gückel et al.1982)
1.29×10^{-3} (Spencer 1983)
1.30×10^{-3}* (25.3°C, gas saturation-GC, measured range 25.3–45°C, Kim et al. 1984; Kim 1985)
$\log (P/\text{mmHg}) = 10.5655 - 4645.07/(T/K)$; temp range 25.3–45°C (gas saturation, Kim 1985)
0.69×10^{-3} (20°C, extrapolated-Clausius-Clapeyron eq., Kim et al. 1984; Kim 1985)
8.13×10^{-4} (20°C, GC-RT correlation, Kim et al. 1984; Kim 1985)
5.0×10^{-3} (20°C, Hartley & Kidd 1987)
1.80×10^{-3}* (gas saturation-GC, measured range 25–125°C Rordorf 1989)
$\log (P_L/\text{Pa}) = 13.006 - 4697.2/(T/K)$; measured range 32.3–160°C (gas saturation-GC, Rordorf 1989)
6.7×10^{-3} (P_L, GC-RT correlation, Hinckley et al. 1990)
8.90×10^{-4} (20°C, Worthing & Hance 1991; Tomlin 1994)
0.0533 (20°C, Montgomery 1993)
6.67×10^{-4} (20°C, selected, Hornsby et al. 1996)
1.30×10^{-3} (20°C, selected, Siebers & Mattusch 1996)
0.00316; 0.0066, 0.0013, 0.00059, 0.0025 (gradient GC method; quoted lit. values, Tsuzuki 2000)
3.23×10^{-3}; 1.12×10^{-3}, 0.00145 (gradient GC method; estimation using modified Watson method: Sugden's parachor, McGowan's parachor, Tsuzuki 2000)

Henry's Law Constant (Pa m^3/mol at 25°C or as indicated):

0.120 (20°C, calculated-P/C, Mackay & Shiu 1981)
0.074 (20°C, volatilization rate, Burkhard & Guth 1981)
0.096 (24°C, calculated-P/C, Chiou et al. 1980)
0.015 (calculated-P/C, Jury et al. 1984, 1987a; Jury & Ghodrati 1989)
0.012 (20°C, calculated-P/C, Suntio et al. 1988)
0.015 (calculated-P/C, Taylor & Glotfelty 1988)
0.0087 (23°C, Fendinger & Glotfelty 1990)
0.057 (calculated-P/C, Howard 1991)
0.030 (calculated-bond contribution method, Meylan Howard 1991)
0.0087 (calculated-P/C, Montgomery 1993)
0.020 (selected, Siebers & Mattusch 1996)

Octanol/Water Partition Coefficient, log K_{OW}:

3.81 (shake flask-GC, Chiou et al. 1977; Freed et al. 1977)
3.40 (shake flask-LSC, Felsot & Dahm 1979)
3.81 (shake flask-GC, Freed et al. 1979)

3.80 (Hansch & Leo 1979)
3.93 (shake flask-UV, Lord et al. 1980)
3.93 (shake flask-GC, Briggs 1981)
3.76 (shake flask-GC, Bowman & Sans 1983b)
3.83 (Hansch & Leo 1985)
2.15–3.93 (Montgomery 1993)
3.83 (recommended, Sangster 1993)
3.83 (Tomlin 1994)
3.83 (recommended, Hansch et al. 1995)
3.45 (RP-HPLC-RT correlation, Finizio et al. 1997)
4.32 (RP-HPLC-RT correlation using short ODP column, Donovan & Pescatore 2002)

Bioconcentration Factor, log BCF:

2.53 (fish in static water, Metcalf & Sanborn 1975)
1.81 (tadpoles, Hall & Kolbe 1980)
2.00, 2.54 (calculated-S, K_{OC}, Kenaga 1980)
3.14 (earthworms, Lord et al. 1980)
4.00 (log BCF_{lipid}, Briggs 1981)
2.68 (calculated-K_{OW}, Hansch & Leo 1985)
2.48 (Am. oysters after 84 d,; Howard 1991)
1.48, 2.34 (av., fathead minnow after 70 d, 820,138 d, Howard 1991)
2.34 (av., fathead minnow after 82–138 d, Howard 1991)
1.91, 2.27, 2.40, 1.43 (av., bluegill after 12 h, 29 h, 46 h, 504 d, Howard 1991)
1.95, 2.39, 2.50 (average, brook trout muscle after 8 h, 6 d, 180 d, Howard 1991)
1.90 (Isnard & Lambert 1988)
2.53 (Pait et al. 1992)

Sorption Partition Coefficient, log K_{OC}:

3.68 (soil, Swoboda & Thomas 1968; quoted, Kenaga 1980; Kenaga & Goring 1980)
4.02 (average, 4 soils, Hamaker & Thompson 1972)
3.30 (average, soils, Chiou et al. 1979)
2.88 (soil, calculated-S as per Kenaga & Goring 1978, Kenaga 1980)
2.90 (calculated-S, Mill et al. 1980)
4.03 (average soils/sediments, Rao & Davidson 1980)
3.02 (soil, sorption isotherm, converted from the reported log K_{OM} of 2.78, Briggs 1981)
3.25, 3.95, 3.42 (estimated-S, calculated-S and mp, calculated-K_{OW}, Karickhoff 1981)
2.26–3.96 (reported as log K_{OM}, Mingelgrin & Gerstl 1983)
2.83 (average, 8 Israeli soils, Gerstl & Mingelgrin 1984)
3.19 (average, 4 Israeli sediments, Gerstl & Mingelgrin 1984)
3.52, 2.58 (quoted, calculated-MCI χ, Gerstl & Helling 1987)
3.04 (screening model calculations, Jury et al. 1987a, b; Jury & Ghodrati 1989)
3.68, 3.33 (reported, estimated as log K_{OM}, Magee 1991)
3.15 (estimated-QSAR and SPARC, Kollig 1993)
2.50–4.20 (Montgomery 1993)
3.70 (20°C, selected, Hornsby et al. 1996)
3.20 (soil, calculated-MCI $^1\chi$, Sabljic et al. 1995)
3.20; 3.57, 3.14 (soil, quoted exptl.; estimated-class-specific model, estimated-general model, Gramatica et al. 2000)
3.05, 3.09, 2.94 (soils: organic carbon $OC \geq 0.1\%$, $OC \geq 0.5\%$, $0.1 \leq OC < 0.5\%$, average, Delle Site 2001)
3.17, 3.09 (average values for sediments with $OC \geq 0.5\%$, Delle Site 2001)

Environmental Fate Rate Constants, k, or Half-Lives, $t_{1/2}$:

Volatilization: exptl. $t_{1/2}$ = 14 d in nonstirred aqueous solutions and $t_{1/2}$ = 9.3 d in stirred aqueous solutions, and estimated $t_{1/2}$ ~ 13 d in nonstirred aqueous solutions and $t_{1/2}$ ~ 8.7 d in stirred aqueous solutions (Chiou et al. 1980).

Photolysis: photoreacted 390 times more rapidly when sorbed by algae than in distilled water (Zepp & Schlotzhauer 1983)

direct photolysis has a $t_{½} < 1$ d to 10 d in surface waters, the presence of photosensitizers, free radicals, hydrogen peroxide, or algae which are found in eutrophic waters may accelerate degradation considerably (GEMS 1986; quoted, Howard 1991)

photodegradation $t_{½} = 88$ h (Hazardous Substances Data Bank 1989; quoted, Montgomery 1993)

$t_{½} = 55$ d without addition of humic substances; $t_{½} = 18$ d and $t_{½} = 9$ d with concn of humic acid 20 mg/L and 50 mg/L, respectively, under light intensity $\lambda \geq 290$ nm (Mansour & Feicht 1994).

Oxidation: rate constant k, for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO3} with NO_3 radical and k_{O3} with O_3 or as indicated, *data at other temperatures see reference:

k_{OH}(calc) $= 92 \times 10^{-12}$ cm^3 molecule^{-1} s^{-1} (Winer & Atkinson 1990).

Hydrolysis:

k(second-order alkaline) $= 1.2 \times 10^{-3}$ M^{-1} s^{-1} at 27°C (Ketelaar 1950; quoted, Wolfe 1980)

$t_{½} = 130$ d at pH 7.4 and 20°C (NIEHS 1975; quoted, Freed et al. 1977, 1979; Montgomery 1993)

$t_{½} = 5240$ h, 180 h, 30 h, 4.47 h at room temp, 50, 70, 90°C, respectively, in estuarine water with salinity of 25.7% at pH 7.8; and $t_{½}$ ranging from 15.7–40.5 h in seawater or distilled water containing NaCl, NaOH or salt at 30 g/L at pH ranging from 1–8.0 at 70°C (Weber 1976)

$t_{½} = 24$ wk at pH 6, $t_{½} = 19$ wk at pH 7.4 and 20°C (Freed et al. 1979; quoted, Howard 1991; Montgomery 1993)

$t_{½} = 43$ wk at pH 5, $t_{½} = 24$ wk at pH 6, and $t_{½} = 15$ wk at pH 8 and 20°C (Chapman & Cole 1982; quoted, Howard 1991; Montgomery 1993)

k(alkaline) $= 2.3 \times 10^{-2}$ M^{-1} s^{-1}, k(neutral) $= 4.5 \times 10^{-8}$ s^{-1} in aqueous buffer at 20°C (Harris 1982)

$k = 2.4$ yr^{-1} at pH 7.0 and 25°C (Kollig 1993); $t_{½} = 3.5$ wk at pH 6 (Montgomery 1993)

$t_{½} = 272$ d at pH 4, $t_{½} = 260$ d at pH 7, and $t_{½} = 130$ d at pH 9 at 22°C (Tomlin 1994).

Biodegradation: generally occurs with a half-life of several weeks but in well acclimated water, complete degradation may occur in two weeks (Eichelberger & Lichtenberg 1971; Sharom et al. 1980; quoted, Howard 1991)

$t_{½} > 4250$ d from biodegradation rate constant in aquatic systems from river water samples (Williams 1977; quoted, Scow 1982);

$k = 0.029$ d^{-1} in soil by die-away tests from soil incubation studies (Rao & Davidson 1980; quoted, Scow 1982)

$t_{½} = 18$ d for a 100 d leaching and screening test in 0–10 cm depth of soil (Rao & Davidson 1980; quoted, Jury et al. 1983, 1984, 1987a, b; Jury & Ghodrati 1989)

$k < 0.00016$ d^{-1} of aerobic degradation observed in incubations of river water samples (Lyman et al. 1990; quoted, Hemond & Fechner 1994).

Biotransformation:

Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants:

Half-Lives in the Environment:

Air: atmospheric transformation lifetime was estimated to be < 1 d (Kelly et al. 1994).

Surface water: persistence of up to 8 wk in river water (Eichelberger & Lichtenberg 1971)

$t_{½} = 3670$ h at pH 5 and $t_{½} = 523$ h at pH 9 in water at 20°C (Gomaa & Faust 1972)

estimated $t_{½} > 4250$ d from biodegradation rate constant in aquatic systems from river water samples (Williams 1977; quoted, Scow 1982);

$t_{½} = 5240$ h, 180 h, 30 h, 4.47 h at room temp, 50, 70, 90°C, respectively, in estuarine water with salinity of 25.7% at pH 7.8; and $t_{½}$ ranging from 15.7–40.5 h in seawater or distilled water containing NaCl, NaOH or salt at 30 g/L at pH ranging from 1–8.0 at 70°C (Weber 1976)

$t_{½} = 7.84$ d in the Indian River water at 24 ppt salinity; pH 8.16 (Wang & Hoffman 1991);

photolysis $t_{½} = 55$ d without addition of humic substances; $t_{½} = 18$ d and 9 d with concn of humic acid 20 mg/L and 50 mg/L, respectively, under light intensity λ- 290 nm (Mansour & Feicht 1994);

$t_{½} = 120$ d at 6°C, $t_{½} = 84$ d at 22°C in darkness for Milli-Q water at pH 6.1; $t_{½} = 120$ d at 6°C, $t_{½} = 86$ d at 22°C in darkness, 8 d under sunlight conditions for river water at pH 7.3; $t_{½} = 122$ d at 6°C, $t_{½} = 33$ d at 22°C in darkness for filtered river water at pH 7.3; $t_{½} = 542$ d at 6°C, $t_{½} = 44$ d at 22°C in darkness, $t_{½} = 18$ d under sunlight conditions for seawater at pH 8.1 (Lartiges & Garrigues 1995).

Ground water:

Sediment:

Soil: persistence of one week (Edwards 1973; quoted, Morrill et al. 1982);
- persistence of less than one month (Wauchope 1978);
- $t_{½} > 24$ wk in sterile sandy loam and $t_{½} < 1.0$ wk in nonsterile sandy loam; $t_{½} > 24$ wk in sterile organic soil and $t_{½} = 1.5$ wk in nonsterile organic soil (Miles et al. 1979);
- estimated first-order $t_{½} = 23.9$ d from biodegradation rate constant $k = 0.029\ d^{-1}$ in soil by die-away tests from soil incubation studies (Rao & Davidson 1980; quoted, Scow 1982);
- moderately persistent in soil with $t_{½} = 20–100$ d (Willis & McDowell 1982);
- reported $t_{½} = 18$ d calculated using screening model calculations (Jury et al. 1987a, b; Jury & Ghodrati 1989; quoted, Montgomery 1993);
- av. degradation rate constant $k = 0.030\ d^{-1}$ in silty clay with $t_{½} = 23$ d and av. degradation rate constant $k = 0.0315\ d^{-1}$ in sandy clay with $t_{½} = 22$ d (Sattar 1990);
- $t_{½} = 14$ d (selected, Halfon et al. 1996);
- field $t_{½} = 14$ d (20–25°C, selected, Hornsby et al. 1996);
- soil $t_{½} = 6$ d (Pait et al. 1992)

Biota: biochemical $t_{½} = 15$ d from screening model calculations (Jury et al. 1987a, b; Jury & Ghodrati 1989).

TABLE 18.1.1.64.1
Reported vapor pressures of parathion at various temperatures and the coefficients for the vapor pressure equations

$\log P = A - B/(T/K)$	(1)	$P = A - B/(T/K)$	(1a)
$\log P = A - B/(C + t/°C)$	(2)	$P = A - B/(C + t/°C)$	(2a)
$\log P = A - B/(C + T/K)$	(3)		
$\log P = A - B/(T/K) - C·\log (T/K)$	(4)		

1.

Bright et al. 1950		Williams 1951		Spencer et al. 1979		Gückel et al. 1982	
gas saturation		dynamic/microdistillation		gas saturation-GC		evaporation rate	
t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa
	calc- eq. 1*				observed		
20	5.04×10^{-3}	20	2.61×10^{-3}	25	1.29×10^{-3}	20	6.41×10^{-4}
25	7.96×10^{-3}	25.4	4.68×10^{-3}	35	4.32×10^{-3}	40	7.29×10^{-3}
30	1.23×10^{-2}	54.5	0.088	45	0.01680	60	6.10×10^{-2}
35	1.86×10^{-2}	70.7	0.373				
40	2.79×10^{-2}	100	2.866	calculated from eq. 1			
45	0.04135	140	58.66	20	6.27×10^{-4}		
		160	142.7	25	1.26×10^{-3}		
eq. 1	P/mmHg		#extrapolated	30	2.45×10^{-3}		
A	7.161			35	4.71×10^{-3}		
B	3395	eq. 1	P/mmHg	40	8.83×10^{-3}		
		A	10.30	45	0.0162		
*calc by Spencer et al. 1979		B	4400				
				eq. 1	P/mmHg		
				A	12.66		
				B	5274		

TABLE 18.1.1.64.1 *(Continued)*

2.

Kim et al. 1984, Kim 1985		**Rordorf 1989**	
gas saturation-GC		**gas saturation-GC**	
t/°C	**P/Pa**	**t/°C**	**P/Pa**
25.3	0.00131	25	0.0018
34.9	0.00409	50	0.030
45.0	0.0120	75	0.330
20.0	0.0693	100	2.60
25.0	0.00131	125	16.0
eq. 1	P/mmHg	eq. 1	P/Pa
A	10.5654	A	13.006
B	4645.07	B	4697.2

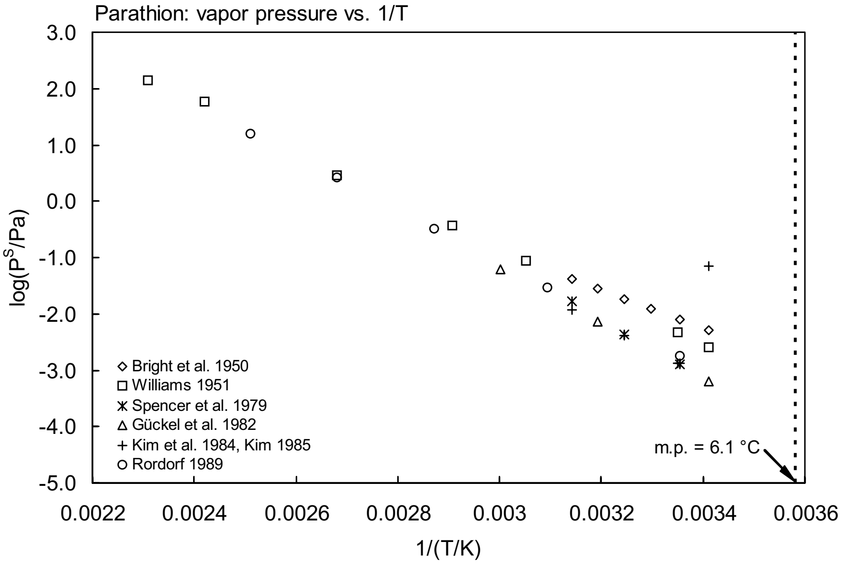
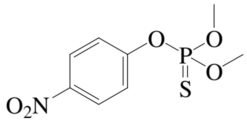


FIGURE 18.1.1.64.1 Logarithm of vapor pressure versus reciprocal temperature for parathion.

18.1.1.65 Parathion-methyl



Common Name: Parathion-methyl
Synonym: Bladan M, Folidol-M, Metacide, Nitrox 80
Chemical Name: *O,O*-dimethyl *O*-4-(nitrophenyl) phosphorothioate; dimethyl 4-nitrophenyl phosphorothioate
Uses: insecticide to control chewing and sucking insects, and mites in a wide range of crops, including fruits, vines, vegetables, ornamentals, cotton, and also used as acaricide.
CAS Registry No: 298-00-0
Molecular Formula: $C_8H_{10}NO_5PS$
Molecular Weight: 263.208
Melting Point (°C):

38	(Lide 2003)

Boiling Point (°C):

109	(at 0.05 mmHg, Freed et al. 1977)
119	(at 0.1 mmHg, Hartley & Kidd 1987)
154	(at 1.0 mmHg, Hartley & Kidd 1987; Tomlin 1994)
143	(Howard 1991)

Density (g/cm^3 at 20°C):

1.358	(Hartley & Kidd 1987; Worthing & Hance 1991; Tomlin 1994)

Molar Volume (cm^3/mol):

207.5	(calculated-Le Bas method at normal boiling point)
194.0	(calculated from density)

Dissociation Constant, pK_a:

7.15	(Kortum et al. 1961; Wolfe 1980)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

24.06	(Plato & Glasgow 1969)

Entropy of Fusion, ΔS_{fus} (J/mol K):
Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F: 0.746 (mp at 38°C)

Water Solubility (g/m^3 or mg/L at 25°C or as indicated):

55	(Melnikov 1971)
60	(Leonard et al. 1976; Khan 1980)
57	(Martin & Worthing 1977)
50	(Smith et al. 1978; Wauchope 1978)
37.7	(19.5°C, shake flask-GC, Bowman & Sans 1979, 1983b)
55	(20°C, Freed et al. 1979)
55–60	(Worthing 1979, 1983; Hartley & Kidd 1987)
60	(Khan 1980)
53	(Weber et al. 1980)
55	(20°C, Worthing & Hance 1991; Tomlin 1994)
60	(20–25°C, selected, Wauchope et al. 1992; Hornsby et al. 1996)

Vapor Pressure (Pa at 25°C or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):

0.00133	(20°C, Wolfdietrich 1965; von Rümker & Horay 1972)
0.00129	(20°C, Gückel et al. 1973)
0.0023	(Grover et al. 1976)
0.00229*	(24.9°C, gas saturation-GC, measured range 24.9–45.1°C, Spencer et al. 1979)

log (P/mmHg) = 14.37 – 3700/(T/K); temp range 24.9–34.9°C (gas saturation, Spencer et al. 1979)
log (P/mmHg) = 10.61 – 4543/(T/K); above mp 35.2–35.4°C (gas saturation, Spencer et al. 1979)

0.0013 (Worthing 1979)
> 0.0133 (20–25°C, Weber et al. 1980)
0.0020* (gas saturation-GC, measured range 25.4–45.1°C, Kim et al. 1984)
log (P/mmHg) = 9.0935 – 4063.65/(T/K); temp range 25.4–45°C (gas saturation method, Kim et al. 1984)
0.00084 (20°C, extrapolated-Clausius-Clapeyron eq., Kim et al. 1984)
log (P/mmHg) = 17.0502 – 6520.21/(T/K); temp range 25.4–34.3°C (gas saturation, Kim 1985)
0.0013 (20°C, Hartley & Kidd 1987)
0.0015 (22°C, selected, Seiber et al. 1989)
0.023 (GC-RT correlation, supercooled liquid P_L, Hinckley et al. 1990)
0.0024 (selected, Taylor & Spencer 1990)
0.0002 (20°C, Worthing & Hance 1991; Tomlin 1994)
0.002 (20–25°C, selected, Wauchope et al. 1992; Hornsby et al. 1996)
0.00041 (Tomlin 1994)
0.00955 (gradient GC method; Tsuzuki 2000)
9.77×10^{-3}; 4.90×10^{-3}, 0.00389 (gradient GC method; estimation using modified Watson method: Sugden's parachor, McGowan's parachor, Tsuzuki 2000)

Henry's Law Constant (Pa·m^3/mol at 25°C or as indicated):
0.0101 (Metcalf et al. 1980)
0.0061 (estimated, Metcalf et al. 1980)
0.0109 (calculated-P/C, Jury et al. 1987a; Jury & Ghodrati 1989)
0.021 (20°C, calculated-P/C, Suntio et al. 1988)
0.0101 (22°C, selected, Seiber et al. 1989)
0.0062 (wetted wall column method-GC, Fendinger & Glotfelty 1990)
0.0170 (calculated-bond contribution method, Meylan & Howard 1991)
0.0062 (23°C, quoted, Schomburg et al. 1991)
0.00383 (20°C, wetted wall column-GC, Rice et al. 1997b)

Octanol/Water Partition Coefficient, log K_{OW}:
2.04 (shake flask-GC, Jaglan & Gunther 1970)
2.04 (shake flask, Leo et al. 1971)
2.99 (shake flask, Mundy et al.1978)
2.68 (shake flask-HPLC, Moody et al.1987)
3.32 (Hansch & Leo 1979)
3.32 (Rao & Davidson 1980)
2.94 (shake flask-GC, Bowman & Sans 1983b)
1.80 (shake flask-GC, Schimmel et al. 1983)
2.86 (Hansch & Leo 1985)
2.86 (recommended, Sangster 1993)
2.71 (RP-HPLC-RT correlation, Sicbaldi & Finizio 1993)
3.00 (Tomlin 1994)
2.86 (recommended, Hansch et al. 1995)
2.71 (RP-HPLC-RT correlation, Finizio et al. 1997)

Bioconcentration Factor, log BCF:
0.778, 0.0 (carp/lipids, carp/muscle, Chigareva 1973)
1.98 (fish in static water, Metcalf 1974)
2.69 (bacteria, Smith et al. 1978)
1.80, 2.89 (calculated-S; calculated-K_{OC}, Kenaga 1980)
3.039 ± 0.005 (guppy, calculated on an extractable lipid wt. basis, De Bruijn & Hermens 1991)
2.98 (guppy, calculated on an extractable lipid wt. basis, De Bruijn & Hermens 1991)
3.04 (*Poecilia reticulata*, De Bruijn & Hermens 1991)
1.85 (Pait et al. 1992)
1.92 (paddy field fish, Tejada 1995)

Sorption Partition Coefficient, log K_{OC}:

3.99 (soil, Hamaker & Thompson 1972; Kenaga 1980; Kenaga & Goring 1980)
1.699 (av. all sediments, Smith et al. 1978)
2.63 (av. of 3 soils, Rao & Davidson 1979)
2.67 (soil, calculated-S as per Kenaga & Goring 1978, Kenaga 1980)
3.71 (Rao & Davidson 1980)
3.02, 3.47, 2.93 (estimated-S, S and mp, K_{OW}, Karickhoff 1981)
3.71 (screening model calculations, Jury et al. 1987a, b; Jury & Ghodrati 1989)
3.84, 1.97 (quoted, calculated-MCI χ, Gerstl & Helling 1987)
3.71–3.99 (soil, Carsel 1989)
3.00 (soil, calculated-MCI $^1\chi$, Sabljic et al. 1995)
3.71 (soil, 20–25°C, selected, Wauchope et al. 1992; Hornsby et al. 1996)
2.68 (sediment, estimated, Paraiba et al. 1999)
3.27, 2.84 (soil, estimated-class-specific model, estimated-general model, Gramatica et al. 2000)
2.82, 2.74 (soils: organic carbon OC $\geq$ 0.1%, OC $\geq$ 0.5%, average, Delle Site 2001)

Environmental Fate Rate Constants, k, or Half-Lives, $t_{1/2}$:

Volatilization: volatilization rate $k < 0.01$ kg ha^{-1} d^{-1} in a flooded rice field (Seiber et al. 1986; Seiber & McChesney 1987; quoted, Seiber et al. 1989)

Photolysis: lab. rate constant $k = 2.7 \times 10^{-7}$ s^{-1} in early January with photolysis $t_{1/2}$ = 240 h, 850 h, 850 h and 170 h in river, pond, eutrophic lake and oligotrophic lake predicted by the one-compartment model (Smith et al. 1978; quoted, Howard et al. 1991);

$t_{1/2}$ = 8 d in summer and $t_{1/2}$ = 38 d in winter for direct sunlight photolysis in natural water (Smith et al. 1978; quoted, Howard 1991; Howard et al. 1991);

photolytic $t_{1/2}$ = 200 h in aquatics (Haque et al. 1980);

photoreacted 390 times more rapidly when sorbed by algae than in distilled water (Zepp & Schlotzhauer 1983).

Oxidation: rate constant k, for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO3} with NO_3 radical and k_{O3} with O_3 or as indicated, *data at other temperatures see reference:

$k = 3.0$ M^{-1} s^{-1} (Smith et al. 1978)

photooxidation half-life of 3.6 d for the vapor-phase reaction with hydroxyl radical in the atmosphere (Atkinson 1985; quoted, Howard 1991);

photooxidation half-life of 1.0–10.5 h based on estimated rate constant for the vapor-phase reaction with OH radical in air (Atkinson 1987; quoted, Howard et al. 1991).

Hydrolysis:

$k = .4 \times 10^{-2}$ mol min^{-1} with $t_{1/2}$ = 125 h for pH <11.0 at 15°C (Ketelaar & Gersmann 1958; quoted, Freed 1976)

$k = 1.1 \times 10^{-7}$ s^{-1} with a half-life of 8.4 h at pH 6 buffer at 70°C in 20% ethanol aqueous solution (Ruzicka et al. 1967; quoted, Freed 1976; Smith et al. 1978)

$t_{1/2}$ = 1.7 wk at pH about 6 and room temp. (Cowart et al. 1971; quoted, Smith et al. 1978)

$k = 1.1 \times 10^{-7}$ s^{-1} with $t_{1/2}$ = 72 d at pH 7 and 25°C (Mabey & Mill 1978; quoted, Howard et al. 1991)

$k = 9 \times 10^{-7}$ s^{-1} (Smith et al. 1978)

k(alkaline) = 5.3×10^{-3} M^{-1} s^{-1} at 27°C and pH 10 (Smith et al. 1978; quoted, Wolfe 1980)

$t_{1/2}$ = 68 d at pH 5, $t_{1/2}$ = 40 d at pH 7, $t_{1/2}$ = 33 d at pH 9 at 25°C (Tomlin 1994).

Biodegradation:

$k = 1.7 \times 10^{-7}$ -g $cell^{-1}$ h^{-1} (Smith et al. 1978);

$t_{1/2}$(aq. aerobic) = 360–1680 h, based on an unacclimated aerobic river die-away test data (Bourquin et al. 1979; Spain et al. 1980; quoted, Howard et al. 1991);

$t_{1/2}$(aq. anaerobic) = 24–168 h, based on unacclimated anaerobic soil and sediment grab sample data (Adhya et al. 1981; Wolfe et al. 1986; quoted, Howard et al. 1991);

$t_{1/2}$ = 15 d for a 100 d leaching and screening test in 0–10 cm depth of soil (Rao & Davidson 1980; quoted, Jury et al. 1983, 1987a, b; Jury & Ghodrati 1989);

$k = (0.003 \pm 0.0003)$ h^{-1} with half-life of 220.9 h in surface aerobic soils at Williamsburg, $k = (0.0017 \pm 0.00009)$ h^{-1} with half-life of 410 h in subsurface aerobic soils at Sault Ste. Marie (Ward 1985)

$k = 0.30$ d^{-1} in river sediment, $k = 0.02$ d^{-1} in river water (Cripe et al. 1987; quoted, Battersby 1990)

Biotransformation:

Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants:

$k_1 = (2.59 \pm 0.88) \times 10^{-3}$ mL g^{-1} d^{-1} (guppy, De Bruijn & Hermens 1991)

$k_2 = (2.38 \pm 0.14)$ d^{-1} (guppy, De Bruijn & Hermens 1991)

$k_2 = 1.71$ d^{-1} (guppy, calculated-K_{OW}, De Bruijn & Hermens 1991)

$k_2 = (0.12 \pm 0.02) \times 10^{-3}$ (NADPH) min^{-1} mg $protein^{-1}$ (rainbow trout, De Bruijn et al. 1993)

$k_2 = (0.11 \pm 0.03) \times 10^{-3}$ (GSH) min^{-1} mg $protein^{-1}$ (rainbow trout, De Bruijn et al. 1993)

Half-Lives in the Environment:

Air: estimated $t_{1/2} = 3.6$ d for the vapor-phase reaction with hydroxyl radical in air (Atkinson 1985; quoted, Howard 1991);

photooxidation $t_{1/2} = 1.0–10.5$ h in air based on estimated rate constant for the vapor-phase reaction with hydroxyl radical in air (Atkinson 1987; quoted, Howard et al. 1991);

reaction rate $k = 4.77 \times 10^{-4}$ min^{-1} in air (Paraiba et al. 1999).

Surface water: persistence up to 4.0 wk in river water (Eichelberger & Lichtenberg 1971);

overall $t_{1/2} = 0.6$ h in river, $t_{1/2} = 15$ h in eutrophic pond, $t_{1/2} = 28.3$ h in eutrophic lake and $t_{1/2} = 157.5$ h oligotrophic lake (Smith et al. 1978);

$t_{1/2} = 8$ d in summer and $t_{1/2} = 38$ d in winter for direct sunlight photolysis in natural water (Howard 1991; Howard et al. 1991);

$t_{1/2} > 28$ d in 100 mL pesticide-seawater solution under indoor conditions, $t_{1/2} = 6.3$ d under outdoor light conditions and $t_{1/2} = 18$ d under outdoor dark conditions (Schimmel et al. 1983);

first-order biodegradation rate constant $k = 0.30$ d^{-1} in river sediment and $k = 0.02$ d^{-1} in river water (Cripe et al. 1987; quoted, Battersby 1990);

$t_{1/2} = 44$ h of dissipation from rice field water (Seiber & McChesney 1987; quoted, Seiber et al. 1989)

$t_{1/2} = 237$ d at 6°C, 46 d at 22°C in darkness for Milli-Q water at pH 6.1; $t_{1/2} = 95$ d at 0°C, 23 d at 22°C in darkness, $t_{1/2} = 11$ d under sunlight conditions for river water at pH 7.3; $t_{1/2} = 173$ d at 6°C, $t_{1/2} = 18$ d at 22°C in darkness for filtered river water at pH 7.3; $t_{1/2} = 233$ d at 6°C, $t_{1/2} = 30$ d at 22°C in darkness, v = 34 d under sunlight conditions for seawater at pH 8.1 (Lartiges & Garrigues 1995);

reaction rate $k = 3.80 \times 10^{-4}$ min^{-1} in water (Paraiba et al. 1999).

Ground water: $t_{1/2} = 24–1680$ h based on estimated aqueous aerobic and anaerobic biodegradation half-life (Howard et al. 1991).

Sediment: $t_{1/2} < 1.2$ d in 10 g sediment/100 mL pesticide-seawater solution under untreated conditions and $t_{1/2} > 28$ d under sterile conditions (Schimmel et al. 1983);

disappearance rate constants: $k = (3.5 \pm 0.6) \times 10^{-3}$ min^{-1} in Beaver Dam sediments samples at pH 6.7, $k = (2.9 \pm 1.2) \times 10^{-3}$ min^{-1} in Memorial Park sediments samples at pH 6.5 and $k = (2.8 \pm 2.4) \times 10^{-3}$ min^{-1} in Hickory Hills sediments samples at pH 6.9 near Athens, Georgia (Wolfe et al. 1986);

reaction rate $k = 2.85 \times 10^{-5}$ min^{-1} in sediment (Paraiba et al. 1999).

Soil: $t_{1/2} = 2,408,640$ h, based on unacclimated aerobic soil grab sample data (Davidson et al. 1980; Butler et al. 1981; quoted, Howard et al. 1991);

measured dissipation rate $k = 0.010–0.034$ d^{-1} (Baker & Applegate 1970; quoted, Nash 1988);

estimated dissipation rate $k = 0.029, 0.042$ d^{-1} (Nash 1988);

persistence of less than one month (Wauchope 1978);

non-persistent in soils with $t_{1/2} < 20$ d (Willis & McDowell 1982);

rate constant $k = 0.16$ d^{-1} with $t_{1/2} = 4$ d under laboratory conditions and rate constant $k = 0.046$ d^{-1} with $t_{1/2} = 15$ d under field conditions (Rao & Davidson 1980);

$t_{1/2} = 15$ d in screening model calculations (Jury et al. 1987a, b; Jury & Ghodrati 1989); selected field $t_{1/2} = 5.0$ d (Wauchope et al. 1992; quoted, Halfon et al. 1996; Hornsby et al. 1996);

soil $t_{1/2} = 44$ d (Pait et al. 1992).

Biota: biochemical $t_{1/2} = 15$ d from screening model calculations (Jury et al. 1987a, b; Jury & Ghodrati 1989).

TABLE 18.1.1.65.1

Reported vapor pressures of parathion-methyl at various temperatures and the coefficients for the vapor pressure equations

$\log P = A - B/(T/K)$	(1)	$\ln P = A - B/(T/K)$	(1a)
$\log P = A - B/(C + t/°C)$	(2)	$\ln P = A - B/(C + t/°C)$	(2a)
$\log P = A - B/(C + T/K)$	(3)		
$\log P = A - B/(T/K) - C \cdot \log (T/K)$	(4)		

Spencer et al. 1979		Kim et al. 1984	
gas saturation-GC		gas saturation-GC	
t/°C	P/Pa	t/°C	P/Pa
24.9	0.00229	25.4	0.00205
30.0	0.00529	30.1	0.00489
34.9	0.00960	34.3	0.00879
38.6	0.0148	38.5	0.0150
39.7	0.0164	41.7	0.0202
41.7	0.0207	45.1	0.0278
45.1	0.0291	20	0.00084#
		25	0.0020#
mp/°C	34.6		#extrapolated
eq. 1	P/mmHg	eq. 1	P/mmHg
A	14.37	A	9.9035
B	5700	B	4063.65
ΔH_V = 109.2 kJ/mol			
above the melting point			
eq. 1	P/mmHg		
A	10.61		
B	4543		
ΔH_V = 87.03 kJ/mol			

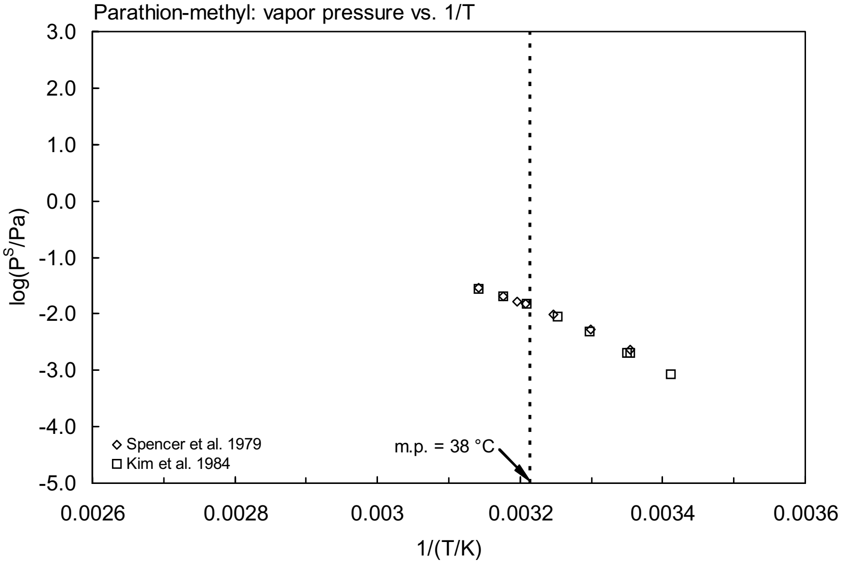
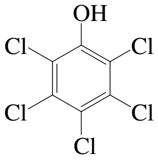


FIGURE 18.1.1.65.1 Logarithm of vapor pressure versus reciprocal temperature for parathion-methyl.

18.1.1.66 Pentachlorophenol

(See also chapter 14. Phenolic Compounds)



Common Name: Pentachlorophenol
Synonym: chlorophen, PCP, penchlorol
Chemical Name: pentachlorophenol
Uses: insecticide/fungicide/herbicide; control of termites; as wood preservatives to protect against fungal rots and wood boring insects; as a pre-harvest defoliant in cotton; and also as a general pre-emergence herbicide.
CAS Registry No: 87-86-5
Molecular Formula: C_6Cl_5OH
Molecular Weight: 266.336
Melting Point (°C):
191 (Firestone 1977; Weast 1982–83; Hartley & Kidd 1987)
187 (Schmidt-Bleek et al. 1982)
174 (Lide 2003)
Boiling Point (°C):
310 (Verschueren 1977, 1983; Callahan et al. 1979)
309–310 (Hartley & Kidd 1987)
310 (dec, Lide 2003)
Density (20°C, g/cm^3):
1.987 (Firestone 1977)
1.978 (Schmidt-Bleek et al. 1982; Verschueren 1983)
1.980 (22°C, Hartley & Kidd 1987)
Dissociation Constant, pK_a:
4.80 (Blackman et al. 1955; Sillén & Martell 1971; McLeese et al. 1979; Kaiser et al. 1984)
5.0 (Farquharson et al. 1958; Renner 1990)
4.92 (Doedens 1967; Jones 1981; Bintein & Devillers 1994)
4.74 (Drahonovsky & Vacek 1971; Callahan et al. 1979; Ugland et al. 1981; Könemann 1981; Könemann & Musch 1981; Dean 1985; Westall et al. 1985; Lagas 1988; Renner 1990; Lee et al. 1990,91)
4.71 (Cessna & Grover 1978; Saarikoski & Viluksela 1982; Saarikoski et al. 1986; Tratnyek & Hoigné 1991)
5.30 (Gebefügi et al. 1979; Xie 1983; Schellenberg et al. 1984)
4.70 (Crosby 1981; Hoigné & Bader 1983)
5.20 (Renberg 1981; Renner 1990; Larsson et al. 1993)
4.90 (Xie & Dryssen 1984; Xie et al. 1986; Shigeoka et al. 1988; Söderström et al. 1994)
4.75 (Leuenberger et al. 1985)
4.60 (Nendza & Seydel 1988)
Molar Volume (cm^3/mol):
207.9 (calculated-Le Bas method at normal boiling point)
134.3 (calculated-density)
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
17.154 (Plato & Glasgow 1969)
Entropy of Fusion, ΔS_{fus} (J/mol K):
Fugacity Ratio at 25°C (assumingΔS_{fus} = 56 J/mol K) F: 0.0345 (mp at 174°C)

Water Solubility (g/m^3 or mg/L at 25°C or as indicated):
15.4 (gravimetric, Carswell & Nason 1938)
18 (27°C, gravimetric, Carswell & Nason 1938)
9.59 (shake flask-UV, at pH 5.1, Blackman et al. 1955)

14	(20°C, shake flask-UV, at pH 3.0, Bevenue & Beckman 1967)
10	(shake flask-gravimetric, at pH 5.0, Toyota & Kuwahara 1967)
14	(gravimetric at pH 5.0, Toyota & Kuwahara 1967)
20–25	(selected, Günther et al. 1968;)
20	(30°C, Firestone 1977)
14	(20°C, Verschueren 1977, 1983)
20	(20°C, Körte et al. 1978)
14	(Kenaga & Goring 1980; Geyer et al. 1982; McKim et al. 1985)
14, 20–25	(selected lit. values, Geyer et al. 1980, Geyer et al. 1984)
15	(23°C, Klöpffer et al. 1982)
20	(20°C, Schmidt-Bleek et al. 1982)
5–10	(at pH 5–6 in contaminated water, Goerlitz et al. 1985)
14	(recommended at pH 4.5–5.5, IUPAC 1985)
80	(20°C, Hartley & Kidd 1987)
41	(predicted-MCI χ, Nirmalakhandan & Speece 1988)
8 ± 2	(shake flask-UV at pH 2.5, Valsaraj et al. 1991)
32 ± 3	(shake flask-UV at pH 5.0, Valsaraj et al. 1991)
19	(quoted, Müller & Klein 1992)
18.4	(shake flask-HPLC/UV, at pH 4.8, Ma et al. 1993)

Vapor Pressure (Pa at 25°C or as indicated):

0.0227	(20°C, static method, Carswell & Nason 1938)
0.0147	(20°C, Bevenue & Beckman 1967)
0.231	(supercooled liq. extrapolated-Antoine eq., Weast 1976–77)
0.10	(Weast 1972–73)
0.0211	(Chiou & Freed 1977)
0.0213	(Firestone 1977)
0.0147–0.0227	(20°C, Goll 1954; Bevenue & Beckman 1967; Neumüller 1974)
0.0956	(supercooled liquid, Hamilton 1980; quoted, Bidleman & Renberg 1985)
0.00415	(23°C, OECD, Klöpffer et al. 1982)
0.0093	(20°C, Schmidt-Bleek et al. 1982)
0.0147	(20°C, Verschueren 1983; Howard 1991)
0.1153	(extrapolated-Antoine eq., Boublik et al. 1984)
0.50	(20°C, quoted, Crossland & Wolff 1985)
0.115	(capillary GC-RT correlation, Bidleman & Renberg 1985)
0.127	(extrapolated-Antoine eq., Stephenson & Malanowski 1987)

Henry's Law Constant (Pa m^3/mol):

0.00248	(calculated-P/C, Hellmann 1987)
0.0127	(estimated-bond contribution, Hellmann 1987)
0.277	(calculated-P/C, Howard 1991)
0.079	(calculated-P/C, this work)

Octanol/Water Partition Coefficient, log K_{OW}:

5.01	(quoted unpublished result, Leo et al. 1971)
5.01	(Firestone 1977)
5.01, 5.12, 5.86, 3.81	(Hansch & Leo 1979)
5.01	(calculated, Veith et al. 1979b; McLeese et al. 1979)
2.97	(Veith et al. 1979)
3.69	(quoted from Kotzias 1980 unpublished result, Geyer et al. 1982)
4.16	(Rao & Davidson 1980)
5.10	(calculated-HPLC-k′ correlation, Butte et al. 1981)
5.19	(calculated-f const., Könemann 1981; Könemann & Musch 1981)
4.00, 0.0	(at pH 4, 8, Renberg 1981)
5.08	(RP-HPLC-k′ correlation, Miyake & Terada 1982)

5.15 (shake flask-GC, Saarikoski & Viluksela 1982; Saarikoski et al. 1986)
5.05 (Kaiser & Valdmanis 1982)
4.84 (shake flask-GC, apparent value at pH 1.2, Kaiser & Valdmanis 1982)
1.30 (shake flask-GC, apparent value at pH 10.5, Kaiser & Valdmanis 1982)
3.69 (Geyer et al. 1982, Schmidt-Bleek et al. 1982)
3.29 (shake flask average, OECD/EEC Lab. comparison tests, Harnisch et al. 1983)
5.01 (Verschueren 1983)
5.85 (calculated as per Leo et al. 1971, Xie 1983)
5.11 ± 0.07 (exptl.-ALPM, Garst & Wilson 1984)
3.69, 3.81 (shake flask, OECD 1981 guidelines, Geyer et al. 1984)
5.24 (shake flask-HPLC/UV, Schellenberg et al. 1984)
5.04, 5.08, 5.85, 5.22 (shake flask-GC, HPLC-k′, calculated-π const., calculated-f const., Xie et al. 1984; Bintein & Devillers 1994)
5.05 (calculated, Xie & Dryssen 1984; quoted, Lagas 1988)
5.24 (OECD 1981 guidelines, Leuenberger et al. 1985)
4.71 (RP-HPLC-RT correlation, Chin et al. 1986)
2.50 (at pH 4.7, Geyer et al. 1987)
4.47 (CPC-RV correlation, Terada et al. 1987)
4.07 (OECD 81 method, Kerler & Schönherr 1988)
5.04 (HPLC-RT correlation, Shigeoka et al. 1988; quoted, Saito et al. 1993)
5.00 (batch equilibration-UV, Beltrame et al. 1988)
5.06 (calculated-CLOGP, Müller & Klein 1992)
5.01, 5.38 (quoted, calculated-original UNIFAC, Chen et al. 1993)
5.24 (EPA CLOGP Data Base, Hulzebos et al. 1993)
5.18 (recommended, LOGKOW databank, Sangster 1993)
5.06, 5.12 (COMPUTOX databank, Kaiser 1993)
5.12 (recommended, Hansch et al. 1995)

Bioconcentration Factor, log BCF:
3.75 (fish, Statham et al. 1976)
3.04 (fish, Körte et al. 1978)
2.89 (fathead minnow, 32-d exposure, Veith et al. 1979)
2.89 (fathead minnow, calculated value, Veith et al. 1979b)
2.64 (algae, calculated, Geyer et al. 1981)
2.00 (trout, Hattula et al. 1981)
3.04, 3.10, 3.02 (activated sludge, algae, golden orfe, Freitag et al. 1982)
2.54 (mussel *Mytilus edulis*, quoted average, Geyer et al. 1982)
3.69 (calculated-K_{OW}, Mackay 1982)
1.60 (killifish, Trujillo et al. 1982)
1.86, 1.72, 1.60 (low-PCP flowing, high-PCP flowing, high-PCP static soft water; Brockway et al. 1984)
1.66, 1.62, 1.26 (low-PCP flowing, high-PCP flowing, high-PCP static hard water; Brockway et al. 1984)
3.10 (*alga chlorella fusca* in culture flasks, Geyer et al. 1984)
3.10, 2.72 (algae: exptl, calculated-K_{OW}, Geyer et al. 1984)
3.10, 3.02, 3.04 (algae, fish, sludge, Klein et al. 1984)
3.00 (quoted, LeBlanc 1984)
3.04, 3.10, 2.42 (activated sludge, algae, golden ide, Freitag et al. 1985)
0.57 (human fat, Geyer et al. 1987)
2.99 (zebrafish, Butte et al. 1987)
0.46 (15°C, initial concn. 1.0 mg/L uptake by *Allolobophora caliginosa* at 24 hours, Haque & Ebing 1988)
0.38 (15°C, initial concn. 10.0 mg/L uptake by *Allolobophora caliginosa* at 24 h, Haque & Ebing 1988)
0.80 (whole *Allolobophora caliginosa*/soil, uptake from soil after 131 d-exposure in outdoor lysimeters, Haque & Ebing 1988)
1.35 (whole *Lumbricus terrestris*/soil, uptake from soil after 131 d-exposure in outdoor lysimeters, Haque & Ebing 1988)
2.80, 2.63 (earthworm *E. fetida andrei*: in Kooyenburg soil, Holten soil, van Gestel & Ma 1988)

–2.66 (daily intake/cow adipose tissue, Travis & Arms 1988)
4.10 (rainbow trout, field bioaccumulation, Thomann 1989)
4.38, 4.50, 4.53, 4.90 (earthworm system, Connell & Markwell 1990)
4.00, 5.30, 3.40, 8.00 (earthworm system, derived data, Connell & Markwell 1990)
2.97 (*P. hoyi*, Landrum & Dupuis 1990)
2.11 (*M. relicta*, Landrum & Dupuis 1990)
2.16–2.53 (soft tissue of freshwater mussel, Mäkelä & Oikari 1990)
2.33; 3.21 (flagfish: whole fish; fish lipid, Smith et al. 1990)
2.78, 2.11, 1.72 (goldfish at pH 7, pH 8, pH 9, Stehly & Hayton 1990)
2.89, 1.11 (fathead minnow, bluegill; Saito et al. 1992)
3.0, 3.4, 3.9, 4.0 (perch bile to water, Söderström et al. 1994)

Sorption Partition Coefficient, log K_{OC}:

2.95 (soil, calculated-K_{OW}, Kenaga & Goring 1980)
3.11–5.65 (soil, calculated-K_{OW}, model of Karickhoff et al. 1979, Sabljic 1987a, b)
3.17–4.54 (soil, calculated-K_{OW}, model of Kenaga & Goring 1980, Sabljic 1987a, b)
3.37–3.69 (soil, calculated-K_{OW}, model of Briggs 1981, Sabljic 1987a, b)
3.00–5.54 (soil, calculated-K_{OW}, model of Means et al. 1982, Sabljic 1987a, b)
2.21–4.49 (soil, calculated-K_{OW}, model of Chiou et al. 1983, Sabljic 1987a, b)
4.52 (sediment, Schellenberg et al. 1984)
2.95, 2.41 (quoted, calculated-MCI χ, Gerstl & Helling 1987)
3.73 (quoted average of Kenaga & Goring 1980 and Schellenberg et al. 1984 values, Sabljic 1987a, b)
3.46 (soil, calculated-MCI χ, Sabljic 1987a, b)
2.95 (soil, calculated-MCI χ, Bahnick & Doucette 1988)
4.04 (estimated, HPLC-k′ correlation, Hodson & Williams 1988)
4.40 (calculated, Lagas 1988)
3.10, 3.26 (totally dissociated as phenolate-calculated, Lagas 1988)
5.27, 5.71 (Bluepoint soil at pH 7.8, pH 7.4, Bellin et al. 1990)
5.58, 5.52 (Glendale soil at pH 7.3, pH 4.3, Bellin et al. 1990)
3.49, 3.57 (Norfolk soil at pH 4.3, pH 4.4, Bellin et al. 1990)
4.32–4.65 (Norfolk + lime soil at pH 6.9, Bellin et al. 1990)

Environmental Fate Rate Constants, k, and Half-Lives, $t_{1/2}$:

Volatilization/evaporation: $t_{1/2}$ = 84 h from the rate of loss experiment on watch glass for an exposure period of 192 h (Dobbs & Grant 1980);

k = 0.028 d^{-1} for nondissociated PCP, assuming diffusion coefficient in air to be 7×10^{-6} m^2/s and in water 7×10^{-10} m^2/s with wind speed 0.1 m above the pond is 2 m/s and the average temperature is 15°C for water depth of 1 m (Crossland & Wolff 1985);

calculated rate constant k = 5×10^{-4} d^{-1} to 1×10^{-7} d^{-1} for total PCP (Crossland & Wolff 1985).

Photolysis: calculated photolysis $t_{1/2}$ = 4.75 h from observed rate k = 3.4×10^{-4} s^{-1} for a depth of 300 cm at pH 7 with light intensity of 0.04 watts/cm^2 between 290 and 330 nm on a midsummer day at the latitude of Cleveland, Ohio (Hiatt et al. 1960; quoted, Callahan et al. 1979);

photolysis $t_{1/2}$ = 1.5 d was estimated from photolytic destruction by sunlight in an aqueous solution at Davis, California (Wong & Crosby 1978; quoted, Callahan et al. 1979);

exposure of aqueous PCP solutions to either sunlight or laboratory ultraviolet light resulted in rapid degradation at pH 7.3 and slower degradation at pH 3.3 (Wong & Crosby 1981);

photolytic $t_{1/2}$ = 10–15 d (Brockway et al. 1984);

k = 0.23 to 0.46 d^{-1} for direct photo-transformation, is the main loss process for PCP from ponds, with $t_{1/2}$ = 1.5 to 3.0 d (Crossland & Wolff 1985);

photo-transformation rate constant k = 0.6 h^{-1} with $t_{1/2}$ = 1 h for distilled water in summer (mean temperature 25°C) and k = 0.37 h^{-1} with $t_{1/2}$ = 2 h in winter (mean temperature 11°C); k = 0.37 h^{-1} with $t_{1/2}$ = 2 h for both poisoned estuarine water and estuarine water in summer and k = 0.27 h^{-1} with $t_{1/2}$ = 3 h in winter during days when exposed to full sunlight and microbes (Hwang et al. 1986);

photo-mineralization rate constant k = 0.11 h^{-1} with $t_{1/2}$ = 6 d for distilled water in summer (mean temperature 25°C) and k = 0.049 h^{-1} with $t_{1/2}$ = 14 d in winter (mean temperature 11°C); k = 0.12 h^{-1} with $t_{1/2}$ = 6 d for poisoned estuarine water in summer and k = 0.07 h^{-1} with $t_{1/2}$ = 10 d in winter; k = 0.25 h^{-1} with $t_{1/2}$ = 10 d for estuarine water in summer and 0.10 h^{-1} with half-life of 7 d for winter during days when exposed to full sunlight and microbes (Hwang et al. 1986);

phototransformation $t_{1/2}$ = 0.75 h in Xenotest 1200 (Svenson & Björndal 1988);

aqueous photolysis $t_{1/2}$ = 1–110 h (Hwang et al. 1986; Sugiura et al. 1984; selected, Howard et al. 1991);

$t_{1/2}$ = 7.43 d assuming a linear rate of photolysis during 96-h period (Smith et al. 1987);

photodegradation rate constant k = 0.60 h^{-1} corresponding to $t_{1/2}$ = 1.0 h (summer), k = 0.37 h^{-1} corresponding to $t_{1/2}$ = 2 h (winter) in distilled water; and k = 0.37 h^{-1} corresponding to $t_{1/2}$ = 2 h (summer), k = 0.27 h^{-1} corresponding to $t_{1/2}$ = 3.0 h (winter) in estuarine water under irradiation by natural sunlight (quoted from Hwang et al. 1987, Sanders et al. 1993).

Oxidation: rate constant k >> 3.0×10^5 $M^{-1} \cdot s^{-1}$ for the reaction with ozone in water at pH 2.0 (Hoigné & Bader 1983);

photooxidation $t_{1/2}$ = 66–3480 h in water, based on reported reaction rate constants for reaction of OH and RO_2 radicals with phenol class in aqueous solution (Mill & Mabey 1985; Guesten et al. 1981; quoted, Howard et al. 1991);

photooxidation $t_{1/2}$ = 139.2–1392 h, based on an estimated rate constant for the vapor-phase reaction with hydroxyl radicals in air (Atkinson 1987; quoted, Howard et al. 1991);

rate constant k = $(0.2 \pm 5.5) \times 10^6$ $M^{-1} \cdot s^{-1}$ for the reaction with singlet oxygen in aqueous phosphate buffer at (27 ± 1)°C (Tratnyek & Hoigné 1991);

atmospheric $t_{1/2}$ < 24 h at noon in mid-summer to $t_{1/2}$ = 216 h in January at latitude of 41.79°N for reaction with OH radicals (Bunce et al. 1991).

Hydrolysis: is not expected to occur (Crossland & Wolff 1985).

Biodegradation: $t_{1/2}$ = 1800–2160 h and 480-∞ h to obtain 75% degradation in mineral medium and seawater, respectively (De Kreuk & Hanstveit 1981);

aqueous aerobic $t_{1/2}$ = 552–4272 h, based on unacclimated and acclimated aerobic sediment grab sample data (Delaune et al. 1983; Baker & Mayfield 1980; quoted, Howard et al. 1991);

aqueous anaerobic $t_{1/2}$ = 1008–36480 h, based on unacclimated anaerobic grab sample data for soil and ground water (Ide et al. 1972; Baker & Mayfield 1980; quoted, Howard et al. 1991);

aerobic degradation rate constant k = 0.0017 L $\mu g^{-1} \cdot d^{-1}$ (Moos et al. 1983);

microbial degradation negligible in darkness (Hwang et al. 1986);

degradation rate constant k = 0.12 ± 0.01 h^{-1} in the absence of light (Minero et al. 1993).

Biotransformation: degradation rate k = 3×10^{-14} $mol \cdot cell^{-1} \cdot h^{-1}$ with microorganisms in Seneca River waters (Banerjee et al. 1984).

Bioconcentration Uptake (k_1) and Elimination (k_2) Rate Constants:

k_1 = 18.3 h^{-1}, 19 h^{-1} (at 1 mM buffer concn), 18.5 h^{-1} (at 10 mM buffer concn) at pH 8 (guppy *P. reticulata* Peters, Saarikoski et al. 1986)

k_1 = 222 d^{-1}, 1677 d^{-1} (flagfish: whole fish; fish lipid, Smith et al. 1990)

k_2 = 1.03 d^{-1}, 1.03 d^{-1} (flagfish: whole fish; fish lipid, Smith et al. 1990)

k_2 = 1.03 d^{-1}, 0.95 d^{-1} (flagfish: BCF based, toxicity based, Smith et al. 1990)

k_2 = 0.00195 ± 0.00063 h^{-1} (*M. relicta*, Landrum & Dupuis 1990)

k_2 = 0.00330 ± 0.00140 h^{-1} (*P. hoyi*, Landrum & Dupuis 1990)

Half-Lives in the Environment:

Air: $t_{1/2}$ = 139.2–1392 h, based on an estimated rate constant for the vapor-phase reaction with hydroxyl radicals in air (Howard et al. 1991);

photolysis $t_{1/2}$ = 6.5 h in noonday summer sunshine (Howard 1991);

$t_{1/2}$ = 216 h at latitude of 43.70°N at noon in January to $t_{1/2}$ < 24 h in mid-summer for reaction with hydroxyl radicals (Bunce et al. 1991).

Surface water: calculated photolysis $t_{1/2}$ = 4.75 h from a determined rate k = 3.4×10^{-4} s^{-1} for a depth of 300 cm at pH 7 with light intensity of 0.04 watts/cm^2 between 290 and 330 nm on a midsummer day at the latitude of Cleveland, Ohio (Hiatt et al. 1960; quoted, Callahan et al. 1979);

photolysis $t_{1/2}$ = 1.5 d was estimated from photolytic destruction by sunlight in an aqueous solution at Davis, California (Wong & Crosby 1978; quoted, Callahan et al. 1979);

photolytic $t_{1/2}$ = 10–15 d (Brockway et al. 1984);

rate constant k >> 3.0×10^5 M^{-1} s^{-1} for the reaction with ozone at pH 2.0 (Hoigné & Bader 1983);

$t_{1/2}$ = 1.5 to 3.0 d for direct photo-transformation from outdoor ponds (Crossland & Wolff 1985);

$t_{1/2}$ = 1 h in summer, $t_{1/2}$ = 2 h in winter for distilled water; $t_{1/2}$ = 2 h in summer, $t_{1/2}$ = 3 h in winter for estuarine water; $t_{1/2}$ = 2 h in summer, $t_{1/2}$ = 3 h in winter for poisoned estuarine water, based on photo-transformation rate constants (Hwang et al. 1986);

$t_{1/2}$ = 6 d in summer, $t_{1/2}$ = 14 d in winter for distilled water; $t_{1/2}$ = 3 d in summer, $t_{1/2}$ = 7 d in winter for estuarine water; $t_{1/2}$ = 6 d in summer, $t_{1/2}$ = 10 d in winter for poisoned estuarine water, based on photo-mineralization rate constants (Hwang et al. 1986);

$t_{1/2}$ = 0.75 h and 0.96 h, based on photochemical transformation in Xenotest 1200 (Svenson & Björndal 1988);

$t_{1/2}$ = 1–110 h, based on aqueous photolysis half-life (Howard et al. 1991);

photodegradation half-lives ranging from hours to days, more rapid at the surface (Howard 1991);

photodegradation $t_{1/2}$ = 1.0 h in summer, 2.0 h in winter in distilled water and $t_{1/2}$ = 2.0 h in summer, 3.0 h in winter in estuarine water under irradiation by natural sunlight (quoted from Hwang et al. 1987, Sanders et al. 1993).

Ground water: $t_{1/2}$ = 1104–36,480 h, based on estimated unacclimated aqueous aerobic sediment grab sample data (Delaune et at. 1983; selected, Howard et al. 1991) and unacclimated anaerobic grab sample data for ground water (Baker & Mayfield 1980; selected, Howard et al. 1991).

Sediment:

Soil: disappearance $t_{1/2}$ = 23.2 d from Kooyenburg soil, $t_{1/2}$ = 47.9 d from Holten soil with earthworm *E. fetida andrei* and $t_{1/2}$ = 27.4 d from Kooyenburg soil, $t_{1/2}$ = 31.8 d from Holten soil with earthworm *L. rubellus* (van Gestel & Ma 1988);

$t_{1/2}$ = 552–4272 h, based on estimated unacclimated aqueous aerobic biodegradation half-life (Howard et al. 1991);

$t_{1/2}$ = 12.0 d in an acidic clay soil with <1.0% organic matter and $t_{1/2}$ = 6.7 d in a slightly basic sandy loam soil with 3.25% organic matter, based on aerobic batch lab. microcosm experiments (Loehr & Matthews 1992).

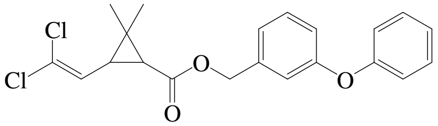
Biota: biological $t_{1/2}$ ~ 30 d in guppy *Lebistes reticulatus* (Landner et al. 1977);

elimination $t_{1/2}$ = 23, 9.3, 6.9, and 6.2 h for fat, liver muscle, and blood, respectively (rainbow trout, Call et al. 1980);

estimated $t_{1/2}$ = 7.0 d in trout (Niimi & Cho 1983; quoted, Niimi & Palazzo 1985);

clearance from flagfish: $t_{1/2}$ = 0.68 d from whole fish and $t_{1/2}$ = 0.68 d from fish lipid (Smith et al. 1990).

18.1.1.67 Permethrin



Common Name: Permethrin

Synonym: Ambush, Dragnet, Ectiban, Exmin, FMC 33297, FMC 41665, ICI-PP 557, Kafil, Kestrel, NDRC-143, NIA 33297, Niagara 33297, Outflank, Outflank-stockade, Perthrine, Picket, Pounce, Pramex, S 3151, SBP-1513, Talcord, WL 43479

Chemical Name: 3-phenoxybenzyl (1*RS*, 3*RS*; 1*RS*, 3*SR*)-3(2,2-dichlorovinyl)-2,2-dimethylcyclo-propanecarbo-xylate; 3-(2,2-dichloroethenyl)-2,2-dimethylcyclopropanecarboxylic acid (3-phenoxyphenyl)methyl ester

Uses: insecticide to control overwintering forms of spider mites, aphids, and scale insects on fruit trees, vines, olives, bananas and ornamentals; used as herbicides to control grass and broadleaf weeds in umbelliferous crops, and in tree nurseries; also used as acaricide and surfactant.

CAS Registry No: 52645-53-1

Molecular Formula: $C_{21}H_{20}Cl_2O_3$

Molecular Weight: 391.288

Melting Point (°C):

liquid	(tech. grade, Worthing & Hance 1991)
34	(Lide 2003)

Boiling Point (°C):

200	(at 0.01 mmHg, Hartley & Kidd 1987; Milne 1995)
200	(tech. grade at 0.1 mmHg, Worthing & Hance 1991; Tomlin 1994)
220	(at 0.05 mmHg, Montgomery 1993)
>290	(Tomlin 1994)

Density (g/cm^3 at 20°C):

1.19–1.27	(Hartley & Kidd 1987; Montgomery 1993; Tomlin 1994; Milne 1995)
1.214	(tech. grade at 25°C, Worthing & Hance 1991)

Molar Volume (cm^3/mol):

431	(calculated-Le Bas method at normal boiling point)
318.1	(calculated-density)

Dissociation Constant, pK_a:

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

Entropy of Fusion, ΔS_{fus} (J/mol K):

Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F: 0.816 (mp at 34°C)

Water Solubility (g/m^3 or mg/L at 25°C or as indicated):

0.20	(Martin & Worthing 1977)
0.04	(shake flask-GC, Coats & O'Donnell-Jefferey 1979)
~ 0.2	(Spencer 1982)
0.05	(in seawater, Schimmel et al. 1983; Zaroogian et al. 1985; Clark et al. 1989)
0.20	(20°C, Hartley & Kidd 1987; Tomlin 1994)
0.20	(30°C, Worthing & Walker 1987, 1991)
0.006	(20–25°C, selected, Wauchope et al. 1992; Hornsby et al. 1996)
0.2	(20°C, Montgomery 1993; Milne 1995)

Vapor Pressure (Pa at 25°C or as indicated. Additional data at other temperatures designated * are compiled at the end of this section):

4.8×10^{-6}	(*cis* isomer, Barlow 1978)
4.9×10^{-6}	(*cis* isomer, Wells et al. 1986)
3.7×10^{-6}	(*trans* isomer, Barlow 1978)
3.1×10^{-6}	(*trans* isomer, Wells et al. 1986)
4.5×10^{-5}	(Hartley & Kidd 1987; Tomlin 1994)

1.0×10^{-5}	(*cis* isomer, GC-RT correlation, supercooled liquid P_L, Hinckley et al. 1990)
8.1×10^{-6}	(*trans* isomer, GC-RT correlation, supercooled liquid P_L, Hinckley et al. 1990)
1.3×10^{-6}	(tech. grade at 20°C, Worthing & Hance 1991)
2.5×10^{-6}	(pure *cis* isomer at 20°C, Worthing & Hance 1991; Montgomery 1993; Tomlin 1994)
1.5×10^{-6}	(pre *trans* isomer at 20°C, Worthing & Hance 1991; Tomlin 1994)
1.7×10^{-6}	(20–25°C, selected, Wauchope et al. 1992; Hornsby et al. 1996)
1.4×10^{-5}*	(*cis* isomer, Knudsen effusion, measured range 40–80°C, Goodman 1997)
8.71×10^{-6}	(solid P^S, converted from P_L determined by GC-RT correlation, Tsuzuki 2001)

Henry's Law Constant (Pa·m³/mol at 25°C or as indicated):

0.0867	(wetted wall column-GC, Fendinger & Glotfelty 1990)
2.50×10^{-5}	(calculated-bond contribution method, Meylan & Howard 1991)
0.00486	(20°C, calculated-P/C, Montgomery 1993)
0.0157	(20–25°C, calculated-P/C, Majewski & Capel 1995)

Octanol/Water Partition Coefficient, log K_{OW}:

3.49	(shake flask-GC, Coats & O'Donnell-Jefferey 1979)
6.60	(calculated, Briggs 1981)
6.50	(shake flask-GC, Schimmel et al. 1983)
6.2 ± 0.9	(*cis*-form, HPLC-RT correlation, Muir et al. 1985)
5.7 ± 0.7	(*trans*-form, HPLC-RT correlation, Muir et al. 1985)
6.10	(tech. grade at 20°C, Worthing & Hance 1991; Tomlin 1994)
6.67	(HPLC-RT correlation, Hu & Leng 1992)
2.88–6.10	(Montgomery 1993)
6.50	(recommended, Sangster 1993)
6.10	(Milne 1995)
5.85	(RP-HPLC-RT correlation, Finizio et al. 1997)
5.73	(RP-HPLC-RT correlation using short ODP column, Donovan & Pescatore 2002)

Bioconcentration Factor, log BCF:

3.18	(calculated-S, Kenaga 1980)
3.28	(Schimmel et al. 1983)
3.23, 3.49, 3.52	(*Pimephales promelas*, Spehar et al. 1983;)
1.49–1.84	(*trans*-form on sediment, 24 h BCF for chironomid larvae in water, Muir et al. 1985)
1.08–2.13	(*trans*-form on sediment, 24 h BCF for chironomid larvae in sediment, Muir et al. 1985)
0.95–1.70	(*trans*-form on sediment, 24 h BCF for chironomid larvae in sediment/pore water, Muir et al. 1985)
0.90–2.22	(*cis*-form on sediment, 24 h BCF for chironomid larvae in water, Muir et al. 1985)
1.46–2.62	(*cis*-form on sediment, 24 h BCF for chironomid larvae in sediment, Muir et al. 1985)
1.32–2.47	(*cis*-form on sediment, 24 h BCF for chironomid larvae in sediment/pore water, Muir et al. 1985)
4.71, 4.83	(oyster, calculated-K_{OW} & models, Zaroogian et al. 1985)
4.71, 4.83	(sheepshead minnow, calculated-K_{OW} & models, Zaroogian et al. 1985)
3.29, 3.39	(*Oncorhynchus mykiss*, Muir et al. 1994; quoted, Devillers et al. 1996)
2.79	(quoted, Pait et al. 1992)

Sorption Partition Coefficient, log K_{OC}:

4.03	(calculated-S, Kenaga 1980)
2.76	(*cis*-form, silt, K_P on 34% DOC, Muir et al. 1985)
2.64	(*cis*-form, clay, K_P on 77% DOC, Muir et al. 1985)
2.64	(*trans*-form, silt, K_P on 23% DOC, Muir et al. 1985)
2.64	(*trans*-form, clay, K_P on 0% DOC, Muir et al. 1985)
5.25	(soil, calculated-χ and fragment contribution, Meylan et al. 1992)
5.00	(soil, 20–25°C, selected, Wauchope et al. 1992; Lohninger 1994; Hornsby et al. 1996)
1.32–2.79	(Montgomery 1993)
4.80	(soil, calculated-MCI $^1\chi$, Sabljic et al. 1995)
4.42, 4.35	(soils: organic carbon OC ≥ 0.1%, OC ≥ 0.5%, average, Delle Site 2001)

Environmental Fate Rate Constants, k, or Half-Lives, $t_{½}$:

Volatilization:

Photolysis: photodegradation rate constant $k = 1.73 \times 10^{-3}$ min^{-1} and $t_{½}$ = 400 min with TiO_2 as catalyst after 20 h irradiation at 222 nm (Hidaka et al. 1992).

Oxidation:

Hydrolysis:

Biodegradation:

$k = 1.24 \times 10^{-2}$ h^{-1} by bacteria strain *A. sobria* with $t_{½}$ = 56 h, $k = 1.13 \times 10^{-2}$ h^{-1} by *E. carotovora* with $t_{½}$ = 61 h, $k = 8.66 \times 10^{-3}$ h^{-1} by *Y. frederiksenii* with $t_{½}$ = 80 h and $k = 1.43 \times 10^{-3}$ h^{-1} for the control, uninoculated solution with $t_{½}$ = 485 d in aqueous soil-fee phase (*cis*-permethrin, Lee et al. 2004)

$k = 1.50 \times 10^{-2}$ h^{-1} by *A. sobria* with $t_{½}$ = 45 h, $k = 1.51 \times 10^{-2}$ h^{-1} by *E. carotovora* with $t_{½}$ = 46 h, $k = 1.85 \times 10^{-2}$ h^{-1} by *Y. frederiksenii* with $t_{½}$ = 37 h and $k = 2.85 \times 10^{-3}$ h^{-1} for the control, uninoculated solution with $t_{½}$ = 259 d in aqueous soil-fee phase (*trans*-permethrin, Lee et al. 2004)

Biotransformation:

Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants:

k_1 = 1.5–2.3 h^{-1} (*Chironomus tentans* larvae in pond sediment-water system for *trans*-permethrin, 96-h exposure, Muir et al. 1983)

k_1 = 1.50 h^{-1} (*Chironomus tentans* larvae in river sediment-water system for *trans*-permethrin, 96-h exposure, Muir et al. 1983)

k_1 = 3.3–12.1 h^{-1} (*Chironomus tentans* larvae in sediment (sand)-water system for *trans*-permethrin, 96-h exposure, Muir et al. 1983)

k_1 = 4.9–14.7 h^{-1} (*Chironomus tentans* larvae in sediment (sand)-water system for *trans*-permethrin, 96-h exposure, calculated by using initial uptake data of 0–12 h, Muir et al. 1983)

k_2 = 0.041 h^{-1} (*Chironomus tentans* larvae in pond sediment-water system for *trans*-permethrin, calculated by concentration decay curve, Muir et al. 1983)

k_2 = 0.021 h^{-1} (*Chironomus tentans* larvae in sediment (sand)-water system for *trans*-permethrin, calculated by concentration decay curve, Muir et al. 1983)

Half-Lives in the Environment:

Air:

Surface water: $t_{½}$ > 21 d in 100 mL pesticide-seawater solution under indoor conditions, $t_{½}$ = 14 d under outdoor light conditions and $t_{½}$ > 14 d under outdoor dark conditions (Schimmel et al. 1983);

biodegradation half-lives by bacteria strains: $t_{½}$ = 56 h by *A. sobria*, $t_{½}$ = 61 h by *E. carotovora*, $t_{½}$ = 80 h by *Y. frederiksenii* and $t_{½}$ = 485 d for the control, uninoculated solution for *cis*-permethrin; $t_{½}$ = 45 h by *A. sobria*, $t_{½}$ = 46 h by *E. carotovora*, $t_{½}$ = 37 h by *Y. frederiksenii* and $t_{½}$ = 259 d for the control, uninoculated solution for *trans*-permethrin (Lee et al. 2004)

Ground water:

Sediment: half-lives in 10 grams sediment/100 mL pesticide-seawater solution: $t_{½}$ < 2.5 d for untreated sediment and $t_{½}$ > 28 d for sterile sediment (Schimmel et al. 1983).

Soil: reported $t_{½}$ < 38 d in soil containing 1.3–51.3% organic matter at pH 4.2–7.7 (Holmstead et al. 1978; quoted, Worthing & Hance 1991; Montgomery 1993; Tomlin 1994);

selected field $t_{½}$ = 30 d (Wauchope et al. 1992; Hornsby et al. 1996);

soil $t_{½}$ = 30 d (Pait et al. 1992);

$t_{½}$ = 32 d for forest soil (Dowd et al. 1993).

Biota: elimination $t_{½}$ ~ 16.7 h in pond sediment-water, $t_{½}$ = 32.9 h in sand-water systems (*Chironomus tentans* larvae, Muir et al. 1983)

TABLE 18.1.1.67.1
Reported vapor pressures of *cis*-permethrin at various temperatures

Goodman 1997	
Knudsen effusion	
t/°C	P/Pa
40	1.4×10^{-5}
50	1.10×10^{-4}
60	5.30×10^{-4}
70	2.30×10^{-3}
80	8.90×10^{-3}
log P = A – B/(T/K)	
	P/Pa
A	18.70
B	7677

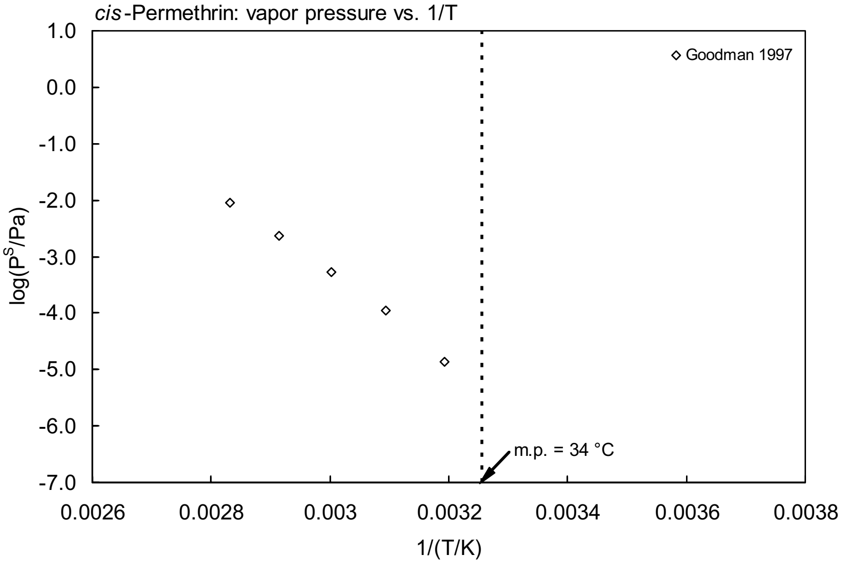
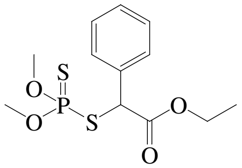


FIGURE 18.1.1.67.1 Logarithm of vapor pressure versus reciprocal temperature for *cis*-permethrin.

18.1.1.68 Phenthoate



Common Name: Phenthoate
Synonym: Cidial, Elsan
Chemical Name: ethyl 2-dimethoxyphosphinothioylthio(phenyl)acetate; ethyl 2-dimethoxy-thiophosphorylthio-2-phenylacetate; *S*-α-ethoxycarbonylbenzyl *O,O*-dimethyl phosphorodithioate; ethyl α-[(dimethoxy-phosphinothioyl)thio]benzeneacetate
Uses: insecticide to control aphids, scale insects, jassids, lepidopterous larvae, bollworms, mealybugs, psyllids, thrips, spider mites, etc. in citrus fruit, pome fruit, olives, cotton, cereals, rice, coffee, tea, sunflower, sugar cane, tobacco, ornamentals, and vegetables; also used as acaricide and for control of mosquito larvae.
CAS Registry No: 2597-03-7
Molecular Formula: $C_{12}H_{17}O_4PS_2$
Molecular Weight: 320.364
Melting Point (°C):
17.5 (Khan 1980; Spencer 1982)
17–18 (Worthing & Hance 1991; Tomlin 1994)
Boiling Point (°C): 78–80 (Spencer 1982)
Density (g/cm^3 at 20°C):
1.226 (Hartley & Kidd 1987; Worthing & Hance 1991; Tomlin 1994)
Molar Volume (cm^3/mol):
261.3 (calculated from density)
Dissociation Constant, pK_a:
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
Entropy of Fusion, ΔS_{fus} (J/mol K):
Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 K/ml K), F: 1.0

Water Solubility (g/m^3 or mg/L at 25°C or as indicated):
200 (Martin & Worthing 1977)
11 (20–25°C, shake flask-GC, Kanazawa 1981)
11 (20°C, Khan 1980; Hartley & Kidd 1987)
11 (24°C, Worthing & Walker 1987, 1991; Tomlin 1994)
11 (20–25°C, selected, Augustijn-Beckers et al. 1994; Hornsby et al. 1996)

Vapor Pressure (Pa at 25°C or as indicated):
0.005 (40°C, Hartley & Kidd 1987)
0.0053 (40°C, Worthing & Hance 1991; Tomlin 1994)
3.5×10^{-4} (20–25°C, selected, Augustijn-Beckers et al. 1994; Hornsby et al. 1996)
9.77×10^{-4}; 2.45×10^{-4}, 6.76×10^{-4} (gradient GC method; estimation using modified Watson method: Sugden's parachor, McGowan's parachor, Tsuzuki 2000)

Henry's Law Constant (Pa·m^3/mol):
0.01019 (calculated-P/C, this work)

Octanol/Water Partition Coefficient, log K_{OW}:
2.89 (shake flask-GC, Kanazawa 1981)
3.96 (shake flask/slow stirring-GC, De Bruijn et al. 1991)
3.69 (Worthing & Hance 1991; Tomlin 1994)
3.32 (RP-HPLC-RT correlation, Saito et al. 1993)
3.69 (recommended, Hansch et al. 1995)

Bioconcentration Factor, log BCF:

1.49	(calculated-S, Kenaga 1980)
1.56	(topmouth gudgeon *Pseudorasbora parva*, Kanazawa 1981)
2.85	(whole body willow shiner after 168 h exposure, Tsuda et al. 1992)
1.57, 1.43, 1.30, 1.51	(whole body carp: 24 h, 72 h, 120 h and 168 h; Tsuda et al. 1993)

Sorption Partition Coefficient, log K_{OC}:

2.38	(soil, calculated-S, Kenaga 1980)
3.00	(20–25°C, estimated, Augustijn-Beckers et al. 1994; Hornsby et al. 1996)

Environmental Fate Rate Constants, k, or Half-Lives, $t_{½}$:

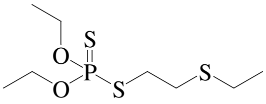
Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants:

excretion rate constant k = 0.05 h^{-1} from whole body willow shiner (Tsuda et al. 1992);
excretion rate constant k = 0.52 h^{-1} with $t_{½}$ = 1.3 h (Tsuda et al. 1993).

Half-Lives in the Environment:

Air:
Surface water:
Ground water:
Sediment:
Soil: selected field $t_{½}$ = 11 d (Augustijn-Beckers et al. 1994; Hornsby et al. 1996);
$t_{½}$ = 10 d in silty clay loam and other soils (Tomlin 1994).
Biota: excretion rate constant k = 0.05 h^{-1} from whole body willow shiner (Tsuda et al. 1992);
excretion rate constant k = 0.52 h^{-1} with $t_{½}$ = 1.3 h (Tsuda et al. 1993).

18.1.1.69 Phorate



Common Name: Phorate

Synonym: AC 3911, American Cyanamid 3911, ENT 24042, Foraat, Gramitox, Granutox, Rampart, Thimate, Thimet, Timet, Vegfu, Vergfru foratox

Chemical Name: *O,O*-diethyl-*S*-(ethylthio)methyl phosphorodithioate; *O,O*-diethyl-*S*-ethylmercaptomethyl dithiophosphate; phosphorodithioic acid *O,O*-diethyl *S*-((ethylthio)methyl) ester

Uses: insecticide to control mites, chewing and sucking insects in fruits and vegetables, cotton, and some ornamentals; also used as acaricide and nematicide.

CAS Registry No: 298-02-2

Molecular Formula: $C_7H_{17}O_2PS_3$

Molecular Weight: 260.378

Melting Point (°C):

–42.9	(Spencer 1982)
<–15	(Montgomery 1993; Lide 2003)

Boiling Point (°C):

118–120	(at 0.8 mmHg, Hartley & Kidd 1987; Montgomery 1993; Milne 1995)
125–127	(at 2 mmHg, Budavari 1989; Milne 1995)
118–120	(tech. grade at 0.8 mmHg, Worthing & Hance 1991)

Density (g/cm^3 at 20°C):

1.156	(25°C, Merck Index 1989; Montgomery 1993; Milne 1995)
1.167	(tech. grade at 25°C, Spencer 1982; Worthing & Hance 1991)

Molar Volume (cm^3/mol):

259.9	(calculated-Le Bas method at normal boiling point)

Dissociation Constant, pK_a:

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

Entropy of Fusion, ΔS_{fus} (J/mol K):

Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F: 1.0

Water Solubility (g/m^3 or mg/L at 25°C or as indicated):

19	(26°C, 95% pure, shake flask-GC, Lord & Burt 1964)
14	(15°C, shake flask-GC, Lord & Burt 1964)
85	(Günther et al. 1968)
70	(Melnikov 1971; Briggs 1981)
50	(Spencer 1973, 1982)
50	(Martin & Worthing 1977; Hartley & Kidd 1987)
80–85	(Wauchope 1978)
20	(shake flask-GC, Felsot & Dahm 1979)
17.9	(20°C, shake flask-GC, Bowman & Sans 1979, 1983b)
50	(room temp., Worthing & Walker 1987; Budavari 1989, Milne 1995)
50	(tech. grade at room temp., Worthing & Hance 1991)
22	(20–25°C, selected, Wauchope 1989; Wauchope et al. 1992; Hornsby et al. 1996)
20	(24°C, Montgomery 1993)

Vapor Pressure (Pa at 25°C or as indicated):

0.112	(20°C, Wolfdietrich 1965; Spencer 1973, 1982)
0.25	(Woolford 1975)
0.148	(gas saturation method, Sutherland et al. 1980)
0.074	(gas saturation-GC, Kim et al. 1984)
0.042	(20°C, extrapolated-Clausius-Clapeyron eq., Kim et al. 1984)

0.0109	(20°C, GC-RT correlation, Kim et al. 1984; Kim 1985)
0.11	(20°C, Hartley & Kidd 1987)
0.112	(20°C, Budavari 1989; Montgomery 1993)
0.11	(GC-RT correlation method, Hinckley et al. 1990)
0.085	(tech. grade, Worthing & Hance 1991)
0.0853	(20–25°C, selected, Wauchope et al. 1992; Hornsby et al. 1996)

Henry's Law Constant (Pa·m^3/mol at 25°C or as indicated):

0.769	(calculated-P/C, Jury et al. 1984, 1987a, 1990; Jury & Ghodrati 1989)
0.65	(20°C, calculated-P/C, Suntio et al. 1988)
0.648	(20–24°C, calculated-P/C, Montgomery 1993)
1.010	(calculated-P/C, this work)

Octanol/Water Partition Coefficient, log K_{OW}:

3.33	(shake flask-GC, Felsot & Dahm 1979)
2.92	(Rao & Davidson 1980)
4.26	(shake flask-UV, Lord et al. 1980)
4.26	(20°C, shake flask-GC, Briggs 1981)
3.83	(22°C, shake flask-GC, Bowman & Sans 1983b)
3.24	(shake flask, Log P Database, Hansch & Leo 1987)
3.92	(Worthing & Hance 1991)
2.91–3.92	(Montgomery 1993)
2.92	(recommended, Sangster 1993)
3.92	(Milne 1995)
3.56	(selected, Hansch et al. 1995)
4.25	(RP-HPLC-RT correlation, Finizio et al. 1997)
3.94	(RP-HPLC-RT correlation using short ODP column, Donovan & Pescatore 2002)

Bioconcentration Factor, log BCF:

1.83, 2.34	(calculated-S, calculated-K_{OC}, Kenaga 1980)
3.34	(earthworms, Lord et al. 1980)
–1.70	(vegetation, correlated-K_{OW}, Travis & Arms 1988)

Sorption Partition Coefficient, log K_{OC}:

3.51	(soil, Hamaker & Thompson 1972; Kenaga 1980; Kenaga & Goring 1980)
2.71	(soil, calculated-S as per Kenaga & Goring 1978, Kenaga 1980)
2.82	(Rao & Davidson 1980; quoted, Jury et al. 1983, 1984, 1990)
2.82	(soil, sorption isotherm, converted form reported log K_{OM} of 2.82, Briggs 1981)
2.32–3.60	(reported as log K_{OM}, Mingelgrin & Gerstl 1983)
2.82	(screening model calculations, Jury et al. 1987a, b; Jury & Ghodrati 1989)
2.58, 2.88	(reported as log K_{OM}, estimated as log K_{OM}, Magee 1991)
2.73	(soil, Worthing & Hance 1991)
3.00	(soil, 20–25°C, estimated, Wauchope et al. 1992; Hornsby et al. 1996)
2.64	(estimated-QSAR & SPARC, Kollig 1993)
2.51–2.80	(Montgomery 1993)
2.82	(selected, Lohninger 1994)
2.70	(soil, calculated-MCI $^1\chi$, Sabljic et al. 1995)
2.70; 2.98, 3.12	(soil, quoted exptl.; estimated-class-specific model, estimated-general model, Gramatica et al. 2000)
2.63	(soil: organic carbon OC -0.5%, average, Delle Site 2001)

Environmental Fate Rate Constants, k, or Half-Lives, $t_{1/2}$:

Volatilization:

Photolysis:

Oxidation:

Hydrolysis: neutral hydrolysis rate constant k = 7.2×10^{-3} h^{-1} with a calculated $t_{1/2}$ = 96 h at pH 7 (Ellington et al. 1987, 1988; quoted, Montgomery 1993);

calculated rate constant k -100×10^{-12} cm^3/molecule·s for the vapor-phase reaction with hydroxyl radical in air (Winer & Atkinson 1990);

$t_{1/2}$ = 3.2 d at pH 7 and $t_{1/2}$ = 3.9 d at pH 9 (Worthing & Hance 1991);

rate constant k = 62 yr^{-1} at pH 7.0 and 25°C (Kollig 1993).

Biodegradation: $t_{1/2}$ = 82 d for a 100 d leaching and screening test in 0–10 cm depth of soil (Rao & Davidson 1980; quoted, Jury et al. 1983);

$t_{1/2}$ = 82 d in soil (Jury et al. 1984, 1987a, b, 1990; Jury & Ghorati 1989);

first-order rate constant k = –0.0403 h^{-1} in nonsterile sediment and k = –0.0209 h^{-1} in sterile sediment by shake-tests at Range Point and first-order rate constant k = –0.0206 h^{-1} in nonsterile water and k = –0.0186 h^{-1} in sterile water by shake-tests at Range Point (Walker et al. 1988);

first-order rate constants k = –0.0241 h^{-1} in nonsterile sediment and k = –0.0185 h^{-1} in sterile sediment by shake-tests at Davis Bayou and first-order rate constants k = –0.0262 h^{-1} in nonsterile water and k = –0.0185 h^{-1} in sterile water by shake-tests at Davis Bayou (Walker et al. 1988).

Biotransformation:

Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants:

Half-Lives in the Environment:

Air:

Surface water:

Ground water:

Sediment:

Soil: $t_{1/2}$ = 68 d in a sandy soil (Way & Scopes 1968; quoted, Montgomery 1993);

estimated persistence of 2 wk (Kearney et al. 1969; Edwards 1973; quoted, Morrill et al. 1982; Jury et al. 1987a);

persistence of less than one month (Wauchope 1978);

biodegradation $t_{1/2}$ = 82 d in soil (Jury et al. 1984, 1987a, b, 1990; Jury & Ghodrati 1989; quoted, Montgomery 1993);

$t_{1/2}$ = 2–14 d (Worthing & Hance 1991);

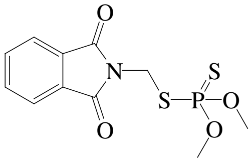
estimated field $t_{1/2}$ = 60 d (Wauchope et al. 1992; quoted, Richards & Baker 1993; selected, Halfon et al. 1996; Hornsby et al. 1996);

soil $t_{1/2}$ = 25 d (Pait et al. 1992).

Biota: $t_{1/2}$ = 1.4 d half-lives in coastal Bermuda grass and alfalfa (Leuck & Bowman 1970; quoted, Montgomery 1993) and $t_{1/2}$ = 3.6 d (Dobson et al. 1960; quoted, Montgomery 1993);

biochemical $t_{1/2}$ = 82 d from screening model calculations (Jury et al. 1987a, b; Jury & Ghodrati 1989).

18.1.1.70 Phosmet



Common Name: Phosmet

Synonym: APPA, Decemthion, Decemthion p-6, ENT 25,705, Ftalophos, Imidan, Percolate, Phthalophos, Prolate, R 1504, Safidon, Smidan, Stauffer R-1504

Chemical Name: *O,O*-dimethyl S-phthalimidomethyl phosphorodithioate; *N*-dimethoxyphosphino-thioylthiomethyl)phthalimide; *S*-[(1,3-dihydro-1,3-dioxo-2*H*-isoindol-2-yl)methyl] *O,O*-dimethyl phosphorodithioate; phosphorodithioic acid, *S*-[(1,3-dihydro-1,3-dioxo-2*H*-isoindol-2-yl)methyl] *O,O*-dimethyl ester

Uses: nonsystemic acaricide and insecticide.

CAS Registry No: 732-11-6

Molecular Formula: $C_{11}H_{12}NO_4PS_2$

Molecular Weight: 317.321

Melting Point (°C):

72.0–72.7, 66.5–69.5 (pure, technical grade, Montgomery 1993; Tomlin 1994)
72 (Lide 2003)

Boiling Point (°C):

decompose rapidly >100°C (Montgomery 1993)

Density (g/cm^3 at 20°C):

Molar Volume (cm^3/mol):

263.3 (calculated-Le Bas method at normal boiling point)

Dissociation Constant, pK$_a$:

Enthalpy of Fusion, ΔH$_{fus}$ (kJ/mol):

30.96 (Plato & Glasgow 1969)

Entropy of Fusion, ΔS$_{fus}$ (J/mol K):

Fugacity Ratio at 25°C (assuming ΔS$_{fus}$ = 56 J/mol K), F: 0.346 (mp at 72°C)

0.3 (20°C, Suntio et al. 1988)

Water Solubility (g/m^3 or mg/L at 25°C or as indicated):

25 (Bright et al. 1950, Melnikov 1971; Spencer 1982)
25 (Hartley & Kidd 1987; Tomlin 1994; Milne 1995)
20 (20–25°C, selected, Wauchope et al. 1992; Hornsby et al. 1996)
22–25 (Montgomery 1993)

Vapor Pressure (Pa at 25°C or as indicated):

6.03×10^{-4} (20°C, Freed et al. 1977)
0.133 (50°C, Spencer 1982; Hartley & Kidd 1987)
6.53×10^{-5} (20–25°C, selected, Wauchope et al. 1992; Hornsby et al. 1996)
6.03×10^{-5}, 0.133 (30, 50°C, Montgomery 1993)
6.50×10^{-5} (Tomlin 1994)
2.0×10^{-5}; 5.90×10^{-5} (gradient GC method; quoted lit. value, Tsuzuki 2000)

Henry's Law Constant (Pa·m^3/mol):

9.50×10^{-4} (calculated-P/C, Suntio et al. 1988)
9.53×10^{-4} (calculated-P/C, Montgomery 1993)
7.62×10^{-4} (calculated-P/C, this work)

Octanol/Water Partition Coefficient, log K$_{OW}$:

2.83 (20°C, shake flask-GC, Chiou et al. 1977)
2.83 (Rao & Davidson 1980)

2.78	(22°C, shake flask-GC, Bowman & Sans 1983)
2.81	(shake flask/slow stirring-GC, De Bruijn & Hermens 1991)
2.78–3.04	(Montgomery 1993)
2.78	(recommended, Sangster 1993)
2.95	(Tomlin 1994)
3.40	(Milne 1995)
2.78	(recommended, Hansch et al. 1995)
3.06	(RP-HPLC-RT correlation, Nakamura et al. 2001)

Bioconcentration Factor, log BCF:

0.90	(bluegill sunfish/fathead minnows, Saito et al. 1992)
1.04	(channel catfish, Saito et al. 1992)
1.56	(av. whole body willow shiner after 24–168 h exposure, Tsuda et al. 1992)
0.23	(av. whole body carp after 24–168 h exposure, Tsuda et al. 1993)

Sorption Partition Coefficient, log K_{OC}:

2.91	(soil, Wauchope et al. 1992, Hornsby et al. 1996)
2.06, 2.34	(soil, estimated-class-specific model, estimated-general model, Gramatica et al. 2000)

Environmental Fate Rate Constants, k, or Half-Lives, $t_{1/2}$:

Volatilization:

Photolysis: $t_{1/2}$ = 53.25 h for absorbance wavelength at 243 nm (Montgomery 1993).

Oxidation:

Hydrolysis: $t_{1/2}$ = 7.2 d at pH 6.1 and $t_{1/2}$ = 7.1 h at pH 7.4 at 20°C; $t_{1/2}$ = 1.1 h at 37.5°C (Freed et al. 1979; quoted, Montgomery 1993);

$t_{1/2}$ = 13 d at pH 4.5, $t_{1/2} < 12$ h at pH 7 and $t_{1/2} < 4$ h at pH 8.3 in buffered aqueous solution at 20°C (Montgomery 1993);

$t_{1/2}$ = 7.0 d at pH 6.1, and $t_{1/2}$ = 7.1 h at pH 7.4 at 20°C (Lartiges & Garrigues 1995).

Biodegradation:

Biotransformation:

Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants:

k_2 = 0.28 h^{-1} (whole body willow shiner, Tsuda et al. 1992)

Half-Lives in the Environment:

Air:

Surface water: $t_{1/2}$ = 33 d at 6°C, $t_{1/2}$ = 5 d at 22°C in darkness for Milli-Q water at pH 6.1 (Lartiges & Garrigues 1995).

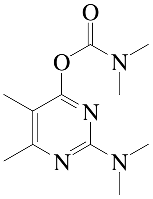
Ground water:

Sediment:

Soil: field $t_{1/2}$ = 10 d (Wauchope et al. 1992; Hornsby et al. 1996).

Biota: $t_{1/2}$ = 6.5 d in Bermuda grass (Montgomery 1993).

18.1.1.71 Pirimicarb



Common Name: Pirimicarb
Synonym: Pirimor, Aphox, Abol, Aficida, Fernos, Rapid
Chemical Name: 2-dimethylamino-5,6-dimethylpyrimidin-4-yl dimethylcarbamate
CAS Registry No: 23103-98-2
Uses: insecticide
Molecular Formula: $C_{11}H_{18}N_4O_2$
Molecular Weight: 238.287
Melting Point (°C):
    90.5 (Spencer 1982; Hartley & Kidd 1987; Worthing 1987; Tomlin 1994; Lide 2003)
Boiling Point (°C):
Density (g/cm^3 at 20°C):
    1.21 (Tomlin 1994)
Molar Volume (cm^3/mol):
Dissociation Constant, pK_a:
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
Entropy of Fusion, ΔS_{fus} (J/mol K):
Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F: 0.228 (mp at 90.5°C)

Water Solubility (g/m^3 or mg/L at 25°C):
    2700 (Kenaga 1980b; Spencer 1982; Hartley & Kidd 1987; Worthing & Walker 1987)
    2000 (pH 4, 20°C, Tomlin 1994)
    2700 (selected, Augustijn-Beckers et al. 1994; Hornsby et al. 1996)

Vapor Pressure (Pa at 25°C):
    0.004 (30°C, Spencer 1982. Hartley & Kidd 1987; Worthing & Walker 1987)
    0.00097 (Tomlin 1994)
    0.004 (selected, Augustijn-Beckers et al. 1994; Hornsby et al. 1996)

Henry's Law Constant (Pa·m^3/mol at 25°C):

Octanol/Water Partition Coefficient, log K_{OW}:
    1.70 (Tomlin 1994)
    1.70 (recommended, Hansch et al. 1995)
    1.70 (LOGPSTAR or CLOGP data, Sabljic et al. 1995)

Octanol/Air Partition Coefficient, log K_{OA}:

Bioconcentration Factor, log BCF or log K_B:
    0.845 (calculated-Solubility, Kenaga 1980b)

Sorption Partition Coefficient, log K_{OC}:
    1.76 (soil, Kenaga 1980b)
    1.57 (soil, estimated and selected value, Augustijn-Beckers et al. 1994)
    1.36 (soil, estimated and selected, Hornsby et al. 1996)
    1.90, 1.52 (soil: quoted, calculated-MCI χ, Meylan et al. 1992)

1.90 (soil, calculated-MCI χ, Sabljic et al 1995)
1.90; 2.30, 1.80 (soil, quoted obs.; estimated-class-specific model, estimated-general model using molecular descriptors, Gramatica et al. 2000)

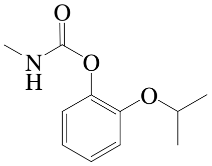
Environmental Fate Rate Constants, k, or Half-Lives, $t_{½}$:

Volatilization:
Photolysis: aqueous solutions are unstable to UV light with $t_{½} < 1$ d at pH 5.7 or 9 (Tomlin 1994).
Oxidation:
Hydrolysis:
Biodegradation: $t_{½}$ = 7–234 d depending on soil type, organic matter ranging from 1.7–51.9% at pH 5.5–8.1 (Tomlin 1994).
Biotransformation:
Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants:

Half-Lives in the Environment:

Air:
Surface water: aqueous solutions are unstable to UV light with $t_{½} < 1$ d at pH 5.7 or 9 (Tomlin 1994).
Ground water:
Sediment:
Soil: $t_{½}$ = 7–234 d depending on soil type, organic matter ranging from 1.7–51.9% at pH 5.5–8.1 (Tomlin 1994); field $t_{½}$ ~ 10 d (estimated, Augustijn-Beckers et al. 1994; Hornsby et al. 1996).
Biota:

18.1.1.72 Propoxur



Common Name: Propoxur
Synonym: Baygon, Blattanex, Under, arprocarb, PHC, Sendran, Suncide, Aracarb, Tugon Fliegendugel
Chemical Name: 2-(1-methylethoxy)phenol methyl carbamate
CAS Registry No: 114-26-1
Uses: insecticide to control cockroaches, flies, fleas, mosquitoes, bugs, ants, millipedes and other insect pests in food storage areas, houses, animal houses, etc.; also to control sucking and chewing insects in fruits, vegetables, ornamentals, vines, maize, lucerne, soya beans, cotton, sugar cane, rice cocoa, forestry, etc.
Molecular Formula: $C_{11}H_{15}NO_3$
Molecular Weight: 209.242
Melting Point (°C)

91.50	(Spencer 1982; Howard 1991; Kühne et al. 1995)
84–87	(Montgomery 1993)
87	(Lide 2003)

Boiling Point (°C):
Density (g/cm³ at 20°C):
Molar Volume (cm³/mol):

244.7	(calculated-Le Bas method at normal boiling point)

Dissociation Constant, pK_a:
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
Entropy of Fusion, ΔS_{fus} (J/mol K):
Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F: 0.246 (mp at 87°C)

Water Solubility (g/m³ or mg/L at 25°C or as indicated):

2000	(20°C, Spencer 1973; 1982)
2000	(Kenaga 1980; Kanazawa 1981)
2000	(20°C, Worthing & Walker 1983, 1987, Worthing & Hance 1991)
1860	(20°C, shake flask-GC, Bowman & Sans 1983)
1800	(20–25°C, selected, Wauchope et al. 1992; Hornsby et al. 1996)
1740, 1930, 2440	(10, 20, 30°C, Montgomery 1993)

Vapor Pressure (Pa at 25°C or as indicated):

1.333	(120°C, Melnikov 1971; Spencer 1973, 1982)
4.13×10^{-4}	(20°C, Hartley & Graham-Bryce 1980)
4.13×10^{-5}	(20°C, selected exptl. value from literature, Kim 1985)
0.0593, 0.0113	(20°C, GC-RT correlation, GC-RT correlation with mp correction, Kim 1985)
4.00×10^{-4}	(20°C, Howard 1991)
1.69×10^{-3}	(20–25°C, selected, Wauchope et al. 1992, Hornsby et al. 1996)
1.30×10^{-3}	(20°C, Montgomery 1993; Siebers et al. 1994)

Henry's Law Constant (Pa·m³/mol at 25°C or as indicated):

0.1308	(20°C, calculated-P/C, Suntio et al. 1988)
4.46×10^{-5}	(calculated-P/C, Howard 1991)
1.32×10^{-4}	(calculated-P/C, Montgomery 1993)
1.40×10^{-4}	(calculated-P/C, Siebers et al. 1994)
1.98×10^{-6}	(calculated-P/C, this work)

Octanol/Water Partition Coefficient, log K_{OW}:

1.52	(shake flask-UV, Fujita et al. 1974)
1.50	(Hansch & Leo 1979)
1.45	(Rao & Davidson 1980)
1.52	(Kenaga & Goring 1980; Kanazawa 1981)
1.552	(shake flask-GC, Bowman & Sans 1983)
1.52	(Hansch & Leo 1985)
1.75	(RP-HPLC-RT correlation, Trapp & Pussemier 1991)
1.45–1.56	(Montgomery 1993)
1.52	(recommended, Sangster 1993)
1.52	(recommended, Hansch et al. 1995)
1.99	(RP-HPLC-RT correlation, Nakamura et al. 2001)

Bioconcentration Factor, log BCF:

0.924	(calculated, Howard 1991)

Sorption Partition Coefficient, log K_{OC}:

1.67	(measurements for average of 2 soils, Kanazawa 1981, 1989)
1.86	(calculated, Howard 1991)
1.48	(soil, Wauchope et al. 1992; Hornsby et al. 1996)
0.48–1.97	(Montgomery 1993)
1.48	(estimated-chemical structure, Lohninger 1994)
1.67	(soil, calculated-MCI $^1\chi$, Sabljic et al. 1995)
1.63, 1.88	(soil, estimated-class-specific model, estimated-general model, Gramatica et al. 2000)

Environmental Fate Rate Constants, k, or Half-Lives, $t_{1/2}$:

Volatilization:

Photolysis: atmospheric and/or aqueous photolysis $t_{1/2}$ = 62.5–87.9 h, based on measured rate of photolysis on bean leaves in sunlight (Ivie & Casida 1971; quoted, Howard et al. 1991) and in aqueous solution under simulated sunlight (Jensen-Korte et al. 1987; quoted, Howard et al. 1991);

photolyze in water with $t_{1/2}$ = 88 h and decreased with humic material to 13–41 h; $t_{1/2}$ = 87.9 h in water when irradiated with light >290 nm (Howard 1991).

Oxidation: photooxidation $t_{1/2}$ = 0.71–7.1 h in air, based on estimated rate constant for the vapor-phase reaction with hydroxyl radical in air (Atkinson 1987; quoted, Howard et al. 1991);

vapor-phase photooxidation $t_{1/2}$ = 4.3 h for reaction with ambient OH radical (Howard 1991).

Hydrolysis: $t_{1/2}$ = 40 min at pH 10 and 20°C, hydrolyzes at a rate of 1.5% d^{-1} in 1% aqueous solution at pH 7 (Spencer 1982);

$t_{1/2}$ = 16, 1.6 and 0.17 d at pH 8, 9, 10, but stable between pH 3–7, $t_{1/2}$ = 40 min at pH 10 (Howard 1991);

$t_{1/2}$ = 290 d at pH 7, $t_{1/2}$ = 17.9 d at pH 8 and $t_{1/2}$ = 48 min at pH 10 (Montgomery et al. 1993);

hydrolysis $t_{1/2}$ = 16 d, 1.6 d and 4.2 h in water at pH 8, 9 and 10 (Aly & El-Dib 1971; quoted, Montgomery 1993).

Biodegradation: aqueous aerobic $t_{1/2}$ = 168–672 h, based on unacclimated aqueous aerobic screening test data (Gummer 1979; Kanazawa 1987; quoted, Howard et al. 1991); aqueous anaerobic $t_{1/2}$ = 672–2688 h, based on estimated unacclimated aqueous aerobic biodegradation half-life (Howard et al. 1991);

$t_{1/2}$ = 44 d under aerobic conditions and $t_{1/2}$ = 59 d under anaerobic conditions in water used a combination of activated sludge, silt loam soil and sediment as an inoculum; $t_{1/2}$ = 78 d under aerobic conditions and $t_{1/2}$ = 125 d under anaerobic conditions at pH 6.9 (Howard 1991).

Biotransformation: metabolism rate k = 3.70×10^{-3} h^{-1} leading to an irradiated moist soil $t_{1/2}$ = 180 h (Graebing & Chib 2004)

Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants:

Half-Lives in the Environment:

Air: $t_{1/2}$ = 0.71–7.1 h, based on estimated rate constant for the vapor-phase reaction with hydroxyl radical in air (Atkinson 1987; quoted, Howard et al. 1991);

$t_{1/2}$ ~ 4 h reacting with photochemically produced hydroxyl radical in air (Howard 1991).

Surface water: $t_{1/2}$ = 38–672 h, based on estimated hydrolysis half-life at pH 9 (Aly & El-Dib 1971; quoted, Howard et al. 1991) and estimated unacclimated aqueous aerobic biodegradation half-life (Howard et al. 1991);

$t_{1/2}$ = 1 d to 1 wk by degradation, photolyze rapidly with $t_{1/2}$ = 13 to 88 h (Howard 1991).

Ground water: $t_{1/2}$ = 38–1344 h, based on estimated hydrolysis half-life at pH 9 (Aly & El-Dib 1971; quoted, Howard et al. 1991) and estimated unacclimated aqueous aerobic biodegradation half-life (Howard et al. 1991).

Sediment:

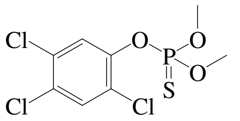
Soil: $t_{1/2}$ = 38–672 h, based on estimated hydrolysis half-life at pH 9 (Aly & El-Dib 1971; quoted, Howard et al. 1991) and estimated unacclimated aqueous aerobic biodegradation half-life (Howard et al. 1991)

Field $t_{1/2}$ = 14–50 d (Wauchope et al. 1992)

On sandy loam soil: first-order rate constants for photolytic decline, $k = 1.65 \times 10^{-3}\ h^{-1}$ irradiated in moisture-maintained soil, $k = 0.91 \times 10^{-3}\ h^{-1}$ irradiated in air-dried soil, $k = 0.91 \times 10^{-3}\ h^{-1}$ in dark control moist soil and $k = 0.23 \times 10^{-3}\ h^{-1}$ in dark control air-dried sandy loam soil from Madia, CA. The initial metabolism rate $k = 3.70 \times 10^{-3}\ h^{-1}$ leading to an irradiated moist soil $t_{1/2}$ = 180 h; in the dark $t_{1/2}$ = 380 h in moist soil Graebing & Chib 2004)

Biota:

18.1.1.73 Ronnel



Common Name: Ronnel

Synonym: Blitex, Dermafos, Dermaphos, dimethyl trichlorophenyl thiophosphate, Dow ET 14, Dow ET 57, Ectoral, ENT 23284, Etrolene, Fenchlorfos, Fenchlorphos, Gesektin K, Karlan, Korlan, Nanchor, Nanker, Nankor, OMS 123, Phenchlorfos, Remelt, Rovan, trichlorometafos, Trolen, Trolene, Viozene

Chemical Name: *O,O*-dimethyl *O*-(2,4,5-trichlorophenyl)thiophosphate; *O,O*-dimethyl *O*-2,4,5-trichlorophenyl phosphorothioate; phosphoric acid *O,O*-dimethyl *O*-(2,4,5-trichlorophenyl)ester

Uses: insecticide.

CAS Registry No: 299-84-3

Molecular Formula: $C_8H_8Cl_3O_3PS$

Molecular Weight: 321.546

Melting Point (°C):

40–42	(Spencer 1982)
41	(Montgomery 1993; Milne 1995; Lide 2003)

Boiling Point (°C):

Density (g/cm^3 at 20°C):

1.48	(25°C, Montgomery 1993)

Molar Volume (cm^3/mol):

257.3	(calculated-Le Bas method at normal boiling point)

Dissociation Constant, pK_a:

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

23.85	(Plato & Glasgow 1969)

Entropy of Fusion, ΔS_{fus} (J/mol K):

Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F: 0.697 (mp at 41°C)

Water Solubility (g/m^3 or mg/L at 25°C or as indicated):

44	(Günther et al. 1968; Melnikov 1971)
1.08	(20°C, shake flask-GC, Chiou et al. 1977)
1.08	(20–25°C, shake flask-GC/ECD, Freed et al. 1979)
2.5	(20°C, Spencer 1982)
0.60	(20°C, shake flask-GC, Bowman & Sans 1979, 1983)
0.98	(20°C, corrected supercooled liq. value, shake flask-GC, Bowman & Sans 1979,83)
6.0	(Dow Chemical unpublished data, Kenaga 1980a, b; Kenaga & Goring 1980)
40	(22°C, Khan 1980)
1.0	(20°C, shake flask-HPLC, Ellgehausen et al. 1981)
1.61	(20°C, selected, Suntio et al. 1988)
40	(Montgomery 1993; Milne 1995)

Vapor Pressure (Pa at 25°C or as indicated):

0.0533	(20°C, Eichler 1965; Melnikov 1971)
0.0071	(20–25°C, Freed et al. 1979)
1.067	(Spencer 1982)
0.0017	(20°C, GC-RT correlation without mo correlation, Kim et al. 1984; Kim 1985)
0.0011	(20°C, GC-RT correlation with mp correction, Kim et al. 1984; Kim 1985)
0.016	(20°C, selected, Suntio et al. 1988)
0.0045	(20°C, Montgomery 1993)

Henry's Law Constant (Pa·m^3/mol at 25°C or as indicated):

3.22	(20°C, calculated-P/C, Suntio et al. 1988)
0.857	(20–25°C, calculated-P/C, Montgomery 1993)

Octanol/Water Partition Coefficient, log K_{OW} at 25°C or as indicated:

4.88 (20°C, shake flask-GC, Chiou et al. 1977)
4.67 (Kenaga 1980b; Kenaga & Goring 1980)
4.88 (20–25°C, shake flask-GC/ECD, Freed et al. 1979)
5.34 (shake flask-HPLC, Ellgehausen et al. 1981)
4.81 (20°C, shake flask-GC, Bowman & Sans 1983)
5.068 ± 0.004 (shake flask/slow-stirring method, De Bruijn et al. 1989)
4.67–5.068 (Montgomery 1993)
4.88 (recommended, Sangster 1993)
5.07 (recommended, Hansch et al. 1995)

Octanol/Air Partition Coefficient, log K_{OA}:

Bioconcentration Factor, log BCF:

2.35 (calculated-S, Kenaga 1980a, b)
–1.38 (average beef fat diet, Kenaga 1980b)
4.64 (guppy *Poecilia reticulata*, lipid wt basis, De Bruijn & Hermens 1991)

Sorption Partition Coefficient, log K_{OC}:

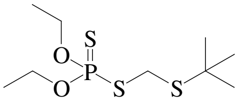
3.20 (soil, calculated-S as per Kenaga & Goring 1978, Kenaga 1980a, b)
2.90 (soil, calculated-MCI χ, Gerstl & Helling 1987)
2.76 (calculated, Montgomery 1993)

Environmental Fate Rate Constants, k, or Half-Lives, $t_{1/2}$:

Volatilization:
Photolysis:
Oxidation:
Hydrolysis: estimated $t_{1/2}$ ~ 3 d at pH 6 (Montgomery 1993).
Biodegradation:
Biotransformation:
Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants:
k_1 = 0.01337 mL g^{-1} d^{-1} (guppy, 0.5–420 h exposure, De Bruijn & Hermens 1991)
k_2 = 0.38 d^{-1} (guppy, De Bruijn & Hermens 1991)
k_2 = 0.14 d^{-1} (calculated-K_{OW}, De Bruijn & Hermens 1991)

Half-Lives in the Environment:

18.1.1.74 Terbufos



Common Name: Terbufos
Synonym: AC 92100, Counter, ST-100
Chemical Name: *S*-(*tert*-butylthio)methyl *O,O*-diethyl phosphorodithioate; *S*-[[(1,1-dimethylethyl)thio]methyl] *O,O*-diethyl phosphorodithioate; phosphorodithioic acid S-((*tert*-butylthio)methyl) *O,O*-diethyl ester
Uses: insecticide in soil to control insects and also used as nematocide to control nematodes in beet, maize, cotton, sorghum, onions, cabbage, and bananas.
CAS Registry No: 13071-79-9
Molecular Formula: $C_9H_{21}O_2PS_3$
Molecular Weight: 288.431
Melting Point (°C):
–29.2 (Worthing & Hance 1991; Howe et al. 1994; Montgomery 1993; Tomlin 1994; Milne 1995)
Boiling Point (°C):
69 (at 0.01 mmHg, Worthing & Hance 1991; Montgomery 1993; Tomlin 1994; Milne 1995)
312 (Brecken-Folse et al. 1994; Howe et al. 1994)
Density (g/cm^3 at 20°C):
1.105 (24°C, Worthing & Hance 1991; Montgomery 1993; Tomlin 1994; Milne 1995)
Molar Volume (cm^3/mol):
261 (24˚C, calculated from density)
Dissociation Constant, pK_a:
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
Entropy of Fusion, ΔS_{fus} (J/mol K):
Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F: 1.0

Water Solubility (g/m^3 or mg/L at 25°C or as indicated):
12 (Martin & Worthing 1977)
5.07 (shake flask-GC, Felsot & Dahm 1979)
≤ 10 (Spencer 1982)
5.5 (19°C, shake flask-GC, Bowman & Sans 1983a, b)
10–15 (Worthing & Hance 1991)
5 (20–25°C, selected, Wauchope et al. 1992; Hornsby et al. 1996)
15 (calculated, Pait et al. 1992)
4.5 (27°C, Montgomery 1993; quoted, Tomlin 1994; Majewski & Capel 1995)
0.10 (Howe et al. 1994)

Vapor Pressure (Pa at 25°C or as indicated):
0.0346 (Worthing & Hance 1991; Tomlin 1994)
0.0427 (20–25°C, selected, Wauchope et al. 1992; Hornsby et al. 1996)
0.0351 (20°C, Montgomery 1993)
0.0174; 0.0346 (liquid P_L, GC-RT correlation; quoted lit., Donovan 1996)
0.0148; 0.00912, 0.0151 (gradient GC method; estimation using modified Watson method: Sugden's parachor, McGowan's parachor, Tsuzuki 2000)

Henry's Law Constant ($Pa{\cdot}m^3/mol$ at 25°C or as indicated):
2.229 (20–27°C, calculated-P/C, Montgomery 1993)
2.463 (calculated-P/C, this work)

Octanol/Water Partition Coefficient, log K_{OW}:
3.68 (shake flask-LSC, Felsot & Dahm 1979)
2.22 (Rao & Davidson 1980)

4.477	(shake flask-GC, Bowman & Sans 1983b)
4.52	(Worthing & Hance 1991; Tomlin 1994)
2.22–4.70	(Montgomery 1993)
4.48	(recommended, Sangster 1993)
3.54	(22°C, shake flask, Brecken-Folse et al. 1994)
0.832	(12°C in reconstituted test water at pH 7.5, Howe et al. 1994)
4.52	(Milne 1995)
4.48	(recommended, Hansch et al. 1995)
4.86	(RP-HPLC-RT correlation, Finizio et al. 1997)
4.51	(RP-HPLC-RT correlation using short ODP column, Donovan & Pescatore 2002)

Bioconcentration Factor, log BCF:

2.73	(topmouth gudgeon, Metcalf & Sanborn 1975)
2.18	(calculated-S, Kenaga 1980; quoted, Pait et al. 1992)
1.0	(*Triaenodes tardus*, Belluck & Felsot 1981)

Sorption Partition Coefficient, log K_{OC} at 25°C or as indicated:

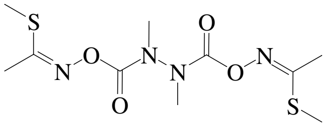
3.04	(soil, calculated-S per Kenaga & Goring 1978, Kenaga 1980)
2.76, 3.29	(quoted, calculated-MCI χ, Gerstl & Helling 1987)
2.70	(soil, 20–25°C, selected, Wauchope et al. 1992; Hornsby et al. 1996)
2.46–3.03	(Montgomery 1993)
2.82	(soil, calculated-MCI ${}^1\chi$, Sabljic et al. 1995)
2.80, 3.30	(soil, estimated-class-specific model, estimated-general model, Gramatica et al. 2000)

Environmental Fate Rate Constants, k, or Half-Lives, $t_{1/2}$:

Half-Lives in the Environment:

Soil: $t_{1/2}$ = 9–27 d in soil (Worthing & Hance 1991; quoted, Montgomery 1993; Tomlin 1994);
selected field $t_{1/2}$ = 5.0 d (Wauchope et al. 1992; quoted, Richards & Baker 1993; Hornsby et al. 1996);
soil $t_{1/2}$ = 5 d (Pait et al. 1992).

18.1.1.75 Thiodicarb



Common Name: Thiodicarb
Synonym: Bismethomyl thioether, Dicarbosulf
Chemical Name: dimethyl *N*,*N*′-(thiobis(methylimino)carbonyloxy)bis(ethanimidothioate)
CAS Registry No: 59669-26-0
Uses: insecticide/molluscicide
Molecular Formula: $C_{10}H_{18}N_4O_4S_3$
Molecular Weight: 354.470
Melting Point (°C):

168–172	(Hartley & Kidd 1987; Montgomery 1993; Tomlin 1994)
173–174	(Tomlin 1994)
173	(Lide 2003)

Boiling Point (°C):
Density (g/cm^3 at 20°C): 1.40 (Montgomery 1993)
Molar Volume (cm^3/mol):
Dissociation Constant, pK_a:
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
Entropy of Fusion, ΔS_{fus} (J/mol K):
Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F: 0.0353 (mp at 173°C)

Water Solubility (g/m^3 or mg/L at 25°C):

35	(Hartley & Kidd 1987; Montgomery 1993; Tomlin 1994)
19.1	(20–25°C, selected, Wauchope et al. 1992; Hornsby et al. 1996)

Vapor Pressure (Pa at 25°C):

0.0043	(20°C, Hartley & Kidd 1987; Montgomery 1993)
1.33×10^{-5}	(20–25°C, Wauchope et al. 1992; Hornsby et al. 1996)
0.0054	(20°C, Tomlin 1994)

Henry's Law Constant (Pa·m^3/mol):

0.044	(calculated-P/C, Montgomery 1993)

Octanol/Water Partition Coefficient, log K_{OW}:

1.70	(shake flask-HPLC, Drabel & Bachmann 1983)
1.2–1.6	(Montgomery 1993)
1.70	(recommended, Sangster 1993)
1.70	(recommended, Hansch et al. 1995)

Octanol/Air Partition Coefficient, log K_{OA}:

Bioconcentration Factor, log BCF or log K_B:

Sorption Partition Coefficient, log K_{OC}:

1.81–3.07; 2.54	(quoted range of reported data; mean, Wauchope et al. 1992)
2.54	(soil, selected, Wauchope et al. 1992; Hornsby et al. 1996)

3.06; 2.25; 2.10–2.69; 2.32–2.52; 2.57 (various soils: clay; loam; sand; sandy loam; silty loam (quoted, Montgomery 1993)
1.81–3.07 (various soils, Montgomery 1993)
2.54; 1.68, 2.57 (soil, quoted obs.; estimated-class-specific model, estimated-general model using molecular descriptors, Gramatica et al. 2000)

Environmental Fate Rate Constants, k, or Half-Lives, $t_{½}$:
Hydrolysis: $t_{½}$ ~ 9 d at pH 3 (Montgomery 1993);
stable at pH 6, rapidly hydrolyzed at pH 9 and slowly at pH 3, $t_{½}$ ~ 9 d (Tomlin 1994).

Half-Lives in the Environment:
Air:
Surface water: hydrolysis $t_{½}$ ~ 9 d at pH 3 (Montgomery 1993);
stable at pH 6, rapidly hydrolyzed at pH 9 and slowly at pH 3, $t_{½}$ ~ 9 d (Tomlin 1994).
Ground water:
Sediment:
Soil: $t_{½}$ = 3–8 d in various soils (Hartley & Kidd 1987)
field $t_{½}$ = 7 d (Wauchope et al. 1992; Hornsby et al. 1996).
Biota:

18.1.1.76 Toxaphene

Common Name: Toxaphene
Synonym: Agricide maggot killer, Alltex, Alltox, Camphochlor, Chem-Phene, chlorinated Camphene, Chloro-camphene, Coopertox, Crestoxo, Cristoxo, ENT 9735, Estonox, Fasco terpene, Geniphene, Gy-phene, Hercules 3956, Huilex, Kamfochlor, Melipax, Motox, NA 2761, NCI-C00259, Octachlorcamphene, Polychlorocamphene, Strobane-T, Texadust, Toxakil, Toxon 63
Chemical Name: mixtures of chlorinated camphene and bornane
Uses: pesticide used primarily on lettuce, cotton, corn, tomatoes, peanuts, wheat and soybean.
CAS Registry No: 8001-35-2
Molecular Formula: $C_{10}H_{16}Cl_8$
Molecular Weight: 413.812

Note: A large number of isomers exist, thus the commercial product is a mixture and the properties below should be regarded as average values for the specific mixture. Considerable variability in properties is thus expected.

Melting Point (°C):
65–90 (Howard 1991; Montgomery 1993; Milne 1995)
35 (dec., Milne 1995)

Boiling Point (°C):
246, 351, 360 (estimated from structure, Tucker et al. 1983)
Density (g/cm^3 at 20°C):
1.65 (25°C, Spencer 1982; Montgomery 1993)
Molar Volume (cm^3/mol):
358.8 (calculated-Le Bas method at normal boiling point)
366.8 (calculated-Le Bas method)
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
Entropy of Fusion, ΔS_{fus} (J/mol K):
Fugacity Ratio at 20°C (assuming ΔS_{fus} = 56 J/mol K), F:
0.30 (Mackay et al. 1986)

Water Solubility (g/m^3 or mg/L at 25°C or as indicated and the reported temperature dependence equations):
3.0 (Brooks 1974)
0.74 (generator column-GC/ECD, Weil et al. 1974)
0.40 (Leonard et al. 1976; Wauchope 1978)
0.40 (Sanborn et al. 1976; Weber et al. 1980)
0.40 (Martin & Worthing 1977)
0.50 (shake flask-GC, Paris et al. 1977)
3.0 (22°C, Khan 1980; Spencer 1982)
0.3–3.0 (U.S. EPA 1984; McLean et al 1988)
3.0 (Worthing & Walker 1987)
0.50 (20°C, selected, Suntio et al. 1988)
0.55 (20°C, Montgomery 1993)
0.63 (calculated from vapor pressure and HLC, Wania & Mackay 1993)
$\log [C/(mol/m^3)] = 0.77 - 1071/(T/K)$ (Wania & Mackay 1993)
3.0 (20–25°C, selected, Hornsby et al. 1996)

Vapor Pressure (Pa at 25°C or as indicated and reported temperature dependence equations):
4.0×10^{-5} (20°C, Spencer 1973)
27–53 (Brooks 1974; Khan 1980)
1.3×10^{-4} (Leonard et al. 1976)
1.3×10^{-4} (20–25°C, Weber et al. 1980)
1.3×10^{-4} (30°C, Seiber et al. 1981)
2.0×10^{-5}, 4.5×10^{-5}, 0.667 (estimated-bp, Tucker et al. 1983)

27.0 (U.S. EPA 1984; quoted, McLean et al. 1988)
8.92×10^{-4} (20°C, estimated, Murphy et al. 1987)
0.0005 (20°C, selected, Suntio et al. 1988)
27–54 (20°C, Montgomery 1993)
0.0016 (calculated from the eq. below, Wania & Mackay 1993)
$\log (P/Pa) = 12.25 - 4487/(T/K)$ (Wania & Mackay 1993)
5.3×10^{-4} (20–25°C, selected, Hornsby et al. 1996)
$(2.3–7.10) \times 10^{-4}$ (supercooled P_L, capillary GC-RT correlation, for 21 toxaphene components-chlorinated bornane and camphene congeners, Bidleman et al. 2003)

Henry's Law Constant (Pa·m^3/mol at 25°C or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):
490 (gas stripping-GC, Warner et al. 1980)
6380 (calculated-P/C, Kavanaugh & Trussel 1980)
45.59 (estimated-group method per Hine & Mookerjee 1975, Tucker et al. 1983)
0.0238 (calculated-P/C, Mackay et al. 1986)
496 (gas stripping-GC, Warner et al. 1987)
0.608 (20°C, estimated, Murphy et al. 1987; quoted, Howard 1991)
0.62 (20°C, average value for toxaphene complex mixture, Murphy et al. 1987)
520 (quoted from WERL Treatability Database, Ryan et al. 1988)
0.42 (20°C, calculated-P/C, Suntio et al. 1988)
3097 (calculated-P/C, Jury et al. 1990)
0.067 (0°C, selected, Cotham & Bidleman 1991)
6382 (Montgomery 1993)
1.054 (calculated-temp dependence eq., Wania & Mackay 1993)
$\log [H/(Pa \cdot m^3/mol)] = 11.48 - 3416/(T/K)$ (Wania & Mackay 1993)
0.36* (technical toxaphene, gas stripping-GC, measured range 10–40°C, Jantunen & Bidleman 2000)
$\log [H/(Pa\ m3/mol)] = 10.42 - 3209/(T/K)$; temp range 10–40°C (technical toxaphene, gas stripping-GC, Jantunen & Bidleman 2000)

Octanol/Water Partition Coefficient, log K_{OW}:
3.52 (shake flask-GC, Paris et al. 1977)
5.30 (HPLC-RT correlation, Veith et al. 1979)
3.23 (Rao & Davidson 1980)
5.28 (Veith & Kosian 1983)
4.83 (from Veith's personal communication, Zaroogian et al. 1985)
5.50 (Garten & Trabalka 1983)
3.85 (Ryan et al. 1988)
5.50 (Isnard & Lambert 1988, 1989; Travis & Arms 1988; Wania & Mackay 1993)
4.63 (estimated-QSAR & SPARC, Kollig 1993)
3.23–5.50 (Montgomery 1993)
4.77–6.64 (range for 36 toxaphene components/congeners, shake flask/slow stirring-GC/ECD, Fisk et al. 1999)

Bioconcentration Factor, log BCF:
–2.79 (beef biotransfer factor log B_b, correlated-K_{OW}, Radeleff et al. 1952; Claborn et al. 1953,60)
–3.20 (milk biotransfer factor log B_m, correlated-K_{OW}, Saha 1969)
3.53 (*Bacillus subtilis*, Paris et al. 1975, 1977)
3.72 (*Flavobacterium harrisonii*, Paris et al. 1975, 1977)
4.23 (*Aspergillus sp.*, Paris et al. 1975, 1977)
4.04 (*Chlorella prenoidosa*, Paris et al. 1975, 1977)
3.63 (*Gambusia*, Sanborn et al. 1976)
4.84 (fathead minnows, Mayer et al. 1977)
3.51–4.23 (microorganisms, Paris et al. 1977)
3.59 (pinfish, 4-d exposure, Schimmel et al. 1977; Veith & Kosian 1983)
3.64 (sheepshead minnow, 4-d exposure, Schimmel et al. 1977)

3.49–4.52, 2.60–3.08 (fish, shrimp, Reish et al. 1978)
4.42, 3.63 (fish: flowing water, static water; Kenaga & Goring 1980)
4.42, 3.02 (fish, calculated-solubility, Kenaga 1980)
3.59 (pinfish, Veith & Kosian 1983)
3.64 (sheepshead minnow, Veith & Kosian 1983)
3.81, 3.72 (fish: flowing system, microcosm, Garten & Trabalka 1983)
3.84, 3.98 (algae: snail, Garten & Trabalka 1983)
3.44, 3.41 (oyster, calculated-K_{OW} and models, Zaroogian et al. 1985)
3.44, 3.41 (pinfish, calculated-K_{OW} and models, Zaroogian et al. 1985)
3.44, 3.41 (sheepshead minnow, calculated-K_{OW} & models, Zaroogian et al. 1985)
4.52, 6.44 (oyster, flow-through 6 months: wet wt basis, lipid wt basis, Geyer et al. 2000)
4.57, 6.50 (oyster, flow-through 6 months: wet wt basis, lipid wt basis, Geyer et al. 2000)
4.84, 6.06 (fathead minnow, flow-through 96-d: wet wt basis, lipid wt basis, Geyer et al. 2000)
4.80, 5.80 (fathead minnow, flow-through 150-d: wet wt basis, lipid wt basis, Geyer et al. 2000)
>4.73, >5.84 (channel catfish, flow-through 100-d: wet wt basis, lipid wt basis, Geyer et al. 2000)
3.04, 3.204 (human, fat: wet wt basis, lipid wt basis, Geyer et al. 2000)

Sorption Partition Coefficient, log K_{OC}:
3.86 (calculated-S, Kenaga 1980; quoted, Howard 1991)
4.99 (soil, McDowell et al. 1981; quoted, Nash 1988)
4.32 (soil, screening model calculations, Jury et al. 1987a, b, 1990; Jury & Ghodrati 1989)
5.32 (sediment, Bomberger et al. 1983; quoted, Howard 1991)
3.17 (calculated-K_{OW} as per Kenaga & Goring 1980, Chapman 1989)
4.31 (estimated-QSAR and SPARC, Kollig 1993)
3.18 (calculated, Montgomery 1993)
5.00 (20–25°C, selected, Hornsby et al. 1996)

Environmental Fate Rate Constants, k, or Half-Lives, $t_{1/2}$:

Volatilization: volatilization $t_{1/2}$ = 2650 d from chemical below soil surface (Jury et al. 1990).

Photolysis:

Hydrolysis: estimated $t_{1/2} > 10$ yr at pH 5–8 and 25°C (Callahan et al. 1979; quoted, Howard 1991)
$k = (8.0 \pm 2.2) \times 10^{-6}\ h^{-1}$ at pH 7 with a calculated $t_{1/2}$ = 10 yr (Ellington et al. 1987, 1988)
$k = 7.0 \times 10^{-2}\ yr^{-1}$ at pH 7.0 and 25°C (Kollig 1993).

Oxidation: rate constant k, for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO3} with NO_3 radical and k_{O3} with O_3 or as indicated, *data at other temperatures see reference:
$t_{1/2}$ = 4–5 d for the vapor-phase reaction with hydroxyl radicals (Howard 1991)
k(aq.) = $8 \times 10^8\ M^{-1}\ s^{-1}$ for the reaction (Fenton with reference to lindane) with hydroxyl radical in aqueous solutions at pH 1.9 ± 0.1 and at 24 ± 1°C (Buxton et al. 1988; quoted, Faust & Hoigné 1990; Haag & Yao 1992)
k(aq.) < $1.3\ M^{-1}\ s^{-1}$ for direct reaction with ozone in water at pH 5.6 and 21°C, with $t_{1/2} > 7$ h at pH 7 (Yao & Haag 1991).
k(aq.) = $(1.2–8.1) \times 10^8\ M^{-1}\ s^{-1}$ for the reaction (Fenton with reference to lindane) with hydroxyl radical in aqueous solutions at pH 1.9 ± 0.1 and at 24 ± 1°C (Haag & Yao 1992)

Biodegradation: very resistant to degradation in soils with reported from $t_{1/2}$ = 0.8 yr (Adams 1967; quoted, Howard 1991) to 14 yr (Nash & Woolson 1967; quoted, Howard 1991).

Biotransformation:

Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants:
$k_2 = 0.016\ d^{-1}$ with $t_{1/2}$ = 43 d and $k_2 = 0.022\ d^{-1}$ with $t_{1/2}$ = 32 d for food concn of 21 ng/g and 136 ng/g, respectively, in a 30-d uptake followed by 160-d depuration studies for a C_7-CHB toxaphene congener (juvenile rainbow trout, Fisk et al. 1998)
$k_2 = 0.007\ d^{-1}$ with $t_{1/2}$ = 95 d and $k_2 = 0.016\ d^{-1}$ with $t_{1/2}$ = 43 d for food concn of 18 ng/g and 121 ng/g, respectively, in a 30-d uptake followed by 160-d depuration studies for a C_8-CHB toxaphene congener (juvenile rainbow trout, Fisk et al. 1998)

k_2 = 0.008 d^{-1} with $t_{½}$ = 83 d and k_2 = 0.017 d^{-1} with $t_{½}$ = 42 d for food concn of 17 ng/g and 134 ng/g, respectively, in a 30-d uptake followed by 160-d depuration studies for C_9-CHB toxaphene congener (juvenile rainbow trout, Fisk et al. 1998)
k_2 = 0.068 yr^{-1}, 0.093 yr^{-1}, 0.160 yr^{-1} in Lake Michigan, Lake Huron and Lake Ontario, respectively, in lake trout (lipid-adjusted, Glassmeyer et al. 2000)
k_2 = 0.085 yr^{-1}, 0.086 yr^{-1}, 0.165 yr^{-1} in Lake Michigan, Lake Huron and Lake Ontario, respectively, in lake trout (wet weight, Glassmeyer et al. 2000)

Half-Lives in the Environment:

Air: $t_{½}$ = 4–5 d for the vapor-phase reaction with hydroxyl radicals (GEMS 1986; quoted, Howard 1991).
Surface water: measured k < 1.3 M^{-1} s^{-1} for direct reaction with ozone in water at pH 2 and 21°C, with $t_{½}$ > 7 h at pH 7 (Yao & Haag 1991);
half-lives in lake water: $t_{½}$ = 18–31 yr in Lake Superior, $t_{½}$ = 5–8 yr in Lake Michigan, $t_{½}$ ~ 8.5 yr in Lake Huron and $t_{½}$ ~ 6 yr in Lake Ontario (Glassmeyer et al. 2000).
Ground water:
Sediment:
Soil: very persistent with reported half-life from $t_{½}$ = 0.8 yr (Adams 1967; quoted, Howard 1991) to 14 yr (Nash & Woolson 1967; quoted, Howard 1991);
$t_{½}$ > 50 d when subject to plant uptake via volatilization (Callahan et al. 1979; quoted, Ryan et al. 1988)
measured dissipation rate k = 0.010 d^{-1} (Seiber et al. 1979; quoted, Nash 1988);
$t_{½}$ = 9 d in screening model calculations (Jury et al 1987b);
estimated dissipation rate k = 0.0011 and 0.013 d^{-1} (Nash 1988);
$t_{½}$ = 3650 d for volatilization to atmosphere from chemical below soil surface (Jury et al. 1990);
field $t_{½}$ = 9 d (20–25°C, selected, Hornsby et al. 1996)
$t_{½}$ = 0.8–14 yr in soil, $t_{½}$ = 10–18 yr in the environment (Geyer et al. 2000)
Biota: field $t_{½}$ = 15.6 d in fruit tree leaves (Decker et al. 1950; quoted, Nash 1983);
microagroecosystem $t_{½}$ = 19 d in cotton leaves (Nash & Harris 1977; quoted, Nash 1983);
field $t_{½}$ ca. 6.3 d in cotton canopy (Willis et al. 1980; quoted, Nash 1983);
$t_{½}$ = 524 d for white suckers, and $t_{½}$ = 232 to 322 d for lake trout (total toxaphene, Delorme et al. 1993);
average fish half-lives in the Great Lakes. $t_{½}$ = 9.1 yr in Lake Michigan, $t_{½}$ = 7.7 yr in Lake Huron and $t_{½}$ = 4.3 yr in Lake Ontario (lake trout, Glassmeyer et al. 2000)
Depuration $t_{½}$ = 32–96 d for a 30-d uptake and 160-d depuration studies (Juvenile rainbow trout, Fisk et al. 1998)

TABLE 18.1.1.76.1
Reported Henry's law constants of toxaphene at various temperatures

Jantunen et al. 2000	
air stripping-GC	
t/°C	H/(Pa m^3/mol)
10	0.10
20	0.36
30	0.69
35	0.86
40	1.50

log H = A – B/(T/K)

	H/(Pa m^3/mol)
A	10.42 ± 0.54
B	3209 ± 162

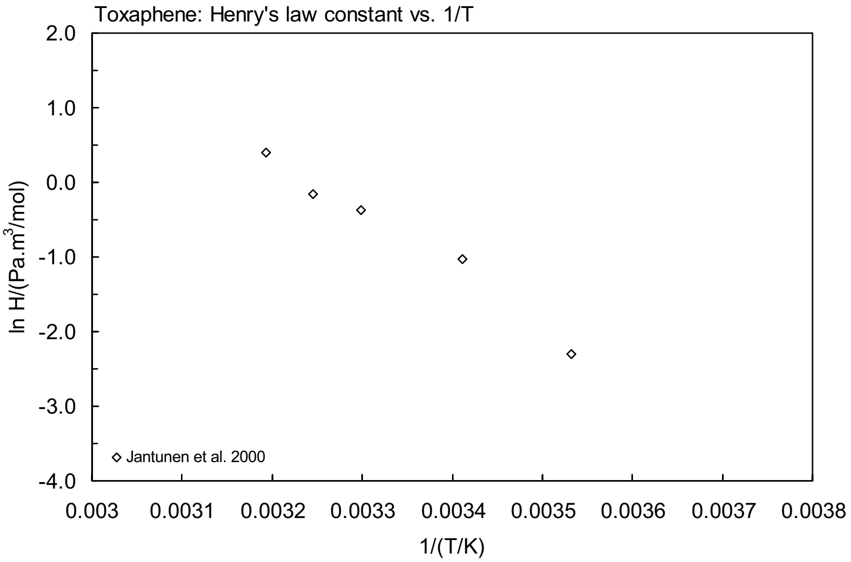
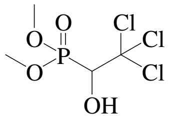


FIGURE 18.1.1.76.1 Logarithm of Henry's law constant versus reciprocal temperature for toxaphene.

18.1.1.77 Trichlorfon



Common Name: Trichlorfon

Synonym: Aerol 1, Agroforotox, Anthion, Bay 15922, Bayer 15922, Bilarcil, Bovinox, Britten, Britton, Cekufon, Chlorak, Chlorfos, Chlorphos, Chloroftalm, Chloroxyphos, Ciclosom, Combat, Combot, Danex, DEP, Depthon, DETF, Dimetox, Dipterax, Diptevur, Ditrifon, Dylox, Dyrex, Dyvon, ENT 19763, Equino-acid, Flibol E, Forotox, Foschlor, Hypodermacid, Leivasom, Loisol, Masoten, Mazoten, Methyl chlorophos, Metifonate, Metrifonate, Metriphonate, NA 2783, NCI-C54831, Neguvon, Phoschlor, Proxol, Ricifon, Ritsifon, Soldep, Sotipox, Trichlorphon, Trichlorphene, Trinex, Tugon, Volfartol, Votexit, Wotexit

Chemical Name: dimethyl 2,2,2-trichloro-hydroxyethylphosphorate; 2,2,2-trichloro-hydroxy-ethylphosphoric acid dimethyl ester

Uses: insecticide to control flies and roaches.

CAS Registry No: 52-68-6

Molecular Formula: $C_4H_8Cl_3O_4P$

Molecular Weight: 257.437

Melting Point (°C):

77	(Lide 2003)

Boiling Point (°C):

100	(at 0.1 mmHg, Spencer 1973; Montgomery 1993; Milne 1995)

Density (g/cm^3 at 20°C):

1.73	(Spencer 1982; Worthing & Hance 1991; Montgomery 1993; Tomlin 1994; Milne 1995)

Molar Volume (cm^3/mol):

194.9	(calculated-Le Bas method at normal boiling point)

Dissociation Constant, pK_a:

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

Entropy of Fusion, ΔS_{fus} (J/mol K):

Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F: 0.309 (mp at 77°C)

Water Solubility (g/m^3 or mg/L at 25°C or as indicated):

154000	(Spencer 1973, 1982; Martin & Worthing 1977; Worthing 1979)
> 5000	(20°C, shake flask-GC, Bowman & Sans 1983a)
150000	(Davies & Lee 1987)
120000	(20°C, Worthing & Hance 1991; Tomlin 1994)
120000	(20–25°C, selected, Wauchope et al. 1992; Hornsby et al. 1996)
154000	(Montgomery 1993; Milne 1995)
90000	(Brecken-Folse et al. 1994)
9000	(Howe et al. 1994)

Vapor Pressure (Pa at 25°C or as indicated):

0.00095	(20°C, vapor density, MacDougall 1964)
0.00104	(20°C, Eichler 1965; Melnikov 1971; Spencer 1973; Hartley & Graham-Bryce 1980)
0.0640	(20°C, GC-RT correlation without mp correction, Kim et al. 1984; Kim 1985)
0.0187	(20°C, GC-RT correlation with mp correction, Kim et al. 1984; Kim 1985)
0.00021	(20°C, Worthing & Hance 1991; Tomlin 1994)
0.00027	(20–25°C, selected, Wauchope et al. 1992; Hornsby et al. 1996)
0.00104	(20°C, Montgomery 1993)
0.00051	(Tomlin 1994)

Henry's Law Constant (Pa·m^3/mol at 25°C or as indicated):

1.7×10^{-6}	(20°C, calculated-P/C, Suntio et al. 1988)
1.7×10^{-6}	(calculated-P/C, Montgomery 1993)

Octanol/Water Partition Coefficient, log K_{OW}:

0.48	(Dow Chemical data, Kenaga & Goring 1980)

0.431 (shake flask-GC, Bowman & Sans 1983b)
0.76 (HPLC-RT correlation, Kawamoto & Urano 1989)
0.43–0.76 (Montgomery 1993)
0.51, 0.72 (shake flask, RP-HPLC-RT correlation, Sicbaldi & Finizio 1993)
1.70 (22°C, shake flask, Brecken-Folse et al. 1994)
0.304 (12°C in reconstituted test water at pH 7.5, Howe et al. 1994)
0.51 (recommended, Sangster 1993)
0.43 (Tomlin 1994)
0.51 (recommended, Hansch et al. 1995)
0.72 (RP-HPLC-RT correlation, Finizio et al. 1997)

Bioconcentration Factor, log BCF:
–0.155 (calculated-S, Kenaga 1980)

Sorption Partition Coefficient, log K_{OC}:
0.778 (calculated-S as per Kenaga & Goring 1978, Kenaga 1980)
1.90 (correlated, Kawamoto & Urano 1989)
1.73 (soil, calculated-MCI χ and fragments contribution, Meylan et al. 1992)
1.00 (soil, 20–25°C, selected, Wauchope et al. 1992; quoted, Dowd et al. 1993; Lohninger 1994; Hornsby et al. 1996)
0.99–1.58 (Montgomery 1993)
1.90 (soil, calculated-MCI $^1\chi$, Sabljic et al. 1995)
1.30 (sediment, estimated, Paraiba et al. 1999)
1.90; 1.87, 2.25 (soil, quoted obs.; estimated-class-specific model, estimated-general model using molecular descriptors, Gramatica et al. 2000)

Environmental Fate Rate Constants, k, or Half-Lives, $t_{1/2}$:

Volatilization:

Photolysis:

Oxidation: photooxidation $t_{1/2}$ = 1–101 h, based on an estimated rate constant for the vapor-phase reaction with hydroxyl radicals in air (Atkinson 1987; quoted, Howard et al. 1991).

Hydrolysis: first-order hydrolysis $t_{1/2}$ = 68 h, based on first-order rate constant at pH 7 and 25°C (Chapman & Cole 1982; quoted, Howard et al. 1991);
$t_{1/2}$ = 510 d at 22°C and at pH 4, $t_{1/2}$ = 46 h at pH 7, and $t_{1/2}$ < 30 min at pH 9 (Tomlin 1994).

Biodegradation: k(aerobic) = 0.28 d^{-1} with $t_{1/2}$ = 2.5 d at 20°C by aerobic activated sludge cultivated by an artificial sewage (batch contacting method, Kawamoto & Urano 1990)
aqueous aerobic $t_{1/2}$ = 24–1080 h, based on unacclimated soil grab sample data (Guirguis & Shafik 1975; Kostovetskii et al. 1976; quoted, Howard et al. 1991);
aqueous anaerobic $t_{1/2}$ = 96–4320 h, based on unacclimated aerobic biodegradation half-life (Howard et al. 1991).

Biotransformation:

Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants:

Half-Lives in the Environment:

Air: photooxidation $t_{1/2}$ = 1–101 h, based on an estimated rate constant for the vapor-phase reaction with hydroxyl radicals in air (Atkinson 1987; quoted, Howard et al. 1991);
reaction rate k = 1.90×10^{-4} min^{-1} in air (Paraiba et al. 1999).

Surface water: $t_{1/2}$ = 22–588 h, based on aqueous hydrolysis half-lives at pH 6 and 8 and 25°C (Chapman & Cole 1982; quoted, Howard et al. 1991);
$t_{1/2}$ = 2.5 d at 20°C by aerobic activated sludge (Kawamoto & Urano 1990)
reaction rate k = 1.90×10^{-4} min^{-1} in water (Paraiba et al. 1999).

Ground water: $t_{1/2}$ = 22–588 h, based on aqueous hydrolysis half-lives at pH 6 and 8 and 25°C (Chapman & Cole 1982; quoted, Howard et al. 1991).

Sediment: reaction rate k = 1.90×10^{-5} min^{-1} in sediment (Paraiba et al. 1999).

Soil: $t_{1/2}$ = 24–1080 h, based on unacclimated soil grab sample data (Guirguis & Shafik 1975; Kostovetskii et al. 1976; quoted, Howard et al. 1991);
selected field $t_{1/2}$ = 10 d (Wauchope et al. 1992; Dowd et al. 1993; Hornsby et al. 1996).

Biota:

18.2 SUMMARY TABLES

TABLE 18.2.1
Common names, chemical names and physical properties of insecticides

Name	Synonym	Chemical name	Molecular formula	Molecular weight, MW g/mol	m.p. °C	Fugacity ratio, F at 25°C	pK$_a$
Acephate [30560-19-1]	Orthene	*O,S*-dimethyl acetylphosphoramidothioate	$C_4H_{10}NO_3PS$	183.166	88	0.241	
Aldicarb [116-06-3]	Temik	2-methyl-2-(methylthio)-propionaldehyde *O*-(methylcarbamoyl) oxime	$C_7H_{14}N_2O_2S$	190.263	99	0.188	
Aldrin [309-00-2]	Aldrec, Aldrex, Aldrite, Octalene	1,2,3,4,10,10-hexachloro-1,4,4a,5,8,8a-hexahydro-1,4-endoexo-5,8-dimethano-naphthalene	$C_{12}H_8Cl_6$	364.910	104	0.168	
Aminocarb [2032-59-9]	Matacil	4-dimethylamino-*m*-tolyl methylcarbamate	$C_{11}H_{16}N_2O_2$	208.257	94	0.210	
Azinphos-methyl [86-50-0]	Guthion	*O,O*-dimethyl-*S*-[4-oxo-1,2,3-benzotriazin-3(4*H*)-yl)methyl]phosphorodithioate	$C_{10}H_{12}N_3O_3PS_2$	317.324	73	0.338	
Bendiocarb [22781-23-3]	Bencarbate, Dycarb, Garvox, Multamat	2,2-dimethyl-1,3-benzodioxol-4-yl-methylcarbamate	$C_{11}H_{13}NO_4$	223.226	130	0.0933	8.8
Bromophos [2104–96–3]	Nexion, S-1942, Omexan, Brofene	*O*-4-bromo-2,5-dichlorophenyl-*O,O*-dimethyl phosphorothioate	$C_8H_8BrCl_2PS$	317.999	54	0.519	
Bromophos-ethyl [4824–78–6]	Nexagen, Filariol	*O*-(4-bromo-2,5-dichlorophenyl) *O,O*-diethyl phosphorothioate	$C_{10}H_{12}Cl_2O_3PS$	394.049			
Carbaryl [63-25-2]	Sevin	1-naphthyl-*N*-methyl carbamate	$C_{12}H_{11}NO_2$	201.221	145	0.0665	
Carbofuran [1563-66-2]	Furadan, Yaltox	2,3-dihydro-2,2-dimethylbenzofuran-7-yl methylcarbamate	$C_{12}H_{15}NO_3$	221.252	151	0.0580	
Carbophenothion [786–19–6]	Carbofenotion, Acarithion, Akarithion	*S*-chlorophenylthio methyl *O,O*-diethyl phosphorothioate	$C_{11}H_{16}ClO_2PS_3$	342.866	liquid	1	
Carbosulfan [55285–14–8]	Marshal, Adventage Posse, FMC 35001	2,3-dihydro-2,2-dimethylbenzofuran-7-yl(dibutylaminothio) methylcarbamate	$C_{20}H_{32}N_2O_3S$	380.544	liquid	1	
Chlordane [57-74-9]	Aspon-chlordane, Chlorindan, Octachlor	1,2,4,5,7,8,8-octachloro-3*a*,4,7,7*a*-tetrahydro-4,7-methanoindane	$C_{10}H_6Cl_8$	409.779	106	0.160	
cis- or α-chlordane [5103–71–9]			$C_{10}H_6Cl_8$	409.799	107–109	0.153	
trans- or β-chlordane [5103–74–2]			$C_{10}H_6Cl_8$	409.799	103–105	0.168	
γ-chlordane [5564–34–7]			$C_{10}H_6Cl_8$	409.799	131	0.0912	
technical grade′[12789–03–6]							
Chlorfenvinphos [470-90-6]	Birlane, Sapecron	2-chloro-1-(2,4-dichlorophenyl) vinyl diethyl phosphate	$C_{12}H_{14}Cl_3O_4P$	359.569	B19	1	
Chlorpyrifos [2921-88-2]	Brodan, Dursban, Dowco 179	*O,O*-diethyl *O*-3,5,6-trichloro 2-pyridyl phosphorothioate	$C_9H_{11}Cl_3NO_3PS$	350.586	42	0.681	
Chlorpyrifos-methyl [5598–13–0]	Reldan, Dowco 214	*O,O*-dimethyl *O*-3,5,6-trichloro-2-pyridyl phosphorothioate	$C_7H_7Cl_3NO_3PS$	322.534	43	0.666	

Crotoxyphos [7700-17-6]	Ciodrin	dimethyl(*E*)-1-methyl-2-(1-phenyl-ethoxycarbonyl)vinyl phosphate	$C_{14}H_{19}O_6P$	314.271	liquid	1
Cyhalothrin [68085–85–8]	Cyhalothrin	(*RS*)-α-cyano-3-phenoxybenzyl(*Z*)-(1*RS*,3*RS*)- (2-chloro-3,3,3-trifluoropropanyl)-2,2-dimethylcyclopropanecarboxylate	$C_{23}H_{19}ClF_3NO_3$	449.850		
lamba-Cyhalothrin [91465–08–6]			$C_{23}H_{19}ClF_3NO_3$	449.850	49.2	0.579
Cypermethrin [52315-07-8]	Polytrin, Ambush C, Kakfil Super, BSI, draft E-ISO	(*RS*)-α-cyano-3-phenoxybenzyl (1*RS*,3*RS*; 1*RS*,3*RS*)-3-(2,2-dichlorovinyl)-2,2-=dimethylcyclopropanecarboxylate	$C_{22}H_{19}Cl_2NO_3$	416.297	70	0.362
α-cypermethrin [67375-30-8]			$C_{22}H_{19}Cl_2NO_3$	416.297	78-81	0.292
β-cypermethrin [65731–84–2]			$C_{22}H_{19}Cl_2NO_3$	416.297	64–71	
ζ-cypermethrin [52315–07–8]			$C_{22}H_{19}Cl_2NO_3$	416.297	–22.4	1
DDD						
p,p'-DDD [72-54-8]	*p,p*'-TDE	1,1-Dichloro-2,2-bis (4-chlorophenyl)ethane	$C_{14}H_{10}Cl_4$	320.041	109.5	0.148
o,p'-DDD [53-10-0]		1,1-dichloro-(2-chlorophenyl)-2-(4-chlorophenyl)ethane	$C_{14}H_{10}Cl_4$	320.041	112	0.140
DDE						
p,p'-DDE [72-55-9]	*p,p*'-DDE	1,1-dichloro-2,2-bis-(p-chlorophenyl)-ethylene	$C_{14}H_8Cl_4$	318.026	89	0.236
o,p'-DDE [3424-82-6]	*o,p*'-DDE	1,1-Dichloro-2(2-chlorophenyl)-2-(4-chlorophenyl)ethylene	$C_{14}H_8Cl_4$	318.026	88-90	0.236
DDT	Agritan		$C_{14}H_9Cl_5$	354.486	108.5	0.152
p,p'-DDT [50-29-3]		1,1,1-trichloro-2,2-bis-(4-chlorophenyl)-ethane				
o,p'-DDT [789-02-6]		1,1,1-trichloro-2-(chlorophenyl)-2-(4-chlorophenyl)-ethane	$C_{14}H_9Cl_5$	354.486		
Deltamethrin [62918-63-5]	Decis, K-Othrine Butox, Butoflin	(*S*)-α-cyano-3-phenoxybenyl(1*R*,3*R*)-3-(2,2-dibromvinyl)-2,2-dimethycyclo-propanecarboxylate	$C_{22}H_{19}Br_2NO_3$	505.199	98-101	0.186
Demeton [8065-48-3]	Systox	*O,O*-diethyl *O*-2-ethylthioethyl phosphorothioate	$C_8H_{19}O_3PS_2$	258.339	liquid	1
Demeton-S-methyl [919-86-8]	Metasystoxi	*S*-2-ethylthioethyl *O,O*-dimethyl phosphorothioate	$C_6H_{15}O_3PS_2$	230.285	liquid	1
Dialifor [10311-84-9]	Torak	*S*-2-chloro-1-phthalimidoethyl *O,O*-diethylphosphorodithioate	$C_{14}H_{17}ClNO_4PS_2$	393.846	68	0.379
Diamidaphos [1754-58-1]	Nellite	phenyl *N,N*'-dimethylphosphoro-diamidate	$C_8H_{13}N_2O_2P$	200.175	103.5	0.170
Diazinon [333-41-5]	Basudin, Diazide, Spectracide	*O,O*-diethyl *O*-2-isopropyl-6-methyl-pyrimidin-4-yl phosphorothioate	$C_{12}H_{21}N_2O_3PS$	304.345	liquid	1
Dicapthon [2463-84-5]	Dicaptan	*O*-(2-chloro-4-nitrophenyl)-*O,O*-dimethyl phosphorothioate	$C_8H_9ClNO_5PS$	297.653	53	0.531
Dichlofenthion [97-17-6]	Mobilawn	*O*-2,4-dichlorophenyl *O,O*-=diethyl phosphorothioate	$C_{10}H_{13}Cl_2O_3PS$	315.153	liquid	1

(*Continued*)

TABLE 18.2.1 (*Continued*)

Name	Synonym	Chemical name	Molecular formula	Molecular weight, MW g/mol	m.p. °C	Fugacity ratio, F at 25°C	pK_a
Dichlorvos [62-73-7]	Vapona, Nuvan, DDVP, Dedevap	2,2-dichlorovinyl-*O,O*-dimethyl phosphate	$C_4H_7Cl_2O_4P$	220.976	liquid	1	
Dicrotophos [141-66-2]	Carbicron, Ektafos, Bidrin	(*E*)-2-dimethylcarbamoyl-1-methylvinyl dimethyl phosphate	$C_8H_{16}NO_5P$	237.191	liquid	1	
Dieldrin [60-57-1]	HEOD	1,2,3,4,10,10-hexachloro-6,7-epoxy-1,4,4a,5,6,7,8,8a-octahydro-*exo*-1,4-*endo*-5,8-dimethanonaphthalene	$C_{12}H_8Cl_6O$	380.909	175.5	0.0334	
Diflubenzuron [35367-38-5]	Deflubenzon, Dimilin	1-(4-chlorophenyl)-3-(2,6-difluoro-benzol) urea	$C_{14}H_9ClF_2N_2O_2$	310.683	239	0.00795	
Dimethoate [60-51-5]	Cygon	*O,O*-dimethyl-*S*-(*N*-methyl-carbamoyl-methyl phosphorodithioate	$C_5H_{12}NO_3PS_2$	229.258	52	0.543	
Dinoseb [88-85-7]	Antox, Aretit, BNP 30, DNBP	2-*sec*-butyl-4,6-dinitrophenol	$C_{10}H_{12}N_2O_5$	240.212	40	0.713	
Disulfoton [298-04-4]	Di-Syston, Dithiosystox	*O,O*-diethyl-*S*-(ethylthio)-ethyl phosphorodithioate	$C_8H_{19}O_2PS_3$	274.405	–25	1	
Endosulfan [115-29-7]	Thiodan, Cyclodan, Malix, Thifor	5-norbornene-2,3-dimethanol-1,4,5,6,7,7-hexachlorocyclic sulfite	$C_9H_6Cl_6O_3S$	406.925	106	0.160	
α-Endosulfan′[959–98–8]			$C_9H_6Cl_6O_3S$	406.925	106	0.160	
β-Endosulfan [33213–65–9]			$C_9H_6Cl_6O_3S$	406.925	207-209	0.0160	
Endosulfan sulfate [1031–07–8]			$C_9H_6Cl_6O_4S$	422.925	181	0.0295	
Endrin [72-20-8]	endrine, nendrin	1,2,3,4,10,10-hexachloro-6,7-epoxy-1,4,4a,5,6,7,8,8a-octahydro-=*exo*-1,4-*exo*-5,8-dimethanonaphthalene	$C_{12}H_8Cl_6O$	380.909	dec 245	0.00694	
Ethiofencarb [29973–13–5]	Croneton, Bay-Hox-1901	α-ethylthio-*o*-tolyl methylcarbamate	$C_{11}H_{15}NO_2S$	225.307	33.4	0.827	
Ethion [563-12-2]	Nialate, diethion	*O,O,O',O'*-tetraethyl-*S,S'*-methylene bis(phosphorodithioate)	$C_9H_{22}O_4P_2S_4$	384.476	–13	1	
Ethoprophos [13194-48-4]	Mocap, ethoprop	*O*-ethyl-*S,S*-dipropyl-phosphorodithioate	$C_8H_{19}O_2PS_2$	242.340	liquid	1	
Fenitrothion [122-14-5]	Sumithion, Folithion Cyfen	*O,O*-dimethyl *O*-4-nitro-*m*-tolyl phosphorothioate	$C_9H_{12}NO_5PS$	277.234	liquid	1	
Fenoxycarb [79127-80-3]	Logic, Pictyl, Varodo	ethyl 2-(4-phenoxyphenoxy)ethyl-carbamate	$C_{17}H_{19}NO_4$	301.338	53	0.531	
Fenpropathrin [64257–84–7]	Rody, Danitol, Meothrin, S-3206	(R,S)-α-cyano-3-phenoxybenzyl 2,2,3,3-tetramethylcyclopropanecarboxylate	$C_{22}H_{23}NO_3$	349.423	47	0.608	
Fensulfothion [115–90–2]	Dassnit, Terracur	*O,O*-diethyl *O*-4-methylsulphinylphenyl phosphorothioate	$C_{11}H_{17}O_4PS_2$	308.354			

Fenthion [55-38-9]	Baytex, Baycid, Mercaptophos,	*O,O*-dimethyl-*O*-(3-methyl-4-(methylthio)phenyl) phosphorothioate	$C_{10}H_{15}O_3PS_2$	278.328	liquid	1
Fenvalerate [51630-58-1]	Sumicidin, Belmark, Pydrin	(*RS*)-α-cyano-3-phenoxybenzyl (*RS*)-2-(4-chlorophenyl)-3-methylbutyrate	$C_{25}H_{22}ClNO_2$	419.901	liquid	1
Flucythrinate [70124-77-5]	Cybolt, Cythrin, Pay-Off	(*RS*)-α-cyano-3-phenoxybenzyl (*S*)-2-(4-difluoromethoxyphenyl)-3-methylbutyrate	$C_{26}H_{23}F_2NO_4$	451.463	liquid	1
Fonofos [944-22-9]	Dyfonate, Fonophos	*O*-ethyl-*S*-phenyl (*RS*)-ethyl-phosphorodithioate	$C_{10}H_{15}OPS_2$	246.329	liquid	1
Heptachlor [76-44-8]	Methanoindene	1,4,5,6,7,8,8-heptachloro-3a-4,7-7a-tetrahydro-4,7-*endo*-methanoindene	$C_{10}H_5Cl_7$	373.318	95.5	0.203
Heptachlor epoxide [1024–57–3]		1,4,5,6,7,8-heptachloro-2,3-epoxy-2,3,3a-4,7,7a-tetrahydro-4,7-methanoindene	$C_{10}H_5Cl_7O$	389.317	160	0.0474
Hexachlorocyclohexane	BHC, HCH	1,2,3,4,5,6-Hexachlorocyclohexane	$C_6H_6Cl_6$	290.830		
α-HCH′[319–84–6]	α-BHC	1,2,3,4,5,6-Hexachlorocyclohexane		290.830	158	0.0496
β-HCH′[319–85–7]	β-BHC	1,2,3,4,5,6-Hexachlorocyclohexane		290.830	309	0.00164
γ-HCH (Lindane)	Gammexane	1,2,3,4,5,6-hexachlorocyclohexane	$C_6H_6Cl_6$	290.830	112.5	0.139
δ-HCH′[319–86–8]	Δ-BHC	1,2,3,4,5,6-hexachlorocyclohexane	$C_6H_6Cl_6$	290.830	141.5	0.0719
Iodofenphos [25311–71–1]	Nuvanol N	*O*-2,5-dichloro-4-iodophenyl *O,O*-dimethyl phosphorothioate	$C_8H_8Cl_2IO_3PS$	345.395	oil	1
Isophorone [78–59–1]	Isooctaphenone	3,5,5-trimethyl-2-cyclohexene-1-one	$C_9H_{14}O$	138.206	–8.1	1
Kepone [143-50-0]	Chlordecone	decachlorooctahydro-1,3,4-metheno-2*H*-cyclobuta [*cd*]pentalen-2-one	$C_{10}H_{10}O$	490.636	350 dec	0.00065
Leptophos [21609-90-5]	Phosvel	*O*-(4-bromo-2,5-dichlorophenyl) *O*-methyl phenylphosphorothioate	$C_{13}H_{10}BrCl_2O_2PS$	412.066	71	0.345
Lindane [58-89-9]	γ-BHC, γ-HCH	1,2,3,4,5,6-hexachlorocyclohexane	$C_6H_6Cl_6$	290.830	112.5	0.139
Malathion [121-75-5]	Karbofos, Cythion, mercaptothion	*S*-[1,2-bis(ethoxycarbenyl)ethyl]-*O,O*-dimethyl phosphorodithioate	$C_{10}H_{19}O_6PS$	330.358	1.4	1
Mecarbam [2595-54-2]	Afos	*S*-(N-ethyoxycarbonyl-*N*-methyl-carbamoylmethyl) *O,O*-diethyl	$C_{10}H_{20}NO_5PS_2$	329.374	oil	1
Methamidophos [10265-92-6]	Monitor, Tamaron	*O,S*-dimethylphosphoramidothioate	$C_2H_8NO_2PS$	141.130	46	0.622
Methiocarb [2032-65-7]	Mesurol, Draza	4-methylthio-3,5-xylyl methylcarbamate	$C_{11}H_{15}NO_2S$	225.308	120	0.117
Methomyl [16752-77-5]	Lannate	*S*-methyl-*N*-(methylcarbamoyl-oxy)-thioaceticimidate	$C_5H_{10}N_2O_2S$	162.210	78	0.302
Methoxychlor [72-43-5]	Marlate	1,1,1-trichloro-2,2-bis(4-methoxy-phenyl)ethane	$C_{16}H_{15}Cl_3O_2$	345.648	87	0.246
Mevinphos [7786-34-7]	Apavinfos, Duraphos	2-carbomethoxy-1-methylvinyl dimethyl phosphate	$C_7H_{13}O_6P$	224.148	–56.1	1
Mirex [2385-85-5]	Dechlorane	1,1a,2,2,3a,4,5,5,5a,5b,6-dodeca-chlorooctahydro-1,3,4-metheno-1*H*-cyclobuta(cd)pentalene	$C_{10}Cl_{12}$	545.543	485 dec	0.000031
Monocrotophos [6923-22-4]	Nuvacron, Azodrin	dimethyl (*E*)-1-methyl-2-(methyl-carbamoyl)vinyl phosphate	$C_7H_{14}NO_5P$	223.164	55	0.508

(*Continued*)

TABLE 18.2.1 (*Continued*)

Name	Synonym	Chemical name	Molecular formula	Molecular weight, MW g/mol	m.p. °C	Fugacity ratio, F at 25°C	pK_a
Naled [300–76–5]	Arthodibrom, Dibrom, Bromex, Bromchlophos	1,2-dibromo-2,2-dichloroethyl dimethyl phosphate	$C_4H_7Br_2Cl_2O_4P$	380.784	27	0.956	
Oxamyl [23135-22-0]	Vydate	*N'N'*-dimethyl-2-methylcarbamoyloxyimino-2-(methylthio)acetamine	$C_7H_{13}N_3O_3S$	219.261	109	0.150	
Parathion [56-38-2]	Folidol, Bladan, Niran	*O,O*-diethyl *O*-4-nitrophenyl phosphorothioate	$C_{10}H_{14}NO_5PS$	291.261	6.1	1	
Parathion-methyl [298-00-0]	Dalf, Nitrox	*O,O*-dimethyl *O*-(*p*-nitrophenyl) phosphorothioate	$C_8H_{10}NO_5PS$	263.208	38	0.746	
Pentachlorophenol [87–86–5]	PCP	pentachlorophenol	C_6H_5OH	266.336	174	0.0345	4.74
Pentachlorophenol sodium salt	(Pentacon)						
Permethrin [52645-53-1]	Ambush, Kafil, Picket, Pramex	3-phenoxybenzyl(1*RS*,3*RS*;1*RS*,3*RS*)-3(2,2-dichlorovinyl)-2,2-=dimethylcyclo-prapanecarboxylate	$C_{21}H_{20}Cl_2O_3$	391.288	34	0.816	
cis-Permethrin					63-65	0.414	
trans-Permethrin					44-47	0.629	
technical grade							
Phenthoate [2597-03-7]	Cidial, Elsan	ethyl 2-dimethoxythiophosphorythio-2-phenylacetate	$C_{12}H_{17}O_4PS_2$	320.364	17-18	1	
Phorate [298-02-2]	Forsaat, Gramitox	*O,O*-diethyl-*S*-(ethylthio)methyl phosphordithioate	$C_7H_{17}O_2PS_3$	260.378	<–15	1	
Phorate-sulfone				292.3			
Phorate-sulfoxide				276.4			
Phosmet [732-11-6]	Imidan	*S*-[(1,3-dihydro-1,3-dioxo-2*H*-isoindol-2-yl)methyl]	$C_{11}H_{12}NO_4PS_2$	317.321	72	0.346	
Phosphamidon [13171-21-6]	Dimecron	2-chloro-2-diethylcarbamoyl-1-methylvinyl dimethyl phosphate	$C_{10}H_{19}ClNO_5P$	299.689	–45	1	
Pirimicarb [23103-98-2]	Pirimor, Aphox	2-dimethylamino-5,6-dimethyl-pyrimidin-4-yl dimethylcarbamate	$C_{11}H_{18}N_4O_2$	238.287	90.5	0.228	
Profenofos [41198-08-7]	Selecron	*O*-4-bromo-2-chlorophenyl *O*-ethyl *S*-propyl phosphorothioate	$C_{11}H_{15}BrClO_3PS$	373.631	liquid	1	
Propoxur [114-26-1]	Baygon	2-(1-Methylethoxy)phenol methyl carbamate	$C_{11}H_{15}NO_3$	209.242	87	0.246	
Ronnel [299-84-3]	Fenchlorphos, Korlan, Etrolene, Trolene	*O,O*-dimethyl *O*-2,4,5-trichlorophenyl-phosphorothioate	$C_8H_8Cl_3O_3PS$	321.546	41	0.697	
Sulfotep [3689-24-5]	dithio, thiotep, ENT, Bladafum	*O,O,O',O'*-tetraethyl dithiopyrophosphate	$C_8H_{20}O_5P_2S_2$	322.320	liquid	1	
Terbacil [5902-51-2]	Sinbar, Turbacil	5-chloro-3-(1,1-dimethyl)-6-methyl-2,4-(1*H*,3*H*)-pyrimidine-dione	$C_9H_{13}Cl_2N_2O_3$	216.664	176	0.0330	9.0

Terbufos [13071-79-9]	Contraven, Counter	*S*-*tert*-butylthiomethyl *O,O*-diethyl phosphorodithioate	$C_9H_{21}O_2PS_3$	288.431	liquid	1
Terbufos sulfone				320.41		
Terbufos sulfoxide				304.41		
Tetramethrin [7696-12-0]	Neo-Pynamin, phthalthrin	cyclohex-1-ene-1,2-dicarboximidomethyl (1*RS*,3*RS*;1*RS*,3*SR*)-2,2-dimethyl-3-methylprop-1-enyl)cyclopropanecarboxylate	$C_{19}H_{25}NO_4$	331.407	65-80	
Thiobencarb [28249-77-6]	Benthiocarb, Bolero, Saturno	*S*-(4-chlorophenyl)methyl diethyl-carbamothioate	$C_{12}H_{16}ClNOS$	257.779	1.7	1
Thiodicarb [59669-26-0]	Cicarbosulf, Larvin, Lepicron	dimethyl *N,N*′-thiobis(methylimino)-carbonyloxy bisethanimidothioate	$C_{10}H_{18}N_4O_4S_3$	354.470	173	0.0353
Toxaphene [8001-35-2]	Camphechlor	chlorinated camphene (67–69% Cl content) - mixture	$C_{10}H_{10}Cl_8$	413.812	65-90	
Trichlorfon [52-68-6]	Tugon, Chlorophos, Dipterex, Neguvon	dimethyl 2,2,2-trichloro-1-hydroxy-ethylphosphonate	$C_4H_8Cl_3O_4P$	257.437	77	0.309
Zinophos [297-92-2]	Thionazin, Namafos Cynem	*O,O*-diethyl-*O*-pyrazin-2-yl phosphorothioate	$C_8H_{13}N_2O_3PS$	248.239	–1.69	1

TABLE 18.2.2
Summary of selected physical-chemical properties of insecticides at 25°C

	Selected properties						Henry's law constant H/(Pa·m³/mol) calcd P/C	log K_{OC} reported
	Vapor pressure		Solubility					
Compound	P^S/Pa	P_L/Pa	S/(g/m³)	C^S/(mol/m³)	C_L/(mol/m³)	log K_{OW}		
Acephate	2.26×10^{-4}	8.96×10^{-4}	818000	4465	17710	–1	5.06×10^{-8}	0.301
Aldicarb	0.004	0.0216	6000	31.54	170	1.1	1.27×10^{-4}	1.48
Aldrin	0.005	0.0302	0.02	5.48×10^{-5}	3.31×10^{-4}	3.01	91.23	2.61
Aminocarb	0.00227	0.0109	915	4.39	21.1	1.73	5.17×10^{-4}	2.00
Azinphos-methyl	3.0×10^{-5}	9.05×10^{-5}	30	0.0945	0.285	2.7	3.17×10^{-4}	2.61
Bendiocarb	6.6×10^{-4}	7.21×10^{-3}	40	0.179	1.96		3.68×10^{-3}	2.76
Carbaryl	2.67×10^{-5}	3.83×10^{-4}	120	0.596	8.56	2.36	4.48×10^{-5}	2.36
Carbofuran	8.0×10^{-5}	1.41×10^{-3}	351	1.59	28.0	2.32	5.04×10^{-5}	2.02
Chlordane								
cis- or α-chlordane	4.0×10^{-4}	2.65×10^{-3}	0.056	1.37×10^{-4}	9.07×10^{-4}	6.0	0.342	5.5
trans- or β-chlordane	5.2×10^{-4}	3.15×10^{-3}	0.056	1.37×10^{-4}	8.30×10^{-4}	6.0	0.262	5.5
Chlorfenvinphos	1.0×10^{-4}	1.0×10^{-4}	124	0.345	0.345	3.82	2.90×10^{-4}	2.47
Chlorpyrifos	0.00227	3.34×10^{-3}	0.73	2.08×10^{-3}	3.07×10^{-3}	4.92	1.09	3.78
Chlorpyrifos-methyl	0.006	9.68×10^{-3}	4.76	0.0148	0.0238		0.407	3.48
Crotoxyphos	0.0019	1.90×10^{-3}	1000	3.18	3.18	2.23	5.97×10^{-4}	2.23
Cypermethrin#	1.87×10^{-7}	6.62×10^{-7}	0.004	9.61×10^{-6}	3.40×10^{-5}	6.6	0.0195	2.59
α-cypermethrin	2.30×10^{-7}	8.21×10^{-7}	0.01	2.40×10^{-5}	8.41×10^{-5}	6.94*	0.0098	
β-cypermethrin	1.80×10^{-7}	5.13×10^{-7}	0.0934	2.24×10^{-4}	6.4×10^{-4}	4.70*	8.02×10^{-7}	
ζ-cypermethrin	2.50×10^{-7}	2.5×10^{-7}	0.045	1.08×10^{-4}	1.08×10^{-4}		2.31×10^{-3}	
DDD								
p,p'-DDD	1.30×10^{-4}	6.93×10^{-4}	0.05	1.56×10^{-4}	1.08×10^{-3}	5.5	0.640	5.0
o,p'-DDD	2.0×10^{-4}*	1.39×10^{-3}	0.10*			6.0		
DDE								
p,p'-DDE	8.66×10^{-4}	3.72×10^{-3}	0.04	1.26×10^{-4}	5.40×10^{-4}	5.7	7.95	5.0
o,p'-DDE	8.0×10^{-4}	3.44×10^{-3}	0.1	3.14×10^{-4}	1.35×10^{-3}	5.8	2.54	
DDT								
p,p'-DDT	2.0×10^{-5}	1.35×10^{-4}	0.0055	1.55×10^{-5}	1.11×10^{-4}	6.19	2.36	5.4
o,p'-DDT	2.53×10^{-5}	1.72×10^{-4}	0.026	7.33×10^{-5}	4.96×10^{-4}		0.347	
Deltamethrin	1.0×10^{-5}	5.52×10^{-5}	0.002	3.96×10^{-6}	2.18×10^{-5}		2.53	5.66
Demeton	0.0347	0.0347	60	0.232	0.232		0.15	1.85
Demeton-S-methyl	0.04	0.040	3300	14.3	14.3		2.79×10^{-3}	
Dialifor	6.50×10^{-5}	1.73×10^{-4}	0.18	4.57×10^{-4}	1.22×10^{-3}	4.7	0.14	

Diamidaphos			50000					
Diazinon	0.008	8.0×10^{-3}	60	0.197	0.197	3.3	0.0406	2.76
Dicapthon	5.0×10^{-4}	1.19×10^{-3}	6.25	0.021	0.05	3.6	0.0238	
Dichlofenthion	25	25.0	0.25	7.93×10^{-4}	7.93×10^{-4}	5.1	31646	
Dichlorvos	7.02	7.02	8000	36.20	36.20	1.45	0.194	1.45
Dicrotophos	0.0213	0.0213	1000000	4216	4216		5.05×10^{-6}	1.88
Dieldrin	0.0005	0.016	0.17	4.46×10^{-4}	0.0142	5.20	1.120	4.08
Diflubenzuron	1.20×10^{-7}	1.31×10^{-5}	0.08	2.57×10^{-4}	0.0281	0.78	4.66×10^{-4}	3.01
Dimethoate	0.01	0.019	20000	87.23	163.2	0.8	1.15×10^{-4}	1.3
Dinoseb	10	14.07	47	0.196	0.275		51.11	2.09
Disulfoton	0.02	0.132	25	0.0911	0.603	4.02	0.220	3.25
DNOC	0.011	0.044	150	1.013	4.063		0.0109	
Endosulfan	0.0013		0.5	1.23×10^{-3}		3.6	1.06	4.09
α-Endosulfan	0.0013	0.008	0.5	1.23×10^{-3}	0.008	3.62		3.4
β-Endosulfan	0.0061	0.394	0.45	1.11×10^{-3}	0.071	3.83		3.5
Endrin	2.0×10^{-5}	1.32×10^{-3}	0.23	6.04×10^{-4}	0.0399	5.2	0.0331	4
Ethion	1.5×10^{-4}	1.50×10^{-4}	1.8	4.68×10^{-3}	4.68×10^{-3}	5.7	0.0320	4.19
Ethoprophos	0.0507	0.0507	750	3.095	3.095	3.59	0.0164	1.85
Fenitrothion	1.3×10^{-4}	1.30×10^{-4}	30	0.108	0.108	3.4	1.20×10^{-3}	3.3
Fenoxycarb	1.70×10^{-6}	3.29×10^{-6}	6	0.0199	0.039	4.3	8.54×10^{-5}	3.0
Fenthion	0.004	4.0×10^{-3}	50	0.180	0.180	4.1	0.0223	3.18
Fenvalerate	4.27×10^{-6}	4.27×10^{-6}	0.085	2.02×10^{-4}	2.02×10^{-4}	6.2	0.0211	4.0
Flucythrinate	1.20×10^{-6}*	1.20×10^{-6}	0.5*	1.11×10^{-3}	1.11×10^{-3}	6.2	1.08×10^{-3}	5.0
Fonofos	0.045	0.045	16	0.0650	0.065	3.9	0.693	2.94
Heptachlor	0.053	0.267	0.056	1.50×10^{-4}	7.56×10^{-4}	5.27	353.4	4.38
Heptachlor epoxide			0.35	8.99×10^{-4}	0.0190	5.0		4.0
Hexachlorocyclohexane								
α-BHC	0.003	0.10	1	3.44×10^{-3}	0.115	3.81	0.872	3.81
β-BHC	4.0×10^{-5}	0.0264	0.1	3.44×10^{-4}	0.227	3.8	0.116	3.36
δ-BHC	0.002	0.0268	8	0.0275	0.369	4.14	0.0727	
Iodofenphos	4.4×10^{-4}	4.4×10^{-4}	18	0.0521	0.0521	4.04	8.45×10^{-3}	
Isophorone	50	50.0	12000	86.83	86.83	1.7	0.576	
Kepone	2.93×10^{-5}	0.05	3	0.0061	10.02	5.4	0.005	4.74
Leptophos	3.0×10^{-6}	6.08×10^{-6}	0.005	1.21×10^{-5}	2.46×10^{-5}	5.9	0.247	3.97
Lindane	0.00374	0.0274	7.3	0.0251	0.184	3.7	0.149	3.0
Malathion	0.001	0.001	145	0.439	0.439	2.8	2.28×10^{-3}	3.26
Mecarbam	negligible		< 1000					
Methamidophos	0.0023	3.59×10^{-3}	200000	142	2210			

(*Continued*)

TABLE 18.2.2 *(Continued)*

	Selected properties						Henry's law constant H/(Pa·m³/mol) calcd P/C	log K_{OC} reported
	Vapor pressure		Solubility					
Compound	P^S/Pa	P_L/Pa	S/(g/m³)	C^S/(mol/m³)	C_L/(mol/m³)	log K_{OW}		
Methiocarb	0.016*	0.130	30	0.133	1.082	2.92	0.120	2.48
Methomyl	0.0067	0.0229	58000	358	1223	0.60	1.87×10^{-5}	
Methoxychlor	0.00013	5.46×10^{-4}	0.045*	1.30×10^{-4}	5.47×10^{-4}	5.08	0.999	4.9
Mevinphos	0.017	0.0170	600000	268	2677	0.5	6.35×10^{-6}	1.64
Mirex	0.0001	3.545	6.5×10^{-5}	1.19×10^{-7}	4.22×10^{-3}	6.9	839.4	6.0
Monocrotophos	0.00933	0.0185	1000000	448	8870	B0.20	2.08×10^{-6}	
Oxamyl	0.0306	0.173	282000	1290	7261	B0.47	2.38×10^{-5}	1.4
Parathion	6.0×10^{-4}	6.0×10^{-4}	12.4	0.0426	0.0426	3.8	0.0141	4.02
Parathion methyl	0.002	2.69×10^{-3}	25	0.095	0.128	3.0	0.0211	3.7
Pentachlorophenol	0.00415	0.12	14	0.053	1.565	5.05	0.79	4
Permethrin	1.70×10^{-6}	2.34×10^{-6}	0.006	1.53×10^{-5}	2.11×10^{-5}	6.1	0.111	4.8
Phenthoate	3.5×10^{-4}	3.50×10^{-4}	11	0.0343	0.034	3.69	0.0102	3.00
Phorate	0.085	0.085	22	0.0845	0.084	3.56	1.01	2.82
Phosmet	6.0×10^{-5}	1.75×10^{-4}	25	0.0788	0.229	2.8	7.62×10^{-4}	2.8
Phosphamidon	0.003	0.003	2.5	8.34×10^{-3}	0.0083		0.360	0.845
Pirimicarb	0.003	0.0133	2200	9.232	41.03		3.25×10^{-4}	
Profenofos	1.2×10^{-4}	1.20×10^{-4}	28	0.0749	0.075		1.60×10^{-3}	3.34
Propoxur	1.70×10^{-5}	7.73×10^{-5}	1800	8.603	39.12	1.5	1.98×10^{-6}	1.48
Pyrethrins	1.33×10^{-6}		0.001	3.05×10^{-6}			0.437	5
Ronnel (Fenchlorofos)	0.107	0.154	0.6	1.87×10^{-3}	2.69×10^{-3}	5.07	57.35	2.9
Sulfotep	0.0227	0.0227	25	0.0776	0.0776		0.293	
Terbacil	4.13×10^{-5}	1.29×10^{-3}	710	3.276	102.06		1.26×10^{-5}	1.74
Terbufos	0.0427	0.0427	5	0.0173	0.017	4.48	2.463	2.70
Thiobencarb	0.00293		19.2	0.0745			0.0393	2.95
Thiodicarb	0.00431	0.117	35	0.0987	2.68		0.0437	
Toxaphene	0.0009		0.5	1.21×10^{-3}		5.50	0.745	5
Trichlorfon	0.001	3.83×10^{-3}	154000	598	2290	0.51	1.67×10^{-6}	1.00
Zinophos	0.4	0.40	1000	4.029	4.03		0.0993	

isomer not specified

* The reported values for this quantity vary considerably, whereas this selected value represents the best judgment of the authors. The reader is cautioned that it may be subject to a large error.

TABLE 18.2.3
Suggested half-life classes of insecticides in various environmental compartments at 25°C

Compound	Air class	Water class	Soil class	Sediment class
Aldicarb	1	5	6	8
Aldrin	4	8	8	9
Carbaryl	3	4	5	6
Carbofuran	1	4	5	6
Chlordane	4	8	8	9
Chloropyrifos	2	4	4	6
DDE	4	9	9	9
p,p'-DDT	4	7	8	9
Diazinon	5	6	6	7
Dieldrin	4	8	8	9
Heptachlor	3	5	6	7
γ-HCH (lindane)	5	8	8	9
Malathion	2	3	3	5
Methoxychlor	2	4	6	7
Mirex	4	6	9	9
Parathion	2	5	5	6
Parathion-methyl	2	5	5	6
Propoxur	1	5	5	6
Toxaphene	4	9	9	9

Class	Mean half-life (hours)	Range (hours)
1	5	< 10
2	17 (~ 1 day)	10–30
3	55 (~ 2 days)	30–100
4	170 (~ 1 week)	100–300
5	550 (~ 3 weeks)	300–1,000
6	1700 (~ 2 months)	1,000–3,000
7	5500 (~ 8 months)	3,000–10,000
8	17000 (~ 2 years)	10,000–30,000
9	~ 5 years	> 30,000

18.3 REFERENCES

Abdullah, A.R., Bajet, C.M., Matin, M.A., Nhan, D.D., Sulaiman, A.H. (1997) Ecotoxicology of pesticides in the tropical paddy field ecosystem. *Environ. Toxicol. Chem.* 16(1), 59–70.

Albert, A. (1963) Ionization constants. In: *Physical Methods in Heterocyclic Chemistry.* Katritzky, A.R., Editor, Academic Press, New York.

Adachi, K., Mitsuhashi, T., Ohkuni, N. (1984) Pesticides and trialkyl phosphates in tap water. *Hyogo-Ken Eisei Kenkyusho Kenkyu Hokoku* 19, 1–6.

Adams, Jr., R.S. (1967) The fate of pesticide residues in soil. *J. Minn. Acad. Sci.* 34, 44–48.

Adams, W.J. (1987) Chapter 16, Bioavailability of neutral lipophilic organic chemicals contained on sediments: A review. In: *Fate and Effects of Sediment-Bound Chemicals in Aquatic Systems*. Dickson, K.L., Maki, A.W., Brungs, W.A., Eds., Pergamon Press, New York.

Addison, J.B. (1981) Measurement of vapour pressures of fenitrothion and metacil. *Chemosphere* 10, 355–364.

Adhya, T.K., Sudhakar-Barik, R., Sethunathan, N. (1981) Fate of fenitrothion, methyl parathion and parathion in anoxic sulfur-containing soil systems. *Pest. Biochem. Phys.* 16, 14.

Agency for Toxic Substances and Disease Registry (1988) Toxicological profile for chlordane. Agency for Toxic Substances and Disease Registry, Atlanta, Georgia.

Agency for Toxic Substances and Disease Registry (1988) Toxicological profile for DDT, DDE, and DDD. Agency for Toxic Substances and Disease Registry, Atlanta, Georgia.

Ahmad, A., Walgenbach, D.D., Sutter, G.R. (1979) Degradation rates of technical carbofuran and a granular formulation in four soils with known insecticide use history. *Bull. Environ. Contam. Toxicol.* 23, 572–574.

Ali, S. (1978) Degradation and Environmental Fate of Endosulfan Isomers and Endosulfan Sulfate in Mouse, Insect and Laboratory Ecosystem. *Diss. Abstr. Int. B.* 39(5), 2117., Ph.D. Thesis, University of Illinois.

Alison, D.T., Hermanutz, R.O. (1977) Toxicity of Diazinon to Brook Trout and Fathead Minnows. EPA 600/3-77-060, U.S. EPA, Duluth, Minnesota.

Alley, E.G. (1973) The use of mirex in control of the imported fire ant. *J. Environ. Quality* 2(1), 52–61.

Altschuh, J., Brüggemann, Santl, H., Eichinger, G., Piringer, O.G.(1999) Henry's law constants for a diverse set of organic chemicals: Experimental determination and comparison of estimation methods. *Chemosphere* 39, 1871–1887.

Aly, O.M., El-Dib, M.A. (1971) Studies on the persistence of some carbamate insecticides in the aquatic environment. I. Hydrolysis of sevin, baygon, pyrolan, and dimetilan in waters. *Water Res.* 5, 1191–1205.

Anderson, R.L., Defoe, D.L. (1980) Toxicity and bioaccumulation of endrin and methoxychlor in aquatic invertebrates and fish. *Environ. Pollut. Ser.* A22, 111.

Andrews, A.K., Van Valin, C.C., Stebbings, B.E. (1966) Some effects of heptachlor on bluegills (*Lepomis macrochirus*). *Trans. Amer. Fish Soc*. 95, 297.

Ankley, G.T., Call, D.J., Cox, J.S., Kahl, M.D., Hoke, R.A., Kosian, P.A. (1994) Organic carbon partitioning as a basis for predicting the toxicity of chlorpyrifos in sediments. *Environ. Toxicol. Chem.* 13, 621–626.

Argyle, R.L., Williams, G.C., Dupree, H.K. (1973) Endrin uptake and release by fingering channel catfish (*Ictalurus puncatus*). *J. Fish Res. Board Can*. 30, 1743.

Armbrust, K.L. (2000) Pesticide hydroxyl radical rate constants: measurements and estimates of their importance in aquatic environments. *Environ. Toxicol. Chem*. 19, 2175–2180.

Ashton, F.M., Crafts, A.S. (1981) *Mode of Action of Herbicides*. John Wiley & Sons, New York.

Atkins, D.H.F., Eggleton, A.E.J. (1971) Studies of atmospheric wash-out and deposition of γ-BHC, dieldrin and *p,p′*-DDT using radio-labelled pesticides. In: *Proc. Symp. on Nucl. Tech. Environ. Pollut.*, pp. 521–533, Vienna.

Atkinson, R. (1985) Kinetics and mechanisms of the gas-phase reactions of hydroxyl radicals with organic compounds under atmospheric conditions. *Chem. Rev.* 85, 69–201.

Atkinson, R. (1987) Structure-activity relationship for the estimation of rate constants for the gas-phase reactions of OH radicals with organic compounds. *Int. J. Chem. Kinetics* 19, 799–828.

Atkinson, R., Carter, W.P.L. (1984) Kinetics and mechanisms of the gas-phase reactions of ozone with organic compounds under atmospheric conditions. *Chem. Rev.* 84, 437–470.

Atkinson, R., Kwok, E.S.C., Arey, J. (1992) Photochemical processes affecting the fate of pesticides in the atmosphere. *Brighton Crop Prot. Conf. - Pests Dis.* 2, 469–476.

Atlas, E., Foster, R., Giam, C.S. (1982) Air-sea exchange of high molecular weight organic pollutants: laboratory studies. *Environ. Sci. Technol.* 16, 283–286.

Augustijn-Beckers, P.W.M., Hornsby, A.G., Wauchope, R.D. (1994) The SCS/ARS/CES pesticide-properties database for environmental decision - making. II. Additional compounds. *Rev. Environ. Contam. Toxicol*. 137, 1–82.

Babers, F.H. (1955) The solubility of DDT in water determined radiometrically. *J. Am. Chem. Soc.* 77, 4666.

Bacci, E., Calamari, D., Gaggi, C., Vighi, M. (1990) Bioconcentration of organic chemical vapors in plant leaves: Experimental measurements and correlation. *Environ. Sci. Technol.* 24, 885–889.

Bacci, E., Gaggi, C. (1987) Chlorinated hydrocarbon vapours and plant foliage: Kinetics and applications. *Chemosphere* 16, 2515–2522.

Bahner, L.H., Oglesby, J.L. (1979) Test of a model for predicting kepone accumulation in selected estuarine species. In: *Aquatic Toxicology SPT 667*, pp. 221–231. American Standard of Testing Materials, Philadelphia, PA.

Bahnick, D.A., Doucette, W.J. (1988) Use of molecular connectivity indices to estimate soil sorption coefficients for organic chemicals. *Chemosphere* 17, 1703–1715.

Baker, M.D., Mayfield, C.I. (1980) Microbial and non-biological decomposition of chlorophenols and phenols in soil. *Water Air Soil Pollut*. 13, 411.

Baker, R.A., Editor (1991) *Organic Substances and Sediments in Water.* Vol. 1 and 2. Lewis Publishers, Chelsea, Michigan.

Baker, R.D., Applegate, H.G. (1970) Effect of temperature and ultraviolet radiation on the persistence of methyl parathion and DDT in soils. *Argon. J.* 62, 509.

Ballschmiter, K., Wittlinger, R. (1991) Interhemisphere exchange of hexachlorohexanes, hexachlorobenzene, polychlorobiphenyls and 1,1,1-trichloro-2,2-bis(*p*-chlorophenyl)-ethane in the lower troposphere. *Environ. Sci. Technol*. 25, 1103–1111.

Balson, E.W. (1947) Studies in vapour pressure measurement. III. An infusion manometer sensitive to 5×10^{-4} mmHg. Vapour pressures of DDT and other slightly volatile substances. *Trans. Faraday Soc.* 43, 54–60.

Banerjee, S., Baughman, G.L. (1991) Bioconcentration factors and lipid solubility. *Environ. Sci. Technol.* 25, 536–539.

Banerjee, S., Howard, P.H., Rosenberg, A.M., Dombrowski, A.E., Sikka, H., Tullis, D.L. (1984) Development of general kinetic model for biodegradation and its application to chlorophenols and related compounds. *Environ. Sci. Technol.* 18, 416–422.

Barlow, F. (1978) Presented at the 4th International Congress of Pesticide Chemistry. Zurich, Switzerland, July 24–28, 1978.

Baron, R.L., Walton, M.S. (1971) Dynamics of HEOD (dieldrin) in adipose tissue of the rats. *Toxicol. Appl. Pharmacol*. 18, 958–963.

Barron, M.G., Plakas, S.M., Wilga, P.C. (1991) Chlorpyrifos pharmacokinetics and metabolism following intravascular and dietary administration in channel catfish. *Toxicol. Appl. Pharmacol*. 108, 474–482.

Battersby, N.S. (1990) A review of biodegradation kinetics in the aquatic environment. *Chemosphere* 21(10–11), 1243–1284.

Baughman, G.L., Lassiter, R.R. (1978) Prediction of environmental pollutant concentration. In: *Estimating the Hazard of Chemical Substances to Aquatic Life.* ASTM STP 657, Cairns, Jr., J., Dickson, K.L., Maki, A.W., Editors, American Society for Testing and Materials, Philadelphia, Pennsylvania.

Baughman, G.L., Paris, D.F. (1981) Microbial bioconcentration of organic pollutants from aquatic systems-A critical review. *CRC Critical Review in Microbiology.* CRC Press, Boca Raton, Florida.

Beall, M.L., Nash, R.G. (1972) Insecticide depth in soil - Effect on soyabean uptake in the greenhouse. *J. Environ. Qual.* 1, 283–288.

Beck, E.W., Johnson, Jr., J.C., Woodham, D.W., Leuck, D.B., Dawsey, L.H., Robbins, J.E., Bowman, M.C. (1966) *J. Econ. Entomol*. 59, 1444.

Behrendt, H., Brüggemann, R. (1993) Modeling the fate of organic chemicals in the soil plant environment: Model study of root uptake of pesticides. *Chemosphere* 27(12), 2325–2332.

Bellin, C.A., O'Connor, G.A., Yin, Y. (1990) Sorption and degradation of pentachlorophenol in sludge-amended soils. *J. Environ. Qual.* 19, 603–608.

Belluck, D., Felsot, A. (1981) Bioconcentration of pesticides by egg masses of the caddisfly, *Triaenodes tardus* milne. *Bull. Environ. Contam. Toxicol*. 26, 299–306.

Beltrame, P., Beltrame, P.L., Cartini, P., Guardione, D., Lanzetta, C. (1988) Inhibiting action of chlorophenols on biodegradation of phenol and its correlation with structured structural properties of inhibitors. *Biotechn. Bioeng.* 31, 821–828.

Bender, M.E. (1969) Uptake and retention of malathion by the carp. *Prog. Fish-Cult.* 31, 155–159.

Bennett, H.J., Day, J.W. (1970) Absorption of endrin by the bluegill sunfish, *Lepomis macrochirus. Pest. Monit. J.* 3, 201.

Berdanier, C.D., de Dennis, S.K. (1977) Effect of exercise on the responses of rats to DDT. *J. Toxicol. Environ. Health* 2, 651–656.

Beste, C.E., Humburg, N.E. (1983) *Herbicide Handbook of the Weed Science Society of America.* 5th Edition, Weed Science Society, Champaign, Illinois.

Bevenue, A., Beckman, H. (1967) Pentachlorophenol: A discussion of its properties and its occurrence as a residue in human and animal tissues. *Res. Rev.* 19, 83–134.

Bhavnagary, H.M., Jayaram, M. (1974) Determination of water solubilities of lindane and dieldrin at different temperatures. *Bull. Grain Technol.* 12(2), 95–99.

Biddinger, G.R., Gloss, S.P. (1984) The importance of trophic transfer in the bioaccumulation of chemical contaminants in organic ecosystem. *Res. Rev.* 91, 103–145.

Bidleman, T.F. (1984) Estimation of vapor pressures for nonpolar organic compounds by capillary gas chromatography. *Anal. Chem.* 56, 2490–2496.

Bidleman, T.F., Billings, W.N., Foreman, W.T. (1986) Vapor-particle partitioning of semivolatile organic compounds-Estimation from field collections. *Environ. Sci. Technol.* 20(10), 1038–1043.

Bidleman, T.F., Leone, A.D., Falconer, R.L. (2003) Vapor pressures and enthalpies of vaporization for toxaphene congeners. *J. Chem. Eng. Data 48*, 1122–1127.

Bidleman, T.F., Renberg, L. (1985) Determination of vapor pressures for chloroguaiacols, chloroveratrols, and nonylphenol by gas chromatography. *Chemosphere* 14, 1475–1481.

Bierman, V., Swain, W. (1982) Mass balance modeling of DDT dynamics in Lakes Michigan and Superior. *Environ. Sci. Technol*. 16, 572–579.

Biggar, J.W., Riggs, I.R. (1974) Apparent solubility of organochlorine insecticides in water at various temperatures. *Hilgardia* 42(10), 383–391.

Biggar, J.W., Doneen, L.D., Riggs, I.R. (1966) Soil interaction with organically polluted water. Summary Report, Department of Water Science and Engineering, University of California, Davis, California.

Biggar, J.W., Dutt, G.R., Riggs, I.R. (1967) Predicting and measuring the solubility of *p,p′*-DDT in water. *Bull. Environ. Contam. Toxicol.* 2(3), 90.

Bilkert, J.N., Rao, P.S.C. (1985) Sorption and leaching of three nonfumigant nematocides in soils. *J. Environ. Sci. Health* B20, 1–26.

Bintein, S., Devillers, J. (1994) QSAR for organic chemical sorption in soils and sediments. *Chemosphere* 28, 1171–1188.

Bishop, W.E., Maki, A.W. (1980) A critical comparison of two bioconcentration test methods. In: *Aquatic Toxicology.* ASTM STP 707, pp. 61–77, American Society for Testing and Materials, Philadelphia, Pennsylvania.

Blackman, G.E., Parke, M.H., Garton, G. (1955) The physiological activity of substituted phenols. I. Relationships between chemical structure and physiological activity. *Arch. Biochem. Biophys.* 54(1), 55–71.

Blum, D.J.W., Suffet, I.H., Duguet, J.P. (1994) Quantitative structure-activity relationship using molecular connectivity for the activated carbon adsorption of organic chemicals in water. *Water Res.* 28, 687–699.

Boehncke, A., Seiber, J., Nolting, H.-G. (1990) Investigations of the evaporation of selected pesticides from natural and model surfaces in field and laboratory. *Chemosphere* 21(9), 1109–1124.

Boehncke, A., Martin, K., Müller, M.G., Cammenga, H.K. (1996) The vapor pressure of lindane (γ-1,2,3,4,5,6-hexachlorocyclohexane)-A comparison of Knudsen effusion measurements with data from other techniques. *J. Chem. Eng. Data* 41, 543–545.

Bomberger, D.C., Gwinn, J.L., Mabey, W.R., Tus, D., Chou, T.W. (1983) Environmental fate and transport at the terrestrial-atmospheric interface. *ACS Symp. Ser.* 225, 197–214.

Bond, C.A., Woodham, D.W., Ahrens, E.H., Medley, J.G. (1975) The accumulation and disappearance of mirex residues. II. In milk and tissues of cows fed two concentrations of the insecticide in their diet. *Bull. Environ. Contam. Toxicol*. 14, 25–31.

Bondarenko, S., Gan, J. (2004) Degradation and sorption of selected organophosphate and carbamate insecticides in urban stream sediments. *Environ. Toxicol. Chem.* 23, 1809–1914.

Boublik, T., Fried, V., Hala, E. (1984) *The Vapor Pressures of Pure Substances.* 2nd Edition, Elsevier, Amsterdam, The Netherlands.

Bourquin, A.W., Garnas, R.I., Pritchard, P.H., Wilkes, F.G., Cripe, C.R., Rubinstein, N.I. (1979) Interdependent microcosms for the assessment of pollutants in the marine environment. *Int. J. Environ. Studies* 13, 131–140.

Bowery, T.G. (1964) In: *Analytical Methods for Pesticides, Plant Growth Regulators, and Food Additives.* Vol. 2, Zweig, G., Editor, Academic Press, New York.

Bowman, B.T., Sans, W.W. (1979) The aqueous solubility of twenty-seven insecticides and related compounds. *J. Environ. Sci. Health* B14(6), 625–634.

Bowman, B.T., Sans, W.W. (1983a) Further water solubility determination of insecticidal compounds. *J. Environ. Sci. Health* B18 (2), 221–227.

Bowman, B.T., Sans, W.W. (1983b) Determination of octanol-water partitioning coefficients (K_{OW}) of 61 organophosphorous and carbamate insecticides and their relationship to respective water solubility (S) values. *J. Environ. Sci. Health* B18 (6), 667–683.

Bowman, M.C., Acree, Jr., F., Corbett, M.K. (1960) Solubility of carbon-14 DDT in water. *J. Agric. Food Chem.* 8 (5), 406–408.

Bowman, M.C., Schechter, M.S., Carter, R.L. (1965) Behavior of chlorinated insecticides in a broad spectrum of soil types. *J. Agric. Food Chem.* 13, 360–365.

Branson, D.R. (1978) Predicting the fate of chemicals in the aquatic environment from laboratory data. pp. 55–70. In: *Estimating the Hazard of Chemical Substances to Aquatic Life*. ASTM STP 657, Cairns, Jr., J., Dickson, K.L., Maki, A.W., Editors, American Society for Testing and Materials, Philadelphia, Pennsylvania.

Brecken-Folse, J.A., Mayer, F.L., Pedigo, L.E., Marking, L.L. (1994) Acute toxicity of 4-nitrophenol, 2,4-dinitrophenol, terbufos and trichlorfon to grass shrimp (*Palaemonetes* spp.) and sheepshead minnows (*Cyprinodon variegatus*) as affected by salinity and temperature. *Environ. Toxicol. Chem.* 13, 67–77.

Briggs, G.G. (1973) A simple relationship between soil adsorption of organic chemicals and their octanol/water partitioning coefficients. *Proc. 7th British Insecticide and Fungicide Conference* 1, 83–86.

Briggs, G.G. (1981) Theoretical and experimental relationships between soil adsorption, octanol-water partition coefficients, water solubilities, bioconcentration factors, and the Parachor. *J. Agric. Food Chem.* 29, 1050–1059.

Bright, N.F.H., Cuthill, J.C., Woodbury, N.H. (1950) The vapor pressure of parathion and related compounds. *J. Sci. Food Agric.* 1, 344.

Brockway, D.L., Smith, P.D., Stancil, F.E. (1984) Fates and effects of pentachlorophenol in hard- and soft-water microcosms. *Chemosphere* 13(12), 1363–1377.

Bromilow, R.H., Baker, R.J., Freeman, M.A.H., Görög, K. (1980) The degradation of aldicarb and oxamyl in soil. *Pest. Sci.* 11(4), 389–395.

Bromilow, R.H., Leistra, M. (1980) Measured and simulated behavior of aldicarb and its oxidation products in fallow soils. *Pest. Sci.* 11, 389–395.

Brooke, D., Nielsen, I., De Bruijn, J., Hermens, J. (1990) An interlaboratory evaluation of the stir-flask method for the determination of octanol water partition coefficients. (LOG POW). *Chemosphere* 21, 119–133.

Brooke, D.N., Dobbs, A.J., Williams, N. (1986) Octanol/water partition coefficients (P): Measurement, estimation, and interpretation, particularly for chemicals with $P > 10^5$. *Ecotoxicol. Environ. Saf.* 11, 251–260.

Brooks, G.T. (1974) *Chlorinated Insecticides*: Volume I: Technology and Applications. CRC Press, Cleveland, Ohio.

Bro-Rasmussen, F., Noddegaard, E., Voldum-Claussen, K. (1970) Comparison of the disappearance of eight organophosphorus insecticides from soil in laboratory and in outdoor experiments. *Pest. Sci.* 1, 179–182.

Broto, P., Moreau, G., Vandycke, C. (1984) Molecular structures: Perception, autocorrelation descriptor and SAR studies. System of atomic contribution for the calculation of the *n*-octanol/water partition coefficients. *Eur. J. Med. Chem. Chim. Term.* 19, 71–78.

Brouwer, D.H., Ravensberg, J.C., De Kort, W.L.A.M., Van Hemmen, J.J. (1994) A personal sampler for inhalable mixed-phase aerosols: modification to an existing sample and validation test with three pesticides. *Chemosphere* 28, 1135–1146.

Bruggeman, W.A., Martron, L.B.J.M., Kooiman, D., Hutzinger, O. (1981) Accumulation and elimination kinetics of di-, tri-, and tetrachlorobiphenyls by goldfish after dietary and aqueous exposure. *Chemosphere* 10, 811–832.

Brusseau, M.L., Rao, P.S.C. (1989) The influence of sorbate-organic matter interactions on sorption nonequilibrium. *Chemosphere* 18, 1691–1706.

Brust, H.F. (1966) A summary of chemical and physical properties of Dursban. *Down to Earth* 22(3), 21–22.

Budavari, S., Editor (1989) *The Merck Index. An Encyclopedia of Chemicals, Drugs and Biologicals.* 11th Edition, Merck and Co., Rahway, New Jersey.

Buehler, S.S., Basu, I., Hites, R. (2004) Causes of variability in pesticide and PCB concentrations in air near the Great Lakes. *Environ. Sci. Technol.* 38, 414–422.

Bunce, N.J., Nakai, J.S., Yawching, M. (1991) A model for estimating the rate of chemical transformation of a VOC in the troposphere by two pathways: Photolysis by sunlight and hydroxyl radical attack. *Chemosphere* 22, 305–315.

Burkhard, L.P., Kuehl, D.W., Veith, G.D. (1985) Evaluation of reverse phase liquid chromatography/mass spectrometry for estimation of *n*-octanol/water partition coefficients. *Chemosphere* 14, 1551–1560.

Burkhard, N., Guth, J.A. (1979) Photolysis of organophosphorous insecticides on soil surfaces. *Pest. Sci.* 10, 313–319.

Burkhard, N., Guth, J.A. (1981) Rate of volatilisation of pesticides from soil surfaces: Comparison of calculated results with those determined in a laboratory model system. *Pest. Sci.* 12(1), 37–44.

Burmaster, D.E., Menzie, C.A., Freshman, J.S., Burris, J.A., Maxwell, N.I., Drew, S.R. (1991) Assessment of methods for estimating aquatic hazards at superfund-type sites: A cautionary tale. *Environ. Toxicol. Chem.* 10, 827–842.

Burns, S.E., Hassett, J.P., Rossi, M.V. (1996) Binding effects on jumic-mindiated photoreaction: intrahumic dechlorination of mirex in water. *Environ. Sci. Technol.* 30, 2934–2941.

Buser, H-R., Müller, M.D. (1995) Isomer and enantioselective degradation of hexachloro-cyclohexane isomers in sewage sludge under anaerobic conditions. *Environ. Sci. Technol.* 29, 664–672.

Butler, P.A. (1971) Influence of pesticides on marine ecosystems. *Proc. Roy. Soc. London* (Ser. B) 177, 321–329.

Butler, L.C., Stauff, D.C., Davis, R.L. (1981) Methyl parathion persistence in soil following simulated spillage. *Arch. Environ. Contam. Toxicol.* 10, 451–458.

Butte, W., Fox, K., Zauke, G.P. (1991) Kinetics of bioaccumulation and clearance of isomeric hexachlorocyclohexanes. *Sci. Total Environ.* 109/110, 377–382.

Butte, W., Fooken, C., Klussman, R., Schuller, D. (1981) Evaluation of lipophilic properties for a series of phenols, using reversed-phase high performance liquid chromatography and high-performance thin-layer chromatography. *J. Chromatogr.* 214, 59–67.

Butte, W., Willing, A., Zanke, G.P. (1987) Bioaccumulation of phenols in zebrafish determined by a dynamic flow through test. In: *QSAR in Environmental Toxicology II.* Kaiser, K.L.E., pp. 43–53, Editor, D. Reidel Publishing Company, Dordrecht, The Netherlands.

Buxton, G.V., Greenstock, C.L., Helman, W.P., Ross, A.B. (1988) Critical review of rate constants for reactions of hydrated electrons, hydrogen atoms and hydroxyl radicals (·OH/·O-) in aqueous solution. *J. Phys. Chem. Ref. Data* 17, 513–886.

Bysshe, S.E. (1982) Chapter 5, Bioconcentration factor in aquatic organisms. In: *Handbook on Chemical Property Estimation Methods, Environmental Behavior of Organic Compounds.* Lyman, W.J., Reehl, W.F., Rosenblatt, D.H., Editors, McGraw-Hill, New York.

Calamari, D., Bacci, E., Forcardi, S., Gaggi, C., Morosini, M., Vighi, M. (1991) Role of plant biomass in the global environmental partitioning of chlorinated hydrocarbons. *Environ. Sci. Technol.* 25, 1489–1495.

Call, D.J., Brooke, L.T., Lu, P.Y. (1980) Uptake, elimination and metabolism of three phenols by fathead minnows. *Arch. Environ. Contam. Toxicol.* 9, 699–714.

Callahan, M.A., Slimak, M.W., Gabel, N.W., May, I.P., Fowler, C.F., Freed, J.R., Jennings, P., Durfee, R.L., Whitmore, F.C., Maestri, B., Mabey, W.R., Holt, B.R., Gould, C. (1979) *Water-Related Environmental Fate of 129 Priority Pollutants.* Vol. 1, EPA Report No. 440/4–79–029a, Versar, Springfield, Virginia.

Canton, J.H., Greve, P.A., Sloof, W., van Esch, G.J. (1975) Toxicity accumulation and elimination studies of alpha-hexacyclohexane (alpha-HCH) with fresh water organisms of different trophic levels. *Water Res.* 9, 1163–1169.

Capel, P.D., Larson, S.J. (1995) A chemodynamic approach for estimating losses of target organic chemicals from water during sample holding time. *Chemosphere* 30, 1097–1107.

Carlberg, G.E., Martinsen, K., Kringstad, A., Gjessing, E., Grande, M., Källqvist, T., Skåre, J.U. (1986) Influence of aquatic humus on the bioavailability of chlorinated micropollutants in Atlantic salmon. *Arch. Environ. Contam. Toxicol.* 15, 543–548.

Carlo, C.P., Ashdown, D., Heller, V.G. (1952) The persistence of parathion, toxaphene and methoxychlor in soil. *Okla. Agric. Exp. Stn. Tech. Bull.* No. T-42, 3–11.

Caro, J.H., Taylor, A.W., Freeman, H.P. (1976) Comparative behaviour of dieldrin and carbofuran in the field. *Arch. Environ. Contam. Toxicol.* 3, 437–447.

Caron, G., Suffet, I.H., Belton, T. (1985) Effect of dissolved organic carbon on the environmental distribution of nonpolar organic compounds. *Chemosphere* 14, 993–1000.

Carringer, R.D., Weber, J.B., Monaco, T.J. (1975) Adsorption-desorption of selected pesticides by organic matter and Montmorillonite. *J. Agric. Food Chem.* 23(3), 568–572.

Carsel, R.F. (1989) Hydrologic processes affecting the movement of organic chemicals in soils. In: *Reactions and Movement of Organic Chemicals in Soils*. SSSA Special Publication No. 22, Sawhney, B.L., Brown, K., Editors, pp. 439–445, Soil Science Society of America and Society of Agronomy, Madison, Wisconsin.

Carswell, T,G., Nason, H.K. (1938) Properties and uses of pentachlorophenol. *Ind. Eng. Chem.* 30, 622–626.

Casida, J.E., Gatterdam, P.E., Getzin, Jr., L.W., Chapman, R.K. (1956) Residual properties of the systemic insecticide O,O-dimethyl 1-carbomethoxy-1-propen-2-yl phosphate. *J. Agric. Food Chem.* 4(3), 236–243.

Castro, T.F., Yoshida, T. (1971) Degradation of organochlorine insecticides in flooded soils in the Philippines. *J. Agric. Food Chem.* 19, 1168–1170.

Cessna, A.J., Grover, R. (1978) Spectrophotometric determination of dissociation constants of selected acidic herbicides. *J. Agric. Food Chem.* 26, 289–292.

Chapman, P.M. (1989) Review of current approaches to developing sediment quality criteria. *Environ. Toxicol. Chem.* 8, 589–599.

Chapman, R.A., Cole, C.M. (1982) Observations on the influence of water and soil pH on the persistence of insecticides. *J. Environ. Sci. Health* B17, 487–504.

Chen, F., Holten-Andersen, J., Tyle, H. (1993) New developments of the UNIFAC model for environmental application. *Chemosphere* 26, 1325–1354.

Chessells, M., Hawker, D.W., Connell, D.W. (1992) Influence of solubility on bioconcentration of hydrophobic compounds. *Ecotoxicol. Environ. Saf.* 23, 260–273.

Cheung, B. (1984) Environmental modelling studies of hazardous substances in Ontario. M.A. Sc. Thesis, University of Toronto, Toronto, Canada.

Chigareva, O.I. (1973) Metaphos distribution in fish organs and tissues. *Tr., Vses. Nauchno-Issled. Inst. Vet. Sanit.* 46, 102.

Chin, Y.P., Weber, Jr., W.J., Chiou, C.T. (1991) Chapter 14, A thermodynamic partition model for binding of nonpolar organic compounds by organic colloids and implications for their sorption to soils and sediments. In: *Organic Substances and Sediments in Water.* Vol. 1. Baker, R.A., Editor, pp. 251–273, Lewis Publishers, Inc., Chelsea, Michigan.

Chin, Y.P., Weber, Jr., W.J., Voice, T.C. (1986) Determination of partition coefficients and aqueous solubilities by reverse phase chromatography-II. *Water Res.* 20(11), 1443–1450.

Chiou, C.T. (1981) Partition coefficient and water solubility in environmental chemistry. In: *Hazard Assessment of Chemicals. Current Development.* Vol. 1, Saxena, J., Fisher, F., Eds, pp. 117–153, Academic Press, N.Y.

Chiou, C.T. (1985) Partition coefficients of organic compounds in lipid-water systems and correlations with fish concentration factors. *Environ. Sci. Technol.* 19, 57–62.

Chiou, C.T., Freed, V.H. (1977) *Chemodynamic Studies on Bench Mark Industrial Chemicals.* NSF/RA-770286 prepared for Research Applied to National Needs, National Science Foundation, Washington DC.

Chiou, C.T., Freed, V.H., Schmedding, D.W., Kohnert, R. (1977) Partition coefficient and bioaccumulation of selected organic chemicals. *Environ. Sci. Technol.* 11(5), 475–478.

Chiou, C.T., Freed, V.H., Peters, L.J., Kohnert, R.L. (1980) Evaporation of solutes from water. *Environ. Internat.* 3, 231–236.

Chiou, C.T., Kile, D.E., Brinton, T.I., Malcolm, R.L., Leenheer, J.A., MacCarthy, P. (1987) A comparison of water solubility enhancements of organic solutes by aquatic humic materials and commercial humic acids. *Environ. Sci. Technol.* 21, 1231.

Chiou, C.T., Kile, D.E., Rutherford, D.W. (1991) The natural oil in commercial linear alkylbenzenesulfonate and its effect on organic solute solubility in water. *Environ. Sci. Technol.* 25, 660–665.

Chiou, C.T., Malcolm, R.L., Brinton, T.I., Kile, D.E. (1986) Water solubility enhancement of some organic pollutants and pesticides by dissolved humic and fulvic acids. *Environ. Sci. Technol.* 20, 502–508.

Chiou, C.T., Peters, L.J., Freed, V.H. (1979) A physical concept of soil-water equilibria for nonionic organic compounds. *Science* 206, 831–832.

Chiou, C T., Porter, P.E., Schmedding, D.W. (1983) Partition equilibria of nonionic organic compounds between soil organic matter and water. *Environ. Sci. Technol.* 17, 227–231.

Chiou, C.T., Schmedding, D.W. (1981) Measurement and interrelation of octanol-water partition coefficient and water solubility of organic chemicals. In: *Test Protocols for Environmental Fate and Movement of Toxicants. J. Assoc. Anal. Chem.*, Arlington, Virginia.

Chiou, C.T., Schmedding, D.W., Manes, M. (1982) Partitioning of organic compounds in octanol-water system. *Environ. Sci. Technol.* 16, 4–10.

Cho, H.-H., Park, J.-W., Liu, C.K. (2002) Effect of molecular structures on the solubility enhancement of hydrophobic organic compounds by environmental amphiphiles. *Environ. Toxicol. Chem.* 21, 999–1003.

Choi, W.-W., Chen, K.Y. (1976) Associations of chlorinated hydrocarbons with fine particles and humic substances in nearshore surficial sediments. *Environ. Sci. Technol.* 10(8), 782–786.

Claborn, H.W., Bowers, J.W., Wells, R.W., Redeleff, R.D., Nickerson, W.J. (1953) Meat contamination from pesticides. *Agric. Chem.* 8, 37–39, 119, 121.

Claborn, H.W., Redeleff, R.D., Bushland, R.C. (1953) *Pesticide Residue in Meat and Milk.* Agriculture Research Service, U.S. Dept. of Agriculture, Washington DC.

Clark, J.R., Goodman, L.R., Borthwick, P.W., Patrick, Jr., J.M., Cripe, G.M., Moody, P.M., Moore, J.C., Lores, E.M. (1989) Toxicity of pyrethroids to marine invertebrates and fish: A literature review and test results with sediment-sorbed chemicals. *Environ. Toxicol. Chem*. 8, 393–401.

CLOGP (1986) Medchem Project of Pomona College, Claremont, California.

Coats, J.R., O'Donnell-Jeffery, N.L. (1979) Toxicity of four synthetic pyrethroid insecticides to rainbow trout. *Bull. Environ. Contam. Toxicol.* 23, 250–258.

Comba, M.E., Nostrom, R.J., Macdonald, C.R., Kaiser, K.L.E. (1993) A Lake Ontario-Gulf of St. Lawrence dynamic mass budget for mirex. *Environ. Sci. Technol.* 27, 2198–2206.

Connell, D.W., Bowman, M., Hawker, D.W. (1988) Bioconcentration of chlorinated hydrocarbons from sediment by oligochaetes. *Ecotoxicol. Environ. Saf.* 16, 293–302.

Connell, D.W., Hawker, D.W. (1986) Bioconcentration of lipophilic compounds by some aquatic organisms. *Ecotoxicol. Environ. Saf.* 11, 184–197.

Connell, D.W., Markwell, R.D. (1990) Bioaccumulation in the soil to earthworm system. *Chemosphere* 20(1–2), 91–100.

Conte, F.S., Parker, J.C. (1975) Effect of aerially-applied malathion on juvenile brown and white shrimp *Penaeus aztecus* and *Penaeus setiferus. Trans. Am. Fish Soc.* 104, 793–799.

Cook, R.F. (1973) Carbofuron. In: *Analytical Methods for Pesticides and Plant Growth Regulators*. Vol. 7, Zweig, G., Editor, pp. 187–210, Academic Press, New York.

Coppedge, J.R., Lindquist, D.A., Bull, D.L., Dorough, H.W. (1967) Fate of 2-methyl-2-(methylthio)propinaldehyde *O*-(methylcarbamoyl) oxime (Temik) in cotton plants and soil. *J. Agric. Food Chem.* 15(5), 902–910.

Corwin, D.L., Farmer, W.J. (1984) Non-single-valued adsorption-desorption of bromacil and diquat by freshwater sediments. *Environ. Sci. Technol.* 18, 507–514.

Cotham, W.E., Bidleman, T.F. (1989) Degradation of malathion, endosulfan and fenvalerate in seawater and seawater/sediment microcosms. *J. Agric. Food Chem.* 37, 824–828.

Cotham, W.E., Bidleman, T F. (1991) Estimating the deposition of organic contaminants to the Arctic. *Chemosphere* 22, 165–188.

Cotham, W.E., Bidleman, T.F. (1992) Laboratory investigations of the partitioning of organochlorine compounds between the gas phase and atmospheric aerosols on glass fiber filters. *Environ. Sci. Technol*. 26, 469–478.

Cowart, R.P., Bonner, F.L., Epps, Jr., E.A. (1971) Rate of hydrolysis of seven organophosphate pesticides. *Bull. Environ. Contam. Toxicol.* 6, 231–234.

Cox, J.L. (1970) Low ambient level uptake of ^{14}C-DDT by three species of marine phytoplankton. *Bull. Environ. Contam. Toxicol*. 5, 218.

Cripe, C.R., Walker, W.W., Pritchard, P.H., Bourquin, A.W. (1987) A shake-flask test for estimation of biodegradability of toxic organic substances in the aquatic environment. *Ecotox. Environ. Saf.* 14, 239–251.

Crosby, D.G., Tucker, R.K. (1971) Accumulation of DDT by *Daphnia magna. Environ. Sci. Technol.* 5, 714–716.

Crosby, T. (1981) Environmental chemistry of pentachlorophenol. *Pure Appl. Chem.* 53, 1051–1080.

Crossland, N.O., Wolff, C.J.M. (1985) Fate and biological effects of pentachlorophenol in outdoor ponds. *Environ. Toxicol. Chem.* 4, 73–86.

Dao, T.H., Lavy, T.L., Dragun, J. (1983) Rationale of the solvent selection for soil extraction of pesticide residues. *Res. Rev.* 87, 91–104.

David, W.A.L., Metcalf, R.L., Winton, M. (1960) The systematic insecticidal properties of certain carbamates. *J. Econ. Entmol.* 53, 1021–1025.

Davidson, J.M., Ou, L.T., Rao, P.S.C. (1980) Adsorption, movement, and biological degradation of high concentration of selected pesticides in soils. EPA-600-/2–80–124. U S EPA, Cincinnati, Ohio.

Davies, J.E., Lee, J.A. (1987) Changing profiles in human health effects of pesticides. *Pestic. Sci. Biotechnol.* 53.

Davies, R.P., Dobbs, A.J. (1984) The prediction of bioconcentration in fish. *Water Res.* 18(10), 1253–1262.

Dean, J., Editor (1985) *Lange's Handbook of Chemistry.* 13th Edition, McGraw-Hill, New York.

Dearth, M.A., Hites, R.A. (1991) Depuration rates of chlordane compounds from rat fat. *Environ. Sci. Technol*. 25(6), 1125–1128.

De Bruijn, J., Busser, F., Seinen, W., Hermens, J. (1989) Determination of octanol/water partition coefficients for hydrophobic organic chemicals with the "slow-stirring" method. *Environ. Toxicol. Chem.* 8, 499–512.

De Bruijn, J., Hermens, J. (1991) Uptake and elimination kinetics of organophosphorus pesticides in the guppy (*Poecilia reticulata*): Correlations with the octanol/water partition coefficient. *Environ. Toxicol. Chem.* 10, 791–804.

De Bruijn, J., Seinen, W., Hermens, J. (1993) Biotransformation of organophosphorus compounds by rainbow trout (*Oncorhynchus mykiss*) liver in relation to bioconcentration. *Environ. Toxicol. Chem.* 12, 1041–1050.

Decker, G.C., Weinman, C.J., Bann, J.M. (1950) A preliminary report on the rate of insecticide residue loss from treated plants. *J. Econ. Entomol.* 43, 919.

Delle Site, A. (2001) Factors affecting sorption of organic compounds in natural sorbent/water systems and sorption coefficients for selected pollutants. A review. *J. Phys. Chem. Ref. Data* 30, 187–439.

De Kock, A.C., Lord, D.A. (1987) A simple procedure for determining octanol-water partition coefficients using reverse phase high performance liquid chromatography (RPHPLC). *Chemosphere* 16(1), 133–142.

De Kreuk, J.F., Hanstveit, A O. (1981) Determination of the biodegradability of the organic fraction of chemical wastes. *Chemosphere* 10, 561–575.

De La Cruz, A.A., Rajanna, B. (1975) Mirex incorporation in the environment: Uptake and distribution in crop seedlings. *Bull. Environ. Contam. Toxicol*. 14, 38–42.

Delaune, R.D., Gambrell, R.P., Reddy, K.S. (1983) Fate of pentachlorophenol in estuarine sediment. *Environ. Pollut. Series* B6, 297–308.

Delorme, P.D., Muir, D.C.G., Lockhart, W.L., Mills, K.H., Ward, F.J. (1993) Depuration of toxaphene in lake trout and white suckers in a natural ecosystem following a single I.P. dose. *Chemosphere* 27(10), 1965–1973.

Demayo, A. (1972) Gas chromatographic determination of the rate constant for the hydrolysis of heptachlor. *Bull. Environ. Contam. Toxicol.* 8(4), 234–237.

Demozay, D., Marechal, G. (1972) Physical and chemical properties in lindane: Monograph of an insecticide, E. Ulman, pp. 15–21, K. Schiller, Freiburg im Breisgau.

Deneer, J.W. (1993) Uptake and elimination of chlorpyrifos in the guppy at sublethal and lethal aqueous concentrations. *Chemosphere* 26(9), 1607–1616.

Deneer, J.W. (1994) Bioconcentration of chlorpyrifos by the three-spined stickleback under laboratory and field conditions. *Chemosphere* 29(7), 1561–1575.

Deutsche Forschungsgemeinschaft (1983) *Hexachlorcyclohexan als Schadstoff in Lebensmitteln*. Verlag Chemie, Weinheim, Germany. 13p.

Devillers, J., Bintein, S., Domine, D. (1996) Comparison of BCF models based on log P. *Chemosphere* 33(6), 1047–1065.

Devillers, J., Thioulouse, J., Domine, D., Chastrette, M., Karcher, W. (1991) Multivariate analysis of the input and output data in the fugacity model level I. In: *Applied Multivariate Analysis in SAR and Environmental Studies.* Devillers, J., Karcher, W. Editors, Kluwer Academic Publishers, Dordrecht, The Netherlands.

Dickson, W. (1956) The vapour pressure of 1:1:p:p'-dichlorodiphenyl trichloroethane (D.D.T.). *Trans. Farad. Soc*. 52, 31–35.

Dierberg, F.E., Pfeuffer, R.J. (1983) Fate of ethion in canals draining a Florida citrus grove. *J. Agric. Food Chem*. 31, 704–709.

Dilling, W.L., Lickly, L.C., Lickly, T.D., Murphy, P.G., McKellar, R.L. (1984) Organic photochemistry. 19. Quantum yields for O,O-diethyl O-(3,5,6-trichloro-2-pyridinal) phosphorothioate and 3,5,6-trichloro-2-pyridinol in dilute aqueous solutions and their environmental transformation rates. *Environ. Sci. Technol*. 18, 540–543.

Di Toro, D.M. (1985) A particle interaction model of reversible organic chemical sorption. *Chemosphere* 14, 1503–1538.

Dobbs, A.J., Cull, M.R. (1982) Volatilization of chemicals-relative loss rates and the estimation of vapor pressures. *Environ. Pollut.* (series B) 3, 289–298.

Dobbs, A.J., Grant, C. (1980) Pesticide volatilisation rates—A new measure of the vapour pressure of pentachlorophenol at room temperature. *Pest. Sci.* 11, 29–32.

Doedens, J.D., Editor (1967) *Lange's Handbook of Chemistry.* McGraw-Hill, New York.

Domsch, K H. (1984) Effects of pesticides and heavy metals on biological processes in soil. *Plant Soil* 76, 367–378.

Donovan, S.F. (1996) New method for estimating vapor pressure by the use of gas chromatography. *J. Chromatogr. A*, 749, 123–129.

Donovan, S.F., Pescatore, M.C. (2002) Method for measuring the logarithm of the octanol-water partition coefficient by using short octadecyl-poly-poly(vinyl alcohol) high-performance liquid chromatography columns. *J. Chromatog*. A, 952, 47–61.

Dörfler, U., Adler-Köhler, R., Schneider, P., Scheunert, I., Korte, F. (1991) A laboratory model system for determining the volatility of pesticides from soil and plant surfaces. *Chemosphere* 23, 485–496.

Dorough, H.W., Hemken, R.W. (1973) Chlordane residues in milk and fat of cows fed HCS 3260 (High Purity Chlordane) in the diet. *Bull. Environ. Contam. Toxicol*. 10, 208–216.

Dorough, H.W., Ivie, G.W. (1974) Fate of mirex-carbon-14 during and after a 28-day feeding period to a lactating cow. *J. Environ. Qual.* 3(1), 65–67.

Dorough, H.W., Huhtanen, K., Marshall, T.C., Bryant, H.E. (1978) Fate of endosulfan in rats and toxicological conditions of apolar metabolites. *Pest. Biochem. Physio*. 8, 241–252.

Dorough, H.W., Pass, B.C. (1973) Residues in corn and soils treated with technical chlordane and high-purity chlordane (HS3260). *J. Econ. Entomol.* 65, 976–979.

Dowd, J.F., Bush, P.B., Neary, D.G., Taylor, J.W., Berisford, Y.C. (1993) Modeling pesticide movement in forested watersheds: Use of PRSM for evaluating pesticide options in loblolly pine stand management. *Environ. Toxicol. Chem.* 12, 429–439.

Drahonovsky, J., Vacek, Z. (1971) Dissoziations konstanten und austauscherchromatographie chlorieter phenole. *Coll. Czech. Chem. Commun.* 36(10), 3431–3440.

Drabel, J., Bachmann, F. (1983) Proinsecticides: structure-activity relationships in carbamoylsulfenyl N-methylcarbamates. In: *Synthesis and Structure-Activity Relationships*. Doyle, P., Fujita, T., Eds., pp. 271–277, Pergamon Press, Oxford, England.

Eadie, B.J., Robbins, J.A. (1987) 11. The role of particulate matter in the movement of contaminants in the Great Lakes. In: *Sources and Fates of Aquatic Pollutants*. Hites, R.A., Eisenreich, S.J., Editors, pp. 318–364, Advances Chemistry Series 216, American Chemical Society, Washington DC.

Eadsforth, C.V. (1986) Application of reverse-phase HPLC for determination of partition coefficients. *Pest. Sci.* 17, 311–325.

Eadsforth, C.V., Moser, P. (1983) Assessment of reverse phase chromatographic methods for determining partition coefficients. *Chemosphere* 12, 1459–1475.

Edwards, C.A. (1973) *Persistence Pesticides in the Environment.* 2nd edition, CRC Press, Cleveland, Ohio.

Eichelberger, J.W., Lichtenberg, J.J. (1971) Persistence of pesticides in river water. *Environ. Sci. Technol.* 5, 541–544.

Eichler, W., Editor (1965) *Hanbuch der Insectizidkunde.* Veb. Verlag Volk. Gesundheit, Berlin.

Elgar, K.E. (1983) Pesticides residues in water - an appraisal. In: *Pesticide Chemistry: Human Welfare and The Environment.* Vol. 4, Miyamoto, J., Kearney, P.C., Editors, International Union of Pure and Applied Chemistry, Pergamon Press, Oxford, England.

Ellgehausen, H., D'Hondt, C., Fuerer, R. (1981) Reversed-phase chromatography as a general method for determining octanol/water partition coefficients. *Pest. Sci.* 12, 219–227.

Ellgehausen, H., Guth, J.A., Esser, H.O. (1980) Factors determining bioaccumulation potential of pesticides in the individual compartments of aquatic food chains. *Ecotoxicol. Environ. Saf.* 4, 134–157.

Ellington, J.J. (1989) Hydrolysis Rate Constants for Enhancing Property-Reactivity Relationships. EPA/600/3-89/063. NTIS PB89-220479. US EPA, Environmental Research Laboratory, Athens, Georgia.

Ellington, J.J., Stancil, F.E., Payne, W.D. (1986) Measurement of Hydrolysis Rate Constants for Evaluation of Hazardous Waste Land Disposal. Volume 1, Data on 32 chemicals. U.S. EPA-600/3-86/043, Washington DC.

Ellington, J.J., Stancil, F.E., Payne, W.D. (1987) Measurement of Hydrolysis Rate Constants for Evaluation of Hazardous Waste Land Disposal. Vol. 2, Data on 54 chemicals. US EPA-600/53-87/019, Washington DC.

Ellington, J.J. et al. (1988) Measurement of Hydrolysis Rate Constants for Evaluation of Hazardous Waste Land Disposal. Volume 3. U.S. EPA 600/3-88/028, Washington DC.

Elzerman, A.W., Coates, J.T. (1987) 10. Hydrophobic organic compounds on sediments: Equilibria and kinetics of sorption. In: *Sources and Fates of Aquatic Pollutants*. Hites, R.A., Eisenreich, S.J., Editors, pp. 263–317, Advances Chemistry Series 216, American Chemical Society, Washington D.C.

Ernst, W. (1977) Determination of the bioconcentration potential of a marine organisms—A steady state approach. *Chemosphere* 6, 731–740.

Evans, M.S., Noguchi, G.E., Rice, C.P. (1991) The biomagnification of polychlorinated biphenyls, toxaphene, and DDT compounds in a Lake Michigan offshore food web. *Arch. Environ. Contam. Toxicol.* 20, 87–93.

Eye, J.D. (1968) Aqueous transport of dieldrin residues in soils. *J. Water Pollut. Control Fed.* 40, R316-R332.

Farquharson, M.E., Gage, J.C., Northover, J. (1958) The biological action of chlorophenols. *Brit. J. Pharmacol.* 13, 20.

Faust, B.C., Hoigné, J. (1990) Photolysis of Fe (III)-hydroxy complexes as sources of OH radicals in clouds, fog and rain. *Atmos. Environ.* 24A, 79–89.

Faust, S.D., Gomaa, H.M. (1972) Chemical hydrolysis of some organic phosphorous and carbamate pesticides in aquatic environments. *Environ. Lett.* 3, 171–201.

Feigenbrugel, V., Le Calvé, S., Mirabel, P. (2004) Temperature dependence of Henry's law constants of metolachlor and diazinon. *Chemosphere* 57, 319–327.

Felsot, A., Dahm, P.A. (1979) Sorption of organophosphorous and carbamate insecticides by soil. *J. Agric. Food Chem.* 27, 557–563.

Felsot, A., Wilson, J. (1980) Adsorption of carbofuran and movement on soil thin layers. *Bull. Environ. Contam. Toxicol.* 24, 778–782.

Ferreira, G.A., Seiber, J.N. (1981) Volatilization and exudation losses of three N-methyl-carbamate insecticides applied systemically to rice. *J. Agric. Food Chem.* 29, 93–99.

Fendinger, N.J., Glotfelty, D.E. (1988) A laboratory method for the experimental determination of air/water Henry's law constants for several pesticides. *Environ. Sci. Technol.* 22, 1289–1293.

Fendinger, N.J., Glotfelty, D.E. (1990) Henry's law constants for selected pesticides, PAHs and PCBs. *Environ. Toxicol. Chem.* 9, 731–735.

Fendinger, N.J., Glotfelty, D.E., Freeman, H.P. (1989) Comparison of two experimental techniques for determining air/water Henry's law constants. *Environ. Sci. Technol.* 23(12), 1528–1531.

Finizio, A., Vighi, M., Sandroni, D. (1997) Determination of *n*-octanol/water partition coefficient (K_{OW}) of pesticide, critical review and comparison of methods. *Chemosphere* 34, 131–161.

Firestone, D. (1977) Chemistry and analysis of pentachlorophenol and its contaminants. Division of Chemistry and Physics, Bureau of Foods. FDA By-Lines No. 2, September, 1977.

Fisher, D.J., Clark, J.R. (1990) Bioaccumulation of kepone by grass shrimp (*Palaemonetes pugio*): importance of dietary accumulation and food ration. *Aqua. Toxicol*. 17, 167–186.

Fisher, D.J., Clark, J.E., Roberts, Jr., M.H., Connolly, J.P., Mueller, L.H. (1986) Bioaccumulation of kepone by spot (*Leiostomus xanthurus*): importance of dietary accumulation and ingestion rate. *Aqua. Toxicol*. 9, 161–178.

Fischer, R.C., Krämer, W., Ballschmiter, K. (1991) Hexachlorocyclohexane isomers as markers in the water flow of Atlantic Ocean. *Chemosphere* 23, 889–900.

Fisher, S.W., Lydy, M.J., Barger, J., Landrum, P.F. (1993) Quantitative structure-activity relationships for predicting the toxicity of pesticides in aquatic systems with sediment. *Environ. Toxicol. Chem*. 12, 1307–1318.

Fisk, A.T., Bosenberg, B., Cymbalisty, C.D., Stern, G.A., Muir, D.C.G. (1999) Octanol/water partition coefficients of toxaphene congeners determined by the "slow-stirring" method. *Chemophere* 39, 2549–2562.

Fisk, A.T., Norstrom, R.J., Cymbalisty, C.D., Muir, D.C.G. (1998) Dietary accumulation and depuration of hydrophobic organochlorines: bioaccumulation parameters and their relationship with the octanol/water partition coefficient. *Environ. Toxicol. Chem*. 17, 951–961.

Fogel, S., Lancione, R., Sewall, A., Boethling, R.S. (1982) Enhanced biodegradation of methoxychlor in soil under enhanced environmental conditions. *Appl. Environ. Microbiol.* 44, 113–120.

Fordham, C.L., Reagan, D.P. (1991) Pathways analysis method for estimating water and sediment criteria at hazardous waster sites. *Environ. Toxicol. Chem.* 10, 949–960.

Foreman, W.T., Bidleman, T.F. (1987) An experimental system for investigating vapor-particle partitioning of trace organic pollutants. *Environ. Sci. Technol.* 21, 869–875.

Frank, R. (1981) Pesticides and PCB in the Grand and Saugeen River Basins. *J. Great Lakes Res.* 7, 440–454.

Fraser, A.J., Burkow, I.C., Wolkers, Mackay, D. (2002) Modeling biomagnification and metabolism of contaminants in harp seals of the Barents Sea. *Environ. Toxicol. Chem.* 21, 55–61.

Freed, V.H. (1976) Solubility, hydrolysis, dissolution constants and other constants of benchmark pesticides. In: *A Literature Survey of Benchmark Pesticides.* George Washington University Medical Center, Washington, DC.

Freed, V.H., Chiou, C.T., Haque, R. (1977) Chemodynamics: Transport and behavior of chemicals in the environment - A problem in environmental health. *Environ. Health Perspect.* 20, 55–70.

Freed, V.H., Chiou, C.T., Schmedding, D.W. (1979) Degradation of selected organophosphorous pesticides in water and soil. *J. Agric. Food Chem.* 27, 706–708.

Freed, V.H., Kaufman, D.D., Metcalf, R.L., Farmer, W.J., Crosby, D.G., Spencer, W. (1976) Chemodynamics: Transport and Behavior of Chemicals in the Environment - A Problem in Environmental Health. George Washington University Medical Center, Washington, D.C.

Freed, V.H., Schmedding, D.W., Kohnert, R., Haque, R. (1979) Physical chemical properties of several organophosphates: Some implications in environmental and biological behavior. *Pest. Biochem. Physiol.* 10, 203–211.

Freeman, H.P., Taylor, A.W., Edwards, W.M. (1975) Heptachlor and dieldren disappearance from a field soil measured by annual residue determinations. *J. Agric. Food Chem.* 23, 1101–1105.

Freitag, D., Geyer, H., Kraus, A., Viswanathan, R., Kozias, D., Attar, A., Klein, W., Korte, F. (1982) Ecotoxicological profile analysis. VII. Screening chemicals for their environmental behavior by comparative evaluation. *Ecotox. Environ. Saf.* 6, 60–81.

Freitag, D., Balhorn, L., Geyer, H., Körte, F. (1985) Environmental hazard profile of organic chemicals. An experimental method for the assessment of the behaviour of chemicals in the ecosphere by simple laboratory tests with C-14 labelled chemicals. *Chemosphere* 14, 1589–1616.

Freitag, D., Lay, J.P., Körte, F. (1984) Environmental hazard profile—Test results as related to structures and translation into the environment. In: *QSAR in Environmental Toxicology.* Kaiser, K.L.E., Editor, pp. 111–136, D. Reidel Publishing Co., Dordrecht, The Netherlands.

Fries, G.F., Marrow, G.S., Gordon, C.H. (1969) Comparative excretion and retention of DDT analogs by dairy cows. *J. Dairy Sci.* 52, 1801–1805.

Fröbe, Z., Drevenkar, V., Štengl, B. (1989) Sorption behaviour of some organophosphorus pesticides in natural sediments. *Toxicol. Environ. Chem.* 19, 69–82.

Fujita, T., Iwasa, J., Hansch, C. (1964) A new substituent constant 'pi' derived from partition coefficients. *J. Am. Chem. Soc.* 86, 5175–5180.

Fujita, T., Kamoshita, K., Nishioka, T., Nakajima, M. (1974) Physicochemical parameters for structure-activity studies of substituted phenyl N-methyl-carbamates. *Agric. Biol. Chem.* 38, 1521–1528.

Fuhremann, T.W., Lichtenstein, E.P. (1980) A comparative study of the persistence, movement, and metabolism of six carbon-14 insecticides in soils and plants. *J. Agric. Food Chem.* 28, 446–452.

Fung, K.K.H., Uren, N.C. (1977) Microbial transformation of *S*-methyl *N*-[(methyl-carbamoyl)oxy]thioacitimidate. *J. Agric. Food Chem.* 25, 966–969.

Garst, J.E. (1984) Accurate, wide range, automated, high performance liquid chromatographic method for the estimation of octanol/water partition coefficients. II: Equilibration in partition coefficient measurements, additivity of substituent-constants and correlation of biological data. *J. Pharm. Sci.* 73(11), 1623–1629.

Garst, J.E., Wilson, W.C. (1984) Accurate, wide-range, automated, high-performance liquid chromatographic method for the estimation of octanol/water partition coefficients. I: Effect of chromatographic conditions and procedure variables on accuracy and reproducibility of the method. *J. Pharm. Sci.* 73(11), 1616–1623.

Garten, Jr., C.T., Trabalka, J.R. (1983) Evaluation of models for predicting terrestrial food chain behavior of xenobiotics. *Environ. Sci. Technol.* 17, 590–595.

Gautier, C., Le Calvé, S., Miabel, P. (2003) Henry's law constants measurements of alachlor and dichlorvos between 283 and 298 K. *Atmos. Environ.* 37, 2437–2453.

Gawlik,. B.M., Feicht, E.A., Karcher, W., Kettup, A., Mujntau, H. (1998) Application of the European reference soil set (EUROSOILS) to a HPLC-screening method for the estimation of soil adsorption coefficients of organic compounds. *Chemosphere* 36, 2903–2919.

Gawlik, B.M., Bo, F., Kettrup, A., Muntau, H. (1999a) Characterisation of a second generation of European reference soils for sorption studies in the framework of chemical testing - Part I: chemical composition and pedological properties. *Sci. Total Environ.* 229, 99–107.

Gawlik, B.M., Kettrup, A., Muntau, H. (1999b) Characterisation of a second generation of European reference soils for sorption studies in the framework of chemical testing - Part II: soil adsorption behaviour of organic chemicals. *Sci. Total Environ.* 229, 109–120.

Gawlik, B.M., Kettrup, A., Muntau, H. (2000) Estimation of soil adsorption coefficients of organic compounds by HPLC screening using the second generation of the European reference soil set. *Chemosphere* 41,7–1347.

Gebefügi, I., Parlar, H., Körte, F. (1979) Occurrence of pentachlorophenol in enclosed environments. *Ecotox. Environ. Saf.* 3, 269–300.

GEMS (1986) Graphical Exposure Modeling Systems. Fate of Atmosphere Pollutants (FAP). Office of Toxic Substances, U.S. EPA, Washington, D.C.

Gerstl, Z. (1984) Adsorption, decomposition and movement of oxamyl in soil. *Pestic. Sci.* 15, 9–17.

Gerstl., Z. (1990) Estimation of organic chemical sorption by soils. *J. Contam. Hydrology* 6, 357–375.

Gerstl, Z., Helling, C.S. (1987) Evaluation of molecular connectivity as a predictive method for the adsorption of pesticides by soils. *J. Environ. Sci. Health* B22, 55–69.

Gerstl, Z., Mingelgrin, U. (1984) Sorption of organic substances by soils and sediments. *J. Environ. Sci. Health* B19(3), 297–312.

Getzin, L.W. (1981a) Degradation of chlorpyrifos in soil: Influence of autoclaving, soil moisture, and temperature. *J. Econ. Entomol.* 74, 158–162.

Getzin, L.W. (1981b) Dissipation of chlorpyrifos from dry soil surfaces. *J. Econ. Entomol.* 74(6), 707–713.

Geyer, H., Kraus, A.G., Klein, W., Richter, E., Körte, F. (1980) Relationship between water solubility and bioaccumulation potential of organic chemicals in rats. *Chemosphere* 9, 277–291.

Geyer, H., Politzki, G., Freitag, D. (1984) Prediction of ecotoxicological behaviour of chemicals: Relationship between *n*-octanol/water partition coefficient and bioaccumulation of organic chemicals by alga *Chlorella. Chemosphere* 13, 269–284.

Geyer, H.J., Rimkus, G.G., Scheunert, I., Kaune, A., Schramm, K.-W., Kettrup, A., Zeeman, M., Muir, D.C.G., Hansen, L.G., Mackay, D. (2000) Bioaccumulation and occurrence of endocrine-disrupting chemicals (EDCs), persistent organic pollutants (POPs), and other organic compounds in fish and orther organisms including humans. In: *The Handbook of Environmental Chemistry, Vol. 2, Part J Bioaccumulation*. Beek, B., Ed., pp. 1–166, Springer-Verlag, Berlin Heidelberg.

Geyer, H., Scheunert, I., Brüggemann, R., Langer, D., Körte, F., Kettrup, A., Mansour, M., Steinberg, C.E.W., Nyholm, N., Muir, D.C.G. (1997) Half-lives and bioconcentration of lindane (γ-HCH) in different fish species and relationship with their lipid content. *Chemosphere* 35, 343–351.

Geyer, H., Scheunert, I., Brüggemann, R., Steinberg, C., Körte, F., Kettrup, A. (1991) QSAR for organic chemical bioconcentration in daphnia, algae, and mussels. *Sci. Total Environ.* 109/110, 387–394.

Geyer, H., Scheunert, I., Körte, F. (1987) Correlation between the bioconcentration potential of organic environmental chemicals in humans and their *n*-octanol/water partition coefficients. *Chemosphere* 16, 239–252.

Geyer, H., Sheehan, P., Kotzias, D., Freitag, D., Korte, F. (1982) Prediction of ecotoxicological behaviour of chemicals: Relationship between physico-chemical properties and bioaccumulation of organic chemicals in the mussel *Mytilus edulis. Chemosphere* 11, 1121–1134.

Geyer, H., Viswanathan, R., Freitag, D., Korte, F. (1981) Relationship between water solubility of organic chemicals and their bioaccumulation by *alga* Chlorella. *Chemosphere* 10, 1307–1313.

Giustini, A., Brunetti, B., Piacente, V. (1998) A sublimation study of lindane. *J. Chem. Eng. Data* 43, 447–450.

Gish, C.D., Hughes, D.L. (1982) Residues of DDT, dieldrin and heptachlor in earthworms during two years following application. *U.S. Fish Wildlife Serv. Spec. Sci. Rep.*: Wildlife. 241.

Given, C.J., Dierberg, F.E. (1985) Effect of pH on the rate of aldicarb hydrolysis. *Bull. Environ. Cantam. Toxicol*. 34, 627–633.

Glassmeyer, S.L., de Vault, D., Hites, R. (2000) Rates at which toxaphene concentration decrease in lake trout form the Great Lakes. *Environ. Sci. Technol*. 34, 1851–1856.

Glooschenko, V. et al. (1979) Bioconcentration of chlordane by the green alga *Senedesmus quadricauda*. *Bull. Environ. Contam. Toxicol.* 21, 515–520.

Glotfelty, D.E. (1981) Atmospheric dispersion of pesticides from treated fields. Ph.D. Thesis, pp. 94–187, University of Maryland, College Park, Maryland.

Glotfelty, D.E., Taylor, A.W., Turner, B.C., Zoller, W.H. (1984) Volatilization of surface-applied pesticides from fallow soils. *J. Agric. Food Chem.* 32, 638–643.

Glotfelty, D E., Leech, M.M., Jersey, J., Taylor, A.W. (1989) Volatilization and wind erosion of soil surface applied atrazine, simazine, alachlor, and toxaphene. *J. Agric. Food Chem*. 37, 546–551.

Glotfelty, D.E., Schomburg, C.J., McChesney, M.M., Sagebiel, J.C., Seiber, J.N. (1990) Studies of the distribution, drift, and volatilization of diazinon resulting from spray application to a dormant peach orchard. *Chemosphere* 21(10–11), 1303–1314.

Gobas, F.A.P.C., Clark, K.E., Shiu, W.Y., Mackay, D. (1989) Bioconcentration of polybrominated benzenes and biphenyls and related superhydrophobic chemicals in fish: Role of bioavailability and elimination into the feces. *Environ. Toxicol. Chem*. 8, 231–245.

Goerlitz, D.F., Troutman, D.E., Godsy, E.M., Franks, B.J. (1985) Migration of wood-preserving chemicals in contaminated ground water in sand aquifer at Pensacola, Florida. *Environ. Sci. Technol.* 19, 955–961.

Goll, O. (1954) Chlorophenol. In: *Ullmans Encyklopädie der Technischen Cheme.* Foerst, W., Ed., pp. 494–499, Urban and Schwarzenberg, Munich/Berlin.

Gomaa, H.M., Suffert, I.H., Faust, S.D. (1969) Kinetics of hydrolysis of diazinon. *Residue Rev.* 29, 171.

Gomaa, H.M., Faust, S.D. (1972) Chemical hydrolysis and oxidation of parathion and paraoxon in aquatic environments. In: *Fate of Organic Pesticides in the Aquatic Environment*. pp. 189–209. Advances Chem. Ser. III. Washington, D.C.

Goodman, M.A. (1997) Vapor pressure of agrochemicals by the Knudsen effusion method using a quartz crystal microbalance. *J. Chem. Eng. Data* 42, 1227–1231.

Görge, G., Nagel, R. (1990) Kinetics and metabolism of 14-C-lindane and 14-C-atrazine in early life stages of zebrafish (*Brachdanio rerio). Chemosphere* 21, 1125–1137.

Grain, C.F. (1982) Chapter 14, Vapor pressure. In: *Handbook on Chemical Property Estimation Methods, Environmental Behavior of Organic Compounds.* Lyman, W.J., Reehl, W.F., Rosenblatt, D.H., Editors, McGraw-Hill, Inc., New York.

Gramatica, P., Corradi, M., Consonni, V (2000) Modelling and prediction of soil sorption coefficients of non-ionic organic pesticides by molecular descriptors. *Chemosphere* 41, 762–777.

Graebing, P., Chib, J.S. (2004) Soil photolysis in a moisture- and temperature-controlled environment. 2. Insecticides. *J. Agric. Food Chem.* 52, 2606–2614.

Grayson, B.T., Fosbracey, L.A. (1982) Determination of the vapor pressure of pesticides. *Pest. Sci.* 13, 269–278.

Grayson, B.T., Langner, E., Wells, D. (1982) Comparison of two gas saturation methods for the determination of the vapor pressure of cypermethrin. *Pest. Sci.* 13, 552–556.

Green, G.H., McKeown, B.A., Oloffs, P.C. (1984) Acephate in rainbow trout (*Salmo gairdneri*); Acute toxicity, uptake, elimination. *J. Environ. Sci. Health* B19, 131–155.

Greenhalgh, R., Dhawan, K., Weinberger, P. (1980) *J. Agric. Food Chem.* 28, 102–105.

Grover, R. (1975) Adsorption and desorption of urea herbicides on soils. *Can. J. Soil. Sci.* 55, 127–135.

Gückel, W., Kästel, R., Lewerenz, J., Synnatschke, G. (1982) A method for determining the volatility of active ingredients used in plant protection. Part III. The temperature relationship between vapor pressure and evaporation rate. *Pest. Sci.* 13, 161–168.

Gückel, W., Synnatsche, G., Rittig, R. (1973) A method for determining the volatility of active ingredients used in plant protection. *Pest. Sci.* 4, 137–147.

Gückel, W., Rittig, R., Synnatsche, G. (1974) A method for determining the volatility of active ingredients used in plant protection. II. Application to formulated products. *Pest. Sci.* 5, 393–400.

Güesten, H., Filby, W.G., Schoop, S. (1981) Prediction of hydroxyl radical reaction rates with organic compounds in the gas-phase. *Atom. Environ.* 15, 1763–1765.

Guinee, J., Heijungs, R. (1993) A proposal for the classification of toxic substances within the framework of life cycle assessment of products. *Chemosphere* 26(1), 1925–1944.

Guirguis, M.W., Shafik, M.T. (1975) Persistence of trichlorfon and dichlorvos in two different autoclaved and non-autoclaved soils. *Bull. Entomol. Soc. Egypt Econ. Ser.* 8, 29–32.

Gummer, W.D. (1979) Pesticide monitoring in the prairies of western Canada. In: Water Quality Interpretive Report No. 4., Inland Waters Directorate, Regina, Saskatchewan, Canada.

Günther, F.A., Günther, J.D. (1971) Residue of pesticides and other foreign chemicals in foods and feeds. *Res. Rev.* 36, 69–77.

Günther, F.A., Westlake, W.E., Jaglan, P.S. (1968) Reported solubilities of 738 pesticide chemicals in water. *Res. Rev.* 20, 1–148.

Haag, W.R., Yao, C.C.D. (1992) Rate constants for the reaction of hydroxyl radicals with several drinking water contaminants. *Environ. Sci. Technol.* 26, 1005–1013.

Hadaway, A.B., Barlow, F., Turner, C.R. (1970) The effect of particle size on the contact toxicity of insecticides to adult mosquitoes. *Bull. Entomol. Res.* 60, 17.

Halfon, E., Galassi, S., Brüggermann, R., Provini, A. (1996) Selection of priority properties to assess environmental hazard of pesticides. *Chemosphere* 33(8), 1543–1562.

Hall, R.J., Kolbe, E. (1980) Bioconcentration of organophosphorous pesticides to hazardous levels by amphibians. *J. Toxicol. Environ. Health* 6, 853–868.

Hamaker, J.W. (1972) Decomposition: Quantitative aspects. In: *Organic Chemicals in the Soil Environment.* Vol. 1, Goring, C.A.I., Hamaker, J.W., Editors, pp. 253–341, Marcel Dekker, Inc., New York.

Hamaker, J.W. (1975) The interpretation of soil leaching experiments. In: *Environmental Dynamics of Pesticides.* Haque, R., Freed, V.H., Editors, pp. 115–133, Plenum Press, New York.

Hamaker, J.W., Thompson, J.M. (1972) Adsorption. In: *Organic Chemistry in the Soil Environment.* Vol. 1, Goring, C.A.I., Hamaker, J.W., Editors, pp. 51–145, Marcel Dekker, Inc., New York.

Hamelink, J.L., Waybrant, R.C. (1976) DDE and lindane in a large-scale model lentic ecosystem. *Trans. Am. Fish Soc.* 105, 124.

Hamilton, D.J. (1980) Gas chromatographic measurement of volatility of herbicide esters. *J. Chromatogr.* 195, 75–83.

Hammers, W.E., Meurs, G.J., De Ligny, C.L. (1982) Correlations between liquid chromatographic capacity ratio data on lichrosorb RP-18 and partition coefficients in the octanol-water system. *J. Chromatogr.* 247, 1–13.

Hansch, C., Leo, A. (1979) *Substituent Constants for Correlation Analysis in Chemistry and Biology.* John Wiley & Sons, New York.

Hansch, C., Leo, A. (1985) Medchem. Project Issue No. 26, Pomona College, Claremont, California.

Hansch, C., Leo, A. (1987) Log P Database, Pomona College Medicinal Chemistry Project. Claremont, CA.

Hansch, C., Leo, A., Hoekman, D. (1995) *Exploring QSAR, Hydrophobic, Electronic, and Steric Constants*. ACS Professional Reference Book, Am. Chem. Soc., Washington, DC.

Hansen, D.J., Wilson, A.J. (1970) Residues in fish, wildlife and estuaries. *Pest. Monit. J.* 4, 51.

Hansen, J L., Spiegel, M.H. (1983) Hydrolysis studies of aldicarb, aldicarb sulfoxide and aldicarb sulfone. *Environ. Toxicol. Chem.* 2, 147–153.

Haque, R., Ebing, W. (1988) Uptake and accumulation of pentachlorophenol and sodium pentachlorophenate by earth worms from water and soil. *Sci. Total Environ.* 68, 113–125.

Haque, R., Falco, J., Cohen, S., Riordan, C. (1980) 8. Role of transport and fate studies in the exposure, assessment and screening of toxic chemicals. In: *Dynamics, Exposure and Hazard Assessment of Toxic Chemicals.* Haque, R., Editor, pp. 47–67, Ann Arbor Science Publishers, Ann Arbor, Michigan.

Harner, T., Mackay, D. (1995) Measurement of octanol-air partition coefficients for chlorobenzenes, PCBs, and DDT. *Environ. Sci. Technol.* 29, 1599–1606.

Harnisch, M., Möckel, H.J., Schultze, G. (1983) Relationship between LOG P_{OW} shake-flask values and capacity factors derived from reversed-phase high-performance liquid chromatography for *n*-alkylbenzenes and some OECD reference substances. *J. Chromatogr.* 282, 315–332.

Harris, J.C. (1982) Chapter 7, Rate of hydrolysis and Chapter 8, Rate of aqueous photolysis. In: *Handbook on Chemical Property Estimation Methods, Environmental Behavior of Organic Compounds.* Lyman, W.J., Reehl, W.F., Rosenblatt, D.H., Editors, McGraw-Hill, New York.

Harris, S.J., Cecil, H.C., Bitman, J. (1974) Effect of several dietary levels of technical methoxychlor on reproduction in rats. *J. Agric. Food Chem.* 22(6), 969–973.

Hartley, D., Kidd, H., Editors (1987) *The Agrochemicals Handbook.* 2nd Edition, The Royal Society of Chemistry, Nottingham, England.

Hartley, D.M., Johnson, J.B. (1983) Use of freshwater clam *Corbicula manilensis* as a monitor for organochlorine pesticides. *Bull. Environ. Contam. Toxicol.* 31, 33–40.

Hartley, G.S., Graham-Bryce, I.J. (1980) *Physical Principles and Pesticide Behavior.* Volume 2, Academic Press, New York.

Harvey, J., Hun, J.C.Y. (1978) Decomposition of oxamyl in soil and water. *J. Agric. Food Chem.* 26, 536–451.

Harvey, J., Reiser, R.W. (1973) Metabolism of methomyl in tobacco, corn and cabbage. *J. Agric. Food Chem.* 21, 775–783.

Hattula, M.L., Wasenius, V.-M., Reunanen, H., Arstila, A.U. (1981) Acute toxicity of some chlorinated phenols, catechols and cresols in trout. *Bull. Environ. Contam. Toxicol.* 26, 295–298.

Hautala, R.P. (1978) Surfactant Effects on Pesticide Photochemistry in Water and Soil. EPA-600/3–78–060, U.S. EPA.

Hawker, D.W., Connell, D.W. (1986) Bioconcentration of lipophilic compounds by some aquatic organisms. *Ecotoxicol. Environ. Saf.* 11, 184–197.

Hawker, D.W., Connell, D.W. (1989) A simple water/octanol partition system for bioconcentration investigations. *Environ. Sci. Technol.* 23, 961–965.

Hazardous Substances Data Bank (1989) National Library of Medicine, Toxicology Information Program.

Heiber, O., Szelagiewicz, M. (1976) Research Report, Central Research Dept., Physical Chemistry Section, Ciba-Geigy Ltd.,.Basel. Reference in Y.H. Kim 1985.

Heller, S.R., Scott, K., Bigwood, D.W. (1989) The need for data evaluation of physical and chemical properties of pesticides: The ARS pesticide properties database. *J. Chem. Inf. Comput. Sci.* 29, 159–162.

Hellmann, H. (1987) Model tests on volatilization of organic trace substances in surface waters. *Frensenius Z. Anal. Chem.* 328, 475–479.

Hemond, H.F., Fechner, E.J. (1994) *Chemical Fate and Transport in the Environment.* Academic Press, New York.

Herbicide Handbook (1978) *Herbicide Handbook*. 4th Ed., Weed Science Society of America, Champaign, Illinois.

Herbicide Handbook (1983) *Herbicide Handbook*. 5th Ed., Weed Science Society of America, Champaign, Illinois.

Hermanutz, R.O. (1978) Endrin and malathion toxicity to flagfish (*Jordanella floridae). Arch. Environ. Contam. Toxicol.* 7, 159–168.

Hermens, J., Leeuwangh, P. (1982) Joint toxicity of mixture of 8 and 24 chemicals to the guppy (*Poecilia reticulata). Ecotoxicol. Environ. Saf.* 6, 302–310.

Hiatt, C.W., Haskins, W.T., Olivier, L. (1960) The action of sunlight on sodium pentachlorophenate. *Am. J. Trop. Med. Hyg.* 9, 527–531.

Hidaka, H., Nohara, K., Zhao, J., Serpone, N., Pelizzetti, E. (1992) Photo-oxidative degradation of the pesticide permethrin catalyzed by irradiated TiO_2 semiconductor slurries in aqueous media. *J. Photochem. Photobiol. A: Chem.* 64, 247–254.

Hill, D.W., McCarty, P.L. (1967) Anaerobic degradation of selected chlorinated hydrocarbon pesticides. *J. Water Pollut. Control Fed.* 39, 1259–1277.

Hill, J.C., Kolling, H.P., Paris, D.F., Wolfe, N.L., Zepp, R.G. (1976) Dynamic Behavior of Vinyl Chloride in Aquatic Ecosystems. U.S. EPA-600/3-76-001.

Hinckley, D.A., Bidleman, T.F., Foreman, W.T. (1990) Determination of vapor pressures for nonpolar and semipolar organic compounds from gas chromatographic retention data. *J. Chem. Eng. Data* 35, 232–237.

Hine, J., Mookerjee, P.K. (1975) The intrinsic hydrophilic character of organic compounds. Correlations in terms of structural contributions. *J. Org. Chem.* 40, 292–298.

Hinman, M.L., Klaine, S.J. (1992) Uptake and translocation of selected organic pesticides by the rooted aquatic plant *Hydrilla verticillata* royale. *Environ. Sci. Technol*. 26, 609–613.

Hodson, J., Williams, N.A. (1988) The estimation of the adsorption coefficient (K_{OC}) for soils by high performance liquid chromatography. *Chemosphere* 17, 67–77.

Hoigné, J., Bader, H. (1983) Rate constants of reactions of ozone with organic and inorganic compounds in water-I. Non-dissociating organic compounds. *Water Res.* 17, 173–183.

Hoigné, J., Bader, H. (1983) Rate constants of reactions of ozone with organic and inorganic compounds in water-II. Dissociating organic compounds. *Water Res.* 17, 185–194.

Hollifield, H.C. (1979) Rapid nephelometric estimate of water solubility of highly insoluble organic chemicals of environmental interests. *Bull. Environ. Contam. Toxicol.* 23, 579–586.

Hollister, T.A., Walsh, G.E., Forester, J. (1975) Mirex and marine unicellular algae: Accumulation, population growth, and oxygen evolution. *Bull. Environ. Contam. Toxicol.* 10, 753.

Holmstead, R.L., Casida, J.E., Luzo, L.O., Fullmer, D.G. (1978) Pyrethroid photo-decomposition: Permethrin. *J. Agric. Food Chem.* 26, 590–595.

Hornsby, A.G., Rao, P.S.C., Jones, R.L. (1990) Fate of aldicarb in the unsaturated zone beneath a citrus grove. *Water Resour. Res.* 26, 2287–2202.

Hornsby, A.G., Wauchope, R.D., Herner, A.E. (1996) *Pesticide Properties in the Environment.* Springer-Verlag, Inc., New York, New York.

Horvath, A.L. (1982) *Halogenated Hydrocarbons, Solubility-Miscibility with Water.* Marcel Dekker, Inc., New York, N.Y.

Horvath, A L., Editor (1991) *Halogenated Hydrocarbons. Solubility-Miscibility with Water.* Marcel Dekker, Inc., New York.

Howard, P.H., Editor (1991) *Handbook of Environmental Fate and Exposure Data for Organic Chemicals. Pesticides.* Vol. III. Lewis Publishers, Chelsea, Michigan.

Howard, P.H., Boethling, R.S., Jarvis, W.F., Meylan, W.M., Michalenko, E.M., Editors (1991) *Handbook of Environmental Degradation Rates.* Lewis Publishers, Chelsea, Michigan.

Howe, G.E., Marking, L.L., Bills, T D., Rach, J.J., Mayer, Jr., F.L. (1994) Effects of water temperature and pH on toxicity of terbufos, trichlorfon, 4-nitrophenol and 2,4-dinitrophenol to the amphipod *Gammarus pseudolimnaeus* and rainbow trout (*Oncorhynchus mykiss*). *Environ. Toxicol. Chem.* 13, 51–66.

Hu, J., Leng, X.-F. (1992) Determination of partition coefficients for some pesticides by using reversed-phase high performance liquid chromatography (HPLC). *Sepu* 10, 344–346.

Huang, J.-Y., Leng, X.-F. (1993) Interaction of rat hepatocyte and cytochrome P450 with pyrethroids in vitro. *Dongwu Xuebao* 39(4), 418–423.

Huckins, J.N., Stalling, D.L., Petty, J.D., Buckler, D.R., Johnson, B.T. (1982) Fate of kepone and mirex in the aquatic environment. *J. Agric. Food Chem.* 30, 1020–1027.

Hulzebos, E.M., Adema, D.M.M., van Breemen, D., Henzen, L., van Dis, W.A., Herbold, H.A., Hoekstra, J.A., Baerselman, R., van Gestel, C.A.M. (1993) Phototoxicity studies with *Lactuca sativa* in soil and nutrient solution. *Environ. Toxicol. Chem.* 12, 1079–1094.

Hussain, M., Fukuto, T.R., Reynolds, H.T. (1974) Physical and chemical basis for systemic movement of organo-phosphorus ester in the cotton plant. *J. Agric. Food Chem.* 22, 225–230.

Hwang, H.-M., Hodson, R.E., Lee, R F. (1986) Degradation of phenol and chlorophenols by sunlight and microbes in estuarine water. *Environ. Sci. Technol.* 20, 1002–1007.

Hwang, H.-M., Hodson, R.E., Lee, R.F. (1987) Photolysis of phenol and chlorophenols in estuarine water. In: *Photochemistry of Environmental Aquatic Systems.* American Chemical Society, Washington DC.

Ide, A., Niki, Y., Sakamoto, F., Watanabe, I. (1972) Decomposition of pentachlorophenol in paddy soil. *Agric. Biol. Chem.* 36, 1937–1944.

Isnard, P., Lambert, S. (1988) Estimating bioconcentration factors from octanol-water partition coefficient and aqueous solubility. *Chemosphere* 17, 21–34.

Isnard, P., Lambert, S. (1989) Aqueous solubility and octanol-water partition coefficient correlations. *Chemosphere* 18, 1837–1853.

IUPAC (1985) *Halogenated Benzenes, Toluenes and Phenols with Water, Solubility Data Series.* Vol. 20, Horvath, A.L., Getzen, F.W., Editors, Pergamon Press, Oxford.

Ivie, G.W., Bull, D.L., Veech, J.A. (1980) Fate of diflubenzuron in water. *J. Agric. Food Chem.* 28, 330–337.

Ivie, G.W., Casida, J.E. (1971) Photosensitizers for the accelerated degradation of chlorinated cyclodienes and other insecticide chemicals exposed to sunlight on bean leaves. *J. Agric. Food Chem.* 19, 410–416.

Ivie, G.W., Gibson, J.R., Bryant, H.E., Begin, J.J., Barnett, J.R., Dorough, H.W. (1974) Accumulation, distribution and excretion of mirex-^{14}C in animals exposed for long periods to the insecticide in the diet. *J. Agric. Food Chem.* 22(4), 646–653.

Iwata, H., Tanabe, S., Sakai, N., Tatsukawa, R. (1993) Distribution of persistent organochlorines in the oceanic air and surface seawater and the role of ocean on their global transport and fate. *Environ. Sci. Technol.* 27, 1080–1098.

Iwata, Y., Westlake, W.E., Berkley, J.H., Carman, G.R., Gunther, F.A. (1977) Aldicarb residues in oranges, citrus by-products, orange leaves, and soil after an aldicarb soil-application in an orange grove. *J. Agric. Food Chem.* 25, 933–937.

Jaber, H.M., Smith, J.H., Cwirla, A.N. (1982) Evaluation of gas saturation methods to measure vapor pressure. (EPA Contract No. 68-01-5117), SRI International, Menlo Park, California.

Jaglan, P.S., Gunther, F.A. (1970) Determination of partitioning values of parathion-methyl and related compounds. *Analyst* 95, 763–765.

Jantunen, L.M.M., Bidleman, T.F. (2000) Temperature dependent Henry's law constant for technical toxaphene. *Chemophere - Global Change Science* 2, 225–231.

Jarvinen, A.W., Tyo, R.M. (1978) Toxicity to fathead minnows of endrin in food and water. *Arch. Environ. Contam. Toxicol.* 7, 409–421.

Jensen-Korte, U., Anderson, C., Spiteller, M. (1987) Photodegradation of pesticides in the presence of humic substances. *Sci. Total Environ.* 62, 335–340.

Johnson, B.T., Saunders, C.R., Sanders, H.O. (1971) Biological magnification and degradation of DDT and aldrin by freshwater invertebrates. *J. Fish Res. Board Can.* 28, 705–709.

Johnson, Jr., J.C., Bowman, M C. (1972) Responses from cows fed diets containing fenthion or fenitrothion. *J. Diary Sci.* 55, 777.

Johnson-Logan, L.R., Broshears, R.E., Klaine, S.J. (1992) Partitioning behavior and the mobility of chlordane in ground water. *Environ. Sci. Technol.* 26, 2234–2239.

Jones, P.A. (1981) Chlorophenols and their impurities in the Canadian environment. Environment Canada, Report SPE 3-EC-81–2F. p. 322.

Jones, R.L., Back, R.C. (1984) Monitoring aldicarb in Florida soil and water. *Environ. Toxicol. Chem.* 3, 9–20.

Jones, R.L., Norris, F.A. (1998) Factors affecting degradation of aldicarb and ethoprop. *J. Nomatology* 30, 45–55.

Jury, W.A., Farmer, W.J., Spencer, W.F. (1984) Behavior assessment model for trace organics in soil: II. Chemical classification and parameter sensitivity. *J. Environ. Qual.* 13, 567–572.

Jury, W.A., Focht, D.D., Farmer, W.J. (1987b) Evaluation of pesticide ground water pollution potential from standard indices of soil-chemical adsorption and biodegradation. *J. Environ. Qual.* 16(4), 422–428.

Jury, W.A., Ghodrati, M. (1989) Overview of organic chemical environmental fate and transport modeling approaches. In: *Reactions and Movement of Organic Chemicals in Soils.* SSSA Special Publication No. 22, pp. 271–304, Soil Sci. Soc. of America and Soc. of Agronomy, Madison, Wisconsin.

Jury, W.A., Russo, D., Streile, G., El Abd, H. (1990) Evaluation of volatilization by organic chemicals residing below the soil surface. *Water Resources Res.* 26, 13–20.

Jury, W.A., Spencer, W.F., Farmer, W.J. (1983) Use of models for assessing relative volatility, mobility, and persistence of pesticides and other trace organics in soil systems. In: *Hazard Assessments of Chemicals: Recent Developments.* Vol. 2, Saxena, J., Editor, Academic Press, New York.

Jury, W.A., Spencer, W.F., Farmer, W.J. (1984) Behavior assessment model for trace organics in soil: III. Application of screening model. *J. Environ. Qual.* 13, 573–579.

Jury, W.A., Winer, A.M., Spencer, W.F., Focht, D.D. (1987a) Transport and transformations of organic chemicals in the soil-air water ecosystem. *Rev. Environ. Contam. Toxicol.* 99, 120–164.

Kaiser, K.L.E. (1983) A non-linear function for the calculation of partition coefficients of aromatic compounds with multiple chlorine substitution. *Chemosphere* 12, 1159–1165.

Kaiser, K.L.E., Dixon, D.G., Hodson, P.V. (1984) QSAR studies on chlorophenols, chlorobenzenes, and *para*-substituted phenols. In: *QSAR in Experimental Toxicology.* Kaiser, K.L.E., Editor, pp. 189–206, D. Reidel Publishing Company, Dordrecht, the Netherlands.

Kaiser, K.L.E., Valdmanis, I. (1982) Apparent octanol/water partition coefficients of pentachlorophenol as a function of pH. *Can. J. Chem.* 60, 2104–2106.

Kanan, M.C., Kanan, S.M., Austin, R.N., Patterson, H.H. (2003) Photodecomposition of carbaryl in the presence of silver-doped zeolite Y and Suwannee River natural organic matter. *Environ. Sic. Technol.* 37, 2280–2285.

Kanazawa, J. (1975) Uptake and excretion of organophosphorus and carbamate insecticides by fresh water, Motsugo (*Pseudorasbora parva*). *Bull. Environ. Contam. Toxicol.* 14, 346–352.

Kanazawa, J. (1978) Bioconcentration ratio of diazinon by freshwater fish and snail. *Bull. Environ. Contam. Toxicol.* 20, 613–617.

Kanazawa, J. (1980) Prediction of biological concentration potential of pesticides in aquatic organisms. *Rev. Plant Protection Res.* (Japan) 13, 27–36.

Kanazawa, J. (1981) Measurement of the bioconcentration factors of pesticides by fresh-water fish and their correlation with physicochemical properties of acute toxicities. *Pest. Sci.* 12, 417–424.

Kanazawa, J. (1983) A method of predicting the bioconcentration potential of pesticides by using fish. *JARQ* 17(3), 173–179.

Kanazawa, J. (1987) Biodegradability of pesticides in water by microbes in activated sludge. *Environ. Monit. Assess.* 9, 57–70.

Kanazawa, J. (1989) Relationship between the soil sorption constants for pesticides and their physicochemical properties. *Environ. Toxicol. Chem.* 8, 477–484.

Kanazawa, J., Yushima, T., Kiritani, K. (1971) Pollution of the ecosystem by insecticides. II. Environmental pollution by organochlorine insecticides. *Kagaku* 41(7), 384–391.

Kapoor, I.P., Metcalf, R.L., Hirwe, A.S., Coats, J.R., Khaisa, M.S. (1973) Structure activity correlations of biodegradability of DDT analogs. *J. Agric. Food Chem.* 21(2), 310–315.

Kapoor, I.P., Metcalf, R.L., Nystrom, R.F., Sangha, G.K. (1970) Comparative metabolism of methoxychlor, methiochlor, and DDT in mouse, insects, and in a model ecosystem. *J. Agric. Food Chem.* 18, 1145–1152.

Karcher, W., Devillers, J. (1990) SAR and QSAR in environmental chemistry and toxicology: Scientific tool or wishful thinking? In: *Practical Applications of Quantitative Structure-Activity Relationships (QSAR) in Environmental Chemistry & Toxicology.* Karcher, W., Devillers, J., Editors, ECSC, EEC, EAEC, Brussels and Luxemburg.

Karickhoff, S.W. (1981) Semi-empirical estimation of sorption of hydrophobic pollutants on natural sediments and soils. *Chemosphere* 10, 833–846.

Karickhoff, S.W. (1985) Pollutant sorption in environmental systems. In: *Environmental Exposure from Chemicals.* Neely, W.B., Blau, G.E., Editors, pp. 49–64, CRC Press, Boca Raton, Florida.

Karickhoff, S.W., Brown, D.S., Scott, T.A. (1979) Sorption of hydrophilic pollutants on natural water sediments. *Water Res.* 13, 241–248.

Katayama, A., Matsumura, F. (1991) Photochemically enhanced microbial degradation of environmental pollutants. *Environ. Sci. Technol.* 25(7), 1329–1333.

Kaufman, D.D. (1976) Soil degradation and persistence of benchmark pesticides. In: *A Literature Survey of Benchmark Pesticides.* pp. 19–71. The George Washington University Medical Center, Dept. of Medical and Public Affairs, Science Communication Division, Washington D.C.

Kavanaugh, M.C., Trussell, R.R. (1980) Design of aeration towers to strip volatile contaminants from drinking water. *J. Am. Water Works Assoc*. 72, 684–692.

Kawamoto, K., Urano, K. (1989) Parameters for predicting fate of organochlorine pesticides in the environment. (I) Octanol-water and air-water partition coefficients. *Chemosphere* 18, 1987–1996.

Kawamoto, K., Urano, K. (1989) Parameters for predicting fate of organochlorine pesticides in the environment. (II) Adsorption constant to soil. *Chemosphere* 19(8/9), 1223–1231.

Kawamoto, K., Urano, K. (1990) Parameters for predicting fate of organochlorine pesticides in the environment. (III) Biodegradation rate constants. *Chemosphere* 21(10–11), 1141–1152.

Kawano, M., Inoue, T., Hidaka, H., Tatsukawa, R. (1986) Chlordane residues in krill, fish and Weddell seal from the Antarctic. *Toxicol. Environ. Chem.* 11, 137.

Kawano, M., Inoue, T., Wada, T., Hidaka, H., Tatsukawa, R. (1988) Bioconcentration and residue of chlordane compounds in marine animals: Invertebrates, fish, mammals, and seabirds. *Environ. Sci. Technol*. 22, 792–797.

Kawano, M., Matsushita, S., Inoue, T., Tanaka, H., Tatsukawa, R. (1986) Biological accumulation of chlordane compounds in marine organisms from the northern North Pacific and Bering Sea. *Mar. Pollut. Bull.* 17, 512–516.

Kearney, P.C., Nash, R.G., Isensee, A.R. (1969) Persistence of pesticides in soil. Chapter 3, pp. 54–67. In: *Chemical Fallout: Current Research on Persistence Pesticides.* Miller, M W., Berg, C.C., Editors, Charles C. Thomas, Springfield, Illinois.

Keil, J.E., Priester, L.E. (1969) DDT uptake and metabolism by a marine diatom. *Bull. Environ. Contam. Toxicol.* 4, 169.

Kelly, T.J., Mukund, R., Spicer, C.W., Pollack, A.J. (1994) Concentrations and transformations of hazardous air pollutants. *Environ. Sci. Technol*. 28, 378A–387A.

Kenaga, E.E. (1972) Factors related to bioconcentration of pesticides. In: *Environmental Toxicology of Pesticides.* Matsumura, F., Boush, G.M., Misato, T., Editors, pp. 193–228, Academic Press, New York.

Kenaga, E.E. (1980a) Predicted bioconcentration factors and soil sorption coefficients of pesticides and other chemicals. *Ecotoxicol. Environ. Saf.* 4, 24–38.

Kenaga, E.E. (1980b) Correlation of bioconcentration factors of chemicals in aquatic and terrestrial organisms with their physical and chemical properties. *Environ. Sci. Technol.* 14, 553–556.

Kenaga E.E., Goring, C.A.I. (1978) Relationship between water solubility, soil-sorption, octanol-water partitioning, and bioconcentration of chemicals in biota. In: *Am. Soc. Test. Mat. 3rd. Aquatic Toxicology Sym.*, New Orleans, Louisiana. 63pp.

Kenaga E.E., Goring, C.A.I. (1980) Relationship between water solubility, soil sorption, octanol-water partitioning, and concentration of chemicals in biota. In: *Aquatic Toxicology.* ASTM STP 707, Eaton, J.G., Parrish, P.R., Hendricks, A.C., Eds., pp. 78–115, Am. Soc. for Testing and Materials, Philadelphia, PA.

Kerler, F., Schönherr, J. (1988) Accumulation of lipophilic chemicals across plant cuticles: Prediction from octanol/water partition coefficients. *Arch. Environ. Contam. Toxicol.* 17, 1–6.

Ketelaar, J.A.A. (1950) Chemical studies of insecticides. II. The hydrolysis of O,O-diethyl- and O,O-dimethyl O-*p*-nitrophenylthiophosphates. *Rev. Trav. Chim.* 69, 649.

Ketelaar, J.A.A., Gersmann, H.R. (1958) Chemical studies on insecticides. VI. The rate of hydrolysis of some phosphorus acid esters. *Rev. Trav. Chim.* 77, 973–981.

Khan, S.U. (1980) *Pesticides in the Soil Environment, Fundamental Aspects of Pollution Control and Environmental Series 5*, Elsevier, Amsterdam, The Netherlands.

Kilzer, L., Scheunert, I., Geyer, H., Klein, W., Körte, F. (1979) Laboratory screening of the volatilization rates of organic chemicals from water and soil. *Chemosphere* 10, 751–761.

Kim, Y.H. (1985) Evaluation of a gas chromatographic method for estimating vapor pressures with organic pollutants. Ph.D. Thesis, University of California, Davis, California.

Kim, Y.H., Woodrow, J.E., Seiber, J.N. (1984) Evaluation of a gas chromatographic method for calculating vapor pressures with organophosphorous pesticides. *J. Chromatogr.* 314, 37–53.

King, P.H., McCarthy, P.L. (1968) A chromatographic model for predicting pesticide migration in soils. *Soil Sci. Soc. Am. Proc*. 106, 248–261.

Kishi, H., Hashimoto, Y. (1989) Evaluation of the procedures for the measurement of water solubility and n-octanol/water partition coefficient of chemicals. *Chemosphere* 18, 1749–1759.

Kishi, H., Kogure, N., Hashimoto, Y. (1990) Contribution of soil constitutents in adsorption coefficient of aromatic compounds, halogenated alicyclic and aromatic compounds to soil. *Chemosphere* 21(7), 867–876.

Kjeldsen, P., Kjølholt, J., Schultz, B., Christensen, T.H., Tjell, J.C. (1990) Sorption and degradation of chlorophenols, nitrophenols and organophosphorus pesticides in the subsoil under landfills-laboratory studies. *J. Contam. Hydrology* 6, 165–184.

Klečka, G.M. (1985) Chapter 6, Biodegradation. In: *Environmental Exposure from Chemicals.* Neely, W.B., Blau, G.E., Editors, pp. 109–156, CRC Press, Boca Raton, Florida.

Klein, W., Geyer, H., Freitag, D., Rohleder, H. (1984) Sensitivity of schemes for ecotoxicological hazard ranking of chemicals. *Chemosphere* 13, 203–211.

Klöpffer, W., Rippen, G., Frische, R. (1982) Physicochemical properties as useful tools for predicting the environmental fate of organic chemicals *Ecotoxicol. Environ. Saf.* 6, 294–301.

Kollig, H.P., Editor (1993) Environmental Rate Constants for Organic Chemicals under Consideration for EPA's Hazardous Waste Identification Projects. EPA/600/R-93/132. Environmental Research Laboratory, U.S. Environmental Protection Agency, Athens, Georgia.

Kollig, H.P., Ellington, J.J., Hamrick, K.J., Jafverts, C.T., Weber, E.J., Wolfe, N.L. (1987) *Hydrolysis Rate Constants, Partition Coefficients, and Water Solubilities for 129 Chemicals.* A Summary of Fate Constants Provided for the Concentration-Based Listing Program. U.S. EPA, Environmental Research Lab., Office of Research and Development, Athens, Georgia.

Könemann, W.H. (1981) Quantity structure-activity relationships in fish toxicity studies. Part 1: Realtionship for 50 industrial pollutants. *Toxicology* 19, 209–221.

Könemann, W.H., Musch, A. (1981) Quantitative structure-activity relationships in fish toxicity studies. Part 2: The influence of pH on the QSAR of chlorophenols. *Toxicology* 19, 223–228.

Konrad, J.G., Chesters, G. (1969) Degradation in soils of ciodrin, an organophosphate insecticide. *J. Agric. Food Chem.* 17, 226.

Kördel, W., Kotthoff, G., Müller, J. (1995a) HPLC-screening method for the determination of adsorption coefficient on soil-Results of a ring-test. *Sci. Total Environ.* 162, 119–125.

Kördel, W., Stuffe, J., Kotthoff, G. (1993) HPLC-screening method for the determination of the adsorption-coefficient on soil.—Comparison of different stationary phases. *Chemosphere* 27, 2341–2352.

Kördel, W., Stutte, J., Kotthoff, G. (1995b) HPLC-screening method to determine the adsorption coefficient in soil-comparison of immobilized humic acid and clay mineral phases for cyanopropyl columns. *Sci. Total Environ.* 162, 119–125.

Körte, F., Freitag, D. (1986) Kriterien zur auswahl umweltgefährlicher alter stoffe. Mobilität einschliesslich abbaubarkeit und akkumulation. Umweltforschungsplan des Bundesministeriums des Innern. Forschungsbericht 106 05 25. GSF im Auftrag des Umweltbundesamtes.

Körte, F., Freitag, D., Geyer, H., Klein, W., Kraus, A.G., Lahaniatis, E. (1978) Ecotoxicologic profile analysis: A concept for establishing ecotoxicologic priority lists for chemicals. *Chemosphere* 1, 79–102.

Kortum, G., Vogel, W., Andrussow, K. (1961) *Dissociation Constants for Organic Acids in Aqueous Solutions.* Butterworths, London.

Kostovetskii, Y.I., Nasishten, S.Y., Tolstopyatova, G.V., Chegrinets, G.Y. (1976) Hygiene aspects of pesticide use in the catchment areas of water bodies. *Vodn. Resur.* 1, 67–72.

Kucklick, J.R., Hinckley, D.A., Bidleman, T.F. (1991) Determination of Henry's law constants for hexachloro-cyclohexane in distilled water and artificial seawater as a function of temperature. *Marine Chem.* 34, 197–209.

Kühne, R., Ebert, R.-U., Kleint, F., Schmidt, G., Schüürmann, G. (1995) Group contribution methods to estimate water solubility of organic chemicals. *Chemosphere* 30(11), 2061–2077.

Kurihara, N., Uchida, M., Fujita, T., Nakajima, M. (1973) Studies on BHC isomers and related compounds. V. Some physicochemical properties of BHC isomers. *Pestic. Biochem. Physiol.* 2(4), 383–390.

Lacorte, S., Barcelo, D. (1994) Rapid degradation of fenitrothion in estuarine waters. *Environ. Sci. Technol.* 28, 1159–1163.

LaFleur, K.S. (1976) Carbaryl desorption and movement in soil columns. *Soil Sci.* 121, 212–216.

Lagas, P. (1988) Sorptions of chlorophenols in soil. *Chemosphere* 17(2), 205–216.

Lamoreaux, R.J., Newland, L.W. (1978) The fate of dichlorvos in soil. *Chemosphere* 10, 807–814.

Landner, L., Lindström, K., Karlsson, M., Nordin, J., Sörensen, L. (1977) Bioaccumulation in fish of chlorinated phenols from Kraft pulp mill bleachery effluents. *Bull. Environ. Contam. Toxicol.* 18, 663–673.

Landrum, R.F., Dupuis, W.S. (1990) Toxicity and toxicokinetics of pentachlorophenol and carbaryl to *Pontoporeia hoyi* and *Mysis relicta.* In: *Aquatic Toxicology and Risk Assessment.* 13th Volume, *ASTM STP* 1096, Landis, W.G., van der Schalie, W.H., Editors, American Society for Testing and Materials, Philadelphia.

Landrum, R.F., Nihart, S R., Edie, B.J., Gardner, W.S. (1984) Reverse-phase separation method for determining pollutant binding to Aldrich humic acid and dissolved organic carbon of natural waters. *Environ. Sci. Technol.* 18, 187–192.

Larsson, P., Bremle, G., Okla, L. (1993) Uptake of pentachlorophenol in fish of acidified and non-acidified lakes. *Bull. Environ. Contam. Toxicol.* 50, 653–658.

Lartiges, S.B., Garrigues, P.P. (1995) Degradation kinetics of organophosphorous and organonitrogen pesticides in different waters under various environmental conditions. *Environ. Sci. Technol.* 29, 1246–1254.

LeBlanc, G.A. (1984) Interspecies relationships in acute toxicity of chemicals to aquatic organisms. *Environ. Toxicol. Chem.* 3, 47–60.

LeBlanc, G.A. (1995) Trophic-level differences in the bioconcentration of chemicals: implication in assessing environmental biomagnification. *Environ. Sci. Technol.* 29, 154–160.

Lee, L.S., Rao, P.S.C., Brusseau, M. (1991) Nonequilibrium sorption and transport of neutral and ionized chlorophenols. *Environ. Sci. Technol.* 25(4), 722–729.

Lee, L.S., Rao, P.S.C., Nkedl-Kizza, P., Delfino, J.J. (1990) Influence of solvent and sorbent characteristics on distribution of pentachlorophenol in octanol-water and soil-water systems. *Environ. Sci. Technol.* 24, 654–661.

Lee, P.W., Stearns, S.M., Hernandez, H., Powell, W.R., Naidu, M.V. (1989) Fate of dicrotophos in the soil environment. *J. Agric. Food Chem.* 37(4), 1169–1174.

Lee, S., Gan, J., Kim, J.-S., Kabashima, J.N., Crowley, D.E. (2004) Microbial transformation of pyrethroid insecticides in aqueous and sediment phases. *Environ. Toxicol. Chem.* 23, 1–6.

Leenheer, J.A., Atrichs, J.L. (1971) *Soil Science Society of America Proceedings* 35, 700–705.

Lemley, A.T., Zhong, W.Z. (1983) Kinetics of aqueous base and acid hydrolysis of *aldicarb*, aldicarb sulfoxide and aldicarb sulfone. *J. Environ. Sci. Health* B18, 189–206.

Lemley, A.T., Wagenet, R.J., Zhong, W.Z. (1988) Sorption of degradation of aldicarb and its oxidation products in a soil-water flow system as a function of pH and temperature. *J. Environ. Qual.* 17, 408–414.

Leo, A., Hansch, C., Elkins, D. (1971) Partition coefficients and their uses. *Chem. Rev.* 71, 525–616.

Leonard, R.A., Bailey, G.W., Swank, Jr., R.R. (1976) Transport, detoxification, fate and effects of pesticides in soil and water environments in land application of waste materials. Soil Conservation Society of America, Ankeny, Iowa. 48pp.

Leshniowsky, W.O., Dugan, P.R., Pfister, R.M., Frea, J.I., Randers, C.I. (1970) Aldrin: removal from lake water by flocculent bacteria. *Science* 169, 993.

Leuck, D.G., Bowman, M.C. (1970) Residues of phorate and five of its metabolites. Their persistence in forage corn and grass. *J. Econ. Entomol*. 63, 1838–1842.

Leuenberger, C., Giger, W., Coney, R., Graydon, J.W., Molnar-Kubica, E. (1985) Persistence chemicals in pulp mill effluents, occurrence and behavior in an activated sludge treatment plant. *Water Res.* 19, 885–894.

Leuenberger, C., Ligocki, M.P., Pankow, P.F. (1985) Trace organic compounds in rain. 4. Identities, concentrations, and scavenging mechanisms for phenols in urban air and rain. *Environ. Sci. Technol.* 19, 1053–1058.

Lewis, D.L., Paris, D.F., Baughman, G.L. (1975) Transformation of malathion by fungus, *Aspergillus oryzae*, isolated from a freshwater pond. *Bull. Environ. Contam. Toxicol.* 13, 596–601.

Lichtenstein, E.P. (1959) Absorption of some chlorinated hydrocarbon insecticides from soils into various crops. *J. Agric. Food Chem*. 7, 430–433.

Lichtenstein, E.P. (1960) Insecticidal residues in various crops grown in soils treated with an abnormal rate of aldrin and heptachlor. *J. Agric. Food Chem.* 8, 448–451.

Lichtenstein, E.P., Fuhremann, T.W., Schultz, K.R. (1971) Persistence and vertical distribution of DDT, lindane and aldrin residues, ten and fifteen years after a single soil application. *J. Agric. Food Chem.* 19, 718–721.

Lichtenstein, E.P., Schultz, K.R. (1961) Persistence of some chlorinated hydrocarbon insecticides influenced by soil types, rates of application and temperature. *J. Econ. Entomol.* 52, 124–131.

Lichtenstein, E.P., Schultz, K.R. (1959) Effect of soil cultivation, soil surface, and water on the persistence of insecticidal residues in soils. *J. Econ. Entomol.* 54, 517.

Lide, D.R., Editor (2003) *Handbook of Chemistry and Physics*. 84th Edition, CRC Press, Boca Raton, Florida.

Lipke, H., Kearns, C.W. (1960) DDT-Dehydrochlorinase III. Solubilization of insecticides by lipoprotein. *J. Econ. Entomol.* 53, 31–35.

Liu, D., Strachan, W.M.J., Thomson, K., Kwasniewska, K. (1981) Determination of the biodegradability of organic compounds. *Environ. Sci. Technol*. 15, 788–793.

Liu, J., Qian, C. (1988) Estimation of n-octanol/water partition coefficients for organic compounds by using high-performance liquid chromatography. *Huanjing Huaxue* 7, 23–27.

Liu, M.H., Kapila, S., Yanders, A.F., Clevenger, T.E., Elseewi, A.A. (1991) Role of entrainers in supercritical fluid extraction of chlorinated aromatics from soils. *Chemosphere* 23, 1085–1095.

Loehr, R.C., Matthews, J.E. (1992) Loss of organic chemicals in soil: Pure compound treatability studies. *J. Soil Contam.* 1(4), 339–360.

Lohninger, H. (1994) Estimation of soil partition coefficients of pesticides from their chemical structure. *Chemosphere* 29, 1611–1626.

Lord, K.A., Briggs, G C., Nearle, M.C., Manlove, R. (1980) Uptake of pesticides from water and soil by earthworms. *Pest. Sci.* 11, 401–408.

Lord, K.A., Burt, P.E. (1964) Effect of temperature on water solubility of phorate and disulfoton. *Chem. Ind.* (London) July 11, 1262–1263.

Lu, P.Y., Metcalf, R.L. (1975) Environmental fate and biodegradability of benzene derivatives as studied in a model aquatic ecosystem. *Environ. Health Perspect.* 10, 269–284.

Lu, X., Tao, S., Cao, J., Dawson, R.W. (1999) Prediction of fish bioconcentration factors of nonpolar organic pollutants based on molecular connectivity indices. *Chemosphere* 39, 987–999.

Lydy, M.J., Bruner, K.A., Fry, D.M., Fisher, S.W. (1990) Effects of sediment and the route of exposure on the toxicity and accumulation of neutral lipophilic and moderately water soluble metabolizable compounds in the midge, *Chironomus riparus.* In: *Aquatic Toxicology and Risk Assessment*. 12th Volume, ASTM STP 1096, pp. 104–164, American Society for Testing and Materials, Philadelphia, Pennsylvania.

Lydy, M.J., Oris, J.T., Baumann, P.C., Fisher, S.W. (1992) Effects of sediment organic carbon content on the elimination rates on neutral lipophilic compounds in the midge *(Chironomus riparus). Environ. Toxicol. Chem.* 11, 347–356.

Lyman, W.J. (1982) Chapter 2, Solubility in water and Chapter 4, Adsorption coefficient for soils and sediments. In: *Handbook on Chemical Property Estimation Methods, Environmental Behavior of Organic Compounds.* Lyman, W., Reehl, W.F., Rosenblatt, D.H., Editors, McGraw-Hill, New York.

Lyman, W.J., Reehl, W.F., Rosenblatt, D.H., Editors (1982) *Handbook on Chemical Property Estimation Methods, Environmental Behavior of Organic Compounds.* McGraw-Hill, New York.

Lyman, W.J., Reehl, W.F., Rosenblatt, D.H., Editors (1990) *Handbook on Chemical Property Estimation Methods, Environmental Behavior of Organic Compounds.* 2nd printing, American Chemical Society, Washington DC.

Ma, K.C., Shiu, W.Y., Mackay, D. (1993) Aqueous solubility of chlorophenols at 25°C. *J. Chem. Eng. Data* 38, 364–366.

Mabey, W.R., Mill, T. (1978) Critical review of hydrolysis of organic compounds in water under environmental conditions. *J. Phys. Chem. Ref. Data* 7, 383–415.

Mabey, W.R., Smith, J.H., Podoll, R.T., Johnson, H.L., Mill, T., Chou, T.W., Gates, J., Waight-Partridge, I., Jaber, H., Vanderberg, D. (1982) Aquatic Fate Process for Organic Priority Pollutants. EPA Report No. 440/4–81–014, U.S. EPA, Washington, DC.

Mabury, S.A., Crosby, D.G. (1996) Pesticide reactivity and its relationship to field persistence. *J. Agric. Food Chem*. 44, 1920–1924.

Macalady, D.L., Wolfe, N.L. (1983) New perspectives on the hydrolytic degradation of the organophosphorothioate insecticide chlorpyrifos. *J. Agric. Food Chem.* 31, 1139–1147.

MacDougall, D. (1964) Dylox. In: *Analytical Methods for Pesticides, Plant Growth Regulators, and Food Additives.* Vol. 2, Zweig, G., Editor, Academic Press, New York.

MacDougall, D. (1972) *Toxicity, Biodegradation.* Swets-Zeitlinger: Lisse, The Netherlands.

MacDougall, D., Archer, T.E. (1964) Di-syston. In: *Analytical Methods for Pesticides, Plant Growth Regulators, and Food Additives*. Vol. II., Zweig, G., Ed., p. 188, Academic Press, New Youk.

Macek, K.J., Petrocelli, S.R., Sleight, B.H. (1979) Consideration in assessing the potential for, and significance of, biomagnification of chemical residues in aquatic food chains. pp. 251–268. In: *Aquatic Toxicology.* ASTM STP 667, Marking, L.L., Kimerle, R.A., Editors, American Society for Testing and Materials, Philadelphia, Pennsylvania.

Mackay, D. (1982) Correlation of bioconcentration factors. *Environ. Sci. Technol.* 16, 274–278.

Mackay, D. (1985) Chapter 5, Air/water exchange coefficients. In: *Environmental Exposure from Chemicals.* Neely, W.B., Blau, G.E., Editors, pp. 91–108, CRC Press, Boca Raton, Florida.

Mackay, D., Bobra, A., Shiu, W.Y., Yalkowsky, S.H. (1980) Relationships between aqueous water solubility and octanol-water partition coefficient. *Chemosphere* 9, 701–711.

Mackay, D., Leinonen, P. (1975) Rate of evaporation of low-solubility contaminants from water bodies to atmosphere. *Environ. Sci. Technol.* 9, 1178–1180.

Mackay, D., Paterson, S. (1991) Evaluating the multimedia fate of organic chemicals: A level III fugacity model. *Environ. Sci. Technol.* 25, 427–436.

Mackay, D., Paterson, S., Chung, B., Neely, W.B. (1985) Evaluation of the environmental behavior of chemicals with a level III fugacity model. *Chemosphere* 14, 335–374.

Mackay, D., Paterson, S., Schroeder, W.H. (1986) Model describing the rates of transfer processes of organic chemicals between atmosphere and water. *Environ. Sci. Technol.* 20, 810–816.

Mackay, D., Shiu, W.Y. (1981) A critical review of Henry's law constants for chemicals of environmental interest. *J. Phys. Chem. Ref. Data* 10, 1175–1199.

Mackay, D., Stiver, W. (1991) Chapter 8, Predictability and environmental chemistry. In: *Environmental Chemistry of Herbicides.* Vol. II, Grover, R., Cessna, A.J., Editors, pp. 281–297, CRC Press, Boca Raton, Florida.

Mackay, D., Wolkoff, A.W. (1973) Rate of evaporation of low-solubility contaminants from water bodies to atmosphere. *Environ. Sci. Technol.* 7, 611–614.

Macy, R. (1948) Partition coefficients of fifty compounds between olive oil and water at 20°C. *J. Ind. Hyg. Toxicol.* 30, 140.

Magee, P.S. (1991) Complex factors in hydrocarbon/water, soil/water, and fish/water partitioning. *Sci. Total Environ*. 109/110, 155–178.

Mailhot, H. (1987) Prediction of algae bioaccumulation and uptake rate of nine organic compounds by ten physicochemical properties. *Environ. Sci. Technol*. 21, 1009–1013.

Maitlen, J.C., Powell, D.M. (1982) Persistence of aldicarb in soil relative to the carry-over of residues into crops. *J. Agric. Food Chem*. 30, 589–592.

Majewski, M.S., Capel, P.D. (1995) *Pesticides in the Atmosphere. Distribution, Trends, and Governing Factors.* Vol. 1 of the series *Pesticides in the Hydrologic System.* Ann Arbor Press, Chelsea, MI.

Mäkelä, P., Oikari, O.J. (1990) Uptake and body distribution of chlorinated phenols in the freshwater mussel, *Anodonta anatina L. Ecotoxicol. Environ. Saf.* 20, 354–362.

Malalayandi, M., Shah, S.M., Lee, P. (1982) Fate of α- and γ-hexachlorocyclohexane isomers under simulated environmental conditions. *J. Environ. Sci. Health* A17(3), 283–297.

Mansour, M., Feicht, E.A. (1994) Transformation of chemical contaminants by biotic and abiotic processes in water and soil. *Chemosphere* 28, 323–332.

Mansour, M., Feicht, E.A., Behechti, A., Scheunert, I. (1997) Experimental approaches to studying the photostability of selected pesticides in water and soil. *Chemosphere* 35, 39–50.

Maquire, R.J., Hale, E.J. (1980) Fenitrothion sprayed on a pond: Kinetics of its distribution and transformation in water and sediment. *J. Agric. Food Chem.* 28, 372–378.

Margot, A., Stammbach, K., (1964) Diazinon. In: *Analytical Methods for Pesticides, Plant Growth Regulators, and Food Additives*. Vol. 11, Zelig, G., Ed., p. 110, Academic Press, New York.

Markwell, R.D., Connell, D.W., Gabric, A.J. (1989) Bioaccumulation of lipophilic compounds from sediments by oligochaetes. *Water Res.* 23(11), 1443–1450.

Martens, R. (1972) Decomposition of endosulfan by soil microorganisms. *Schrifter Ver Wasser-, Bodden-, Luftig, Berlin-Dahlem* 37, 167–173.

Marti, C. (1976) Ciba-Geigy Research Report. Basel, West Germany. Data provided by W.F. Spencer and presented in Ph.D. thesis of Y.-H. Kim 1985.

Martin, H. (1961) *Guide to the Chemicals used in Crop Protection.* 4th Edition, Canadian Dept. of Agriculture Publication 1093, Ottawa, Ontario.

Martin, H. (1972) *Pesticide Manual*, 3rd Edition, British Crop Protection Council, Worcester, England.

Martin, H., Worthing, C.R., Editors (1977) *Pesticide Manual.* 5th Edition, British Crop Protection Council. Thornton Heath, United Kingdom.

Mason, J.W., Rowe, D.R. (1976) The accumulation and loss of dieldrin and endrin in the eastern oyster. *Arch. Environ. Contam. Toxicol.* 4, 349–360.

Masterton, W.L., Lee, T.P. (1972) Effects of dissolved salts on water solubility of lindane. *Environ. Sci. Technol.* 6, 919–921.

Matsumura, F., Benezet, H.J. (1973) Studies on the bioaccumulation and microbial degradation of 2,3,7,8-tetrachlorodibenzo-*p*-dioxin. *Environ. Health Perspect.* 253–258.

Maule, A., Plyte, S., Quick, A.V. (1987) Dehalogenation of organochlorine insecticides by mixed anaerobic microbial populations. *Pestic. Biochem. Physiol.* 277, 229–236.

Maund, S.J., Hamer, M.J., Lane, M.C.G., Farrelly, E., Rapley, J.H., Goggin, U.M., Gentle, W.E. (2002) Partitioning, bioavailability, and toxicity of the pyrethroid insecticide cypermethrin in sediments. *Environ. Toxicol. Chem.* 21, 9–15.

Mayer, F.L., Mehrle, P.M., Dwyer, W.P. (1977) Toxaphene: Chronic Toxicity to Fathead Minnows and Channel Catfish. EPA-600/3–77–069, U.S. Environmental Protection Agency.

McCall, P.J., Swann, R.L., Laskowski, D.A., Unger, S.M., Vrona, S.A., Dishburger, H.J. (1980) Estimation of chemical mobility in soil from liquid chromatographic retention times. *Bull. Environ. Contam. Toxicol.* 24, 190–195.

McConnell, L.L., Cotham, W.E., Bildleman, T.F. (1993) Gas exchange of hexachloro-cyclohexane in the Great Lakes. *Environ. Sci. Technol.* 27, 1304–1311.

McDowell, L.L., Willis, G., Murphree, C.E., Southwick, L.M., Smith, S. (1981) Toxaphene and sediments yields in runoff from a Mississippi delta watershed. *J. Environ. Qual.* 10, 120.

McDuffie, B. (1981) Estimation of octanol/water partition coefficients for organic pollutants using reverse-phase HPLC. *Chemosphere* 10, 73–83.

McKellar, R.L., Dishburger, H.J., Rice, J.R., Craig, L F., Pennington, J.J. (1976) Residues of chlorpyrifos, its oxygen analogue, and 3,5,6-trichloro-2-pyridinol in milk and cream from cows fed chlorpyrifos. *J. Agric. Food Chem.* 24, 283–286.

McKim, J., Schnieder, P., Veith, G. (1985) Absorption dynamics of organic chemical transport across trout gills as related to octanol-water partition coefficients. *Toxicol. Appl. Pharmacol.* 77, 1–10.

McLachlan, M., Mackay, D., Jones, P.H. (1990) A conceptual model of organic chemical volatilization at waterfalls. *Environ. Sci. Technol.* 24, 252–257.

McLean, J.E., Sims, R.C., Doucette, W.J., Caupp, C.R., Grenney, W.J. (1988) Evaluation of mobility of pesticides in soil using U.S. EPA methodology. *J. Environ. Eng.* 114, 689–703.

McLeese, D.W., Metcalf, C.D., Zitko, V. (1980) Lethality of permethrin, cypermethrin and fenvalerate to salmon, lobster and shrimp. *Bull. Environ. Contam. Toxicol.* 25, 950–955.

McLeese, D.W., Sergent, D.B., Metcalf, C.D., Zitko, V., Burridge, L.E. (1979) Uptake and excretion of aminocarb, nonylphenol and pesticide diluent 585 by mussels (*Mytilus edulis*). *Bull. Environ. Contam. Toxicol.* 24, 575–581.

McLeese, D.W., Zetko, V., Sergent, D.B. (1976) Uptake and excretion of fenitrothion by clams and mussel. *Bull. Environ. Contam. Toxicol.* 16, 508–515.

Means, J.C., Woods, S.G., Hassett, J.J., Banwart, W.L. (1982) Sorption of amino- and carboxy-substituted polynuclear aromatic hydrocarbons by sediments and soils. *Environ. Sci. Technol.* 16, 93–98.

Medchem (1988) Medchem Database, Release 3.54 of 1988. Daylight Chemical Information System Inc., California.

Meijer, S.N., Halsall, C.J., Harner, T., Peters, A.J., Ockenden, W.A., Johnston, A.E., Jones, K.C. (2001) Organochlorine pesticide residues in archived UK soils. *Environ. Sci. Technol.* 35, 1989–1995.

Meikle, R.W., Kurihara, N.H., DeVries, D.H. (1983) Chlorpyrifos: The photodecomposition rates in dilute aqueous solution and on a surface, and the volatilization rate from a surface. *Arch. Environ. Contam. Toxicol.* 12, 189.

Melnikov, N.N. (1971) Chemistry of pesticides. *Res. Rev.* 36, 1–447.

Menn, J.J. (1969) Stauffer Chemical Co., Mountain View, California.

Menn, J.J., Patchett, G.G., Batchelder, G.H. (1964) Trithion. In: Analytical Methods, for Pesticides, Plant Growth Regulators, and Food Additives. Vol. II, Zweig, G., Ed., p. 546, Academic Press, New York.

Menzie, C.A., Burmaster, D.E., Freshman, J.S., Callahan, C.A. (1992) Assessment of methods for estimating ecological risk in the terrestrial component: A case study at the Baird and McGuire Supefund site in Holbrook, Massachusetts. *Environ. Toxicol. Chem.* 11, 245–260.

Menzie, C.M. (1972) Fate of pesticides in the environment. *Ann. Rev. Entomol.* 17, 199.

The Merck Index (1983) *An Encyclopedia of Chemicals, Drugs and Biologicals.* 10th Edition, Widholz, M., Editor, Merck and Co., Rahway, New Jersey.

The Merck Index (1989) *An Encyclopedia of Chemicals, Drugs and Biologicals.* 11th Edition, Budavari, S., Editor, Merck and Co., Rahway, New Jersey.

Metcalf, C.D., McLeese, D.W., Zitko, V. (1980) Rate of volatilization of fenitrothion from fresh water. *Chemosphere* 9, 151–155.

Metcalf, R.L. (1971) The chemistry and biology of pesticides. In: *Pesticides in the Environment*. White-Stevens, J., Ed., Part I, Vol. 1, p. 50, Marcel Dekker, New York.

Metcalf, R.L. (1974) In: Comparative Studies of Food and Environmental Contaminants. Proceedings of the FAO/IAEA/WHO Symposium, Otaniemi, International Atomic Energy Agency, Vienna. pp. 3–22.

Metcalf, R.L., Kapoor, I.P., Lu, P-Y., Schuth, C.K., Sherman, P. (1973) Model ecosystem studies of the environmental fate of six organochlorine pesticides. *Environ. Health Perspect.* 4, 35–44.

Metcalf, R.L., Sanborn, J.R. (1975) *Illinois Natural History Survey Bulletin* 31, 381–436.

Metcalf, R.L., Sanborn, J.R., Lu, P.-Y., Nye, D. (1975) Laboratory model ecosystem studies of the degradation and fate of radiolabeled tri-, tetra-, and pentachlorobiphenyl compared with DDE. *Arch. Environ. Contam. Toxicol.* 3, 151–165.

Meylan, W., Howard, P.H. (1991) Bond contribution method for estimating Henry's law constants. *Environ. Toxicol. Chem.* 10, 1283–1293.

Meylan, W., Howard, P.H., Boethling, R.S. (1992) Molecular topology/fragment contribution method for predicting soil sorption coefficients. *Environ. Sci. Technol.* 26, 1560–1567.

Miles, J.R.W. (1976) Fates of insecticides applied to lands and crops. *Pest. Monit. J.* 10, 87–91.

Miles, J.R.W., Delfino, J.J. (1985) Fate of aldicarb, aldicarb sulfoxide, and aldicarb sulfone in Floridan ground water. *J. Agric. Food Chem.* 33(3), 455–460.

Miles, J.R.W., Harris, C.R. (1978) Insecticide residues in water, sediment, and fish of the drainage system of the Holland Marsh, Ontario, Canada. *J. Econ. Entomol.* 71, 125–131.

Miles, J.R.W., Tu, C M., Harris, C R. (1979) Persistence of eight organophosphorous insecticides in sterile and non-sterile mineral and organic soils. *Bull. Environ. Contam. Toxicol.* 22, 312–318.

Mill, T., Hendry, D.M., Mabey, W.E., Johnson, D.J. (1980) Laboratory protocols for evaluating fate of organic chemicals in air and water. EPA-600/3–80–069. U.S. Environmental Protection Agency, Washington DC.

Mill, T., Mabey, W.E. (1985) Photochemical transformations. In: *Environmental Exposure from Chemicals*. Neely, W.B., Blau, G.E., Editors, pp. 175–213, CRC Press, Boca Raton, Florida.

Miller, C.T., Weber, W.J., Jr. (1986) Sorptions of hydrophobic organic pollutants in saturated soil systems. *J. Contam. Hydrol.* 1, 243.

Mills, W.B., Dean, J.D., Porcella, D.B., Gherini, S.A., Hudson, R.J.M., Frick, W.E., Rupp, G.L. (1982) Water quality assessment: A screening procedure for toxic and conventional pollutants. Part 1, U.S. EPA Report No. EPA-600/6–82–004a, Environmental Research Lab., U.S. Environmental Protection Agency, Athens, Georgia.

Milne, G.W.A., Editor (1995) *CRC Handbook of Pesticides.* CRC Press, Boca Raton, Florida.

Minero, C., Pelizzetti, E., Malato, S., Blanco, J. (1993) Large solar plant photocatalytic water decontamination: degradation of pentachlorophenol. *Chemosphere* 26, 2103–2119.

Mingelgrin, U., Gerstl, Z. (1983) Reevaluation of partitioning as a mechanism of nonionic chemicals adsorption in soils. *J. Environ. Qual.* 12(1), 1–11.

Mink, F.L., Risher, J.F., Stara, J.F. (1989) The environmental dynamics of the carbamate insecticide aldricarb in soil and water. *Environ. Pollut.* 61, 127–155.

Miyake, K., Terada, H. (1982) Determination of partition coefficients of very hydrophobic compounds by high-performance liquid chromatography on glycerol-coated controlled-pore glass. *J. Chromatogr.* 240, 9–20.

Moody, R.P., Carroll, J.M., Kresta, A.M.E. (1987) Automated high performance liquid chromatography and liquid scintillation counting determination of pesticide mixture octanol/water partition rates. *Toxicol. Ind. Health* 3, 479–490.

Montgomery, J.H. (1993) *Agrochemicals Desk Reference. Environmental Data*. Lewis Publishers, Chelsea, Michigan.

Moody, R.P., arroll, J.M., Kresta, A.M.E. (1987) Automated high performance liquid chromatography and liquid scintillation counting determination of pesticide mixture octanol/water partition rates. *Toxicol. Ind. Health* 3, 479–490.

Moorefield, H.H. (1974) Data on Temik aldicarb pesticide environmental impact. (Cited in UA EPA 1975) Moos, L.P., Kiesch, E.J., Wukasch, R.F., Grady, Jr., C.P.L. (1983) Pentachlorophenol biodegradation-I. Aerobic. *Water Res.* 17, 1575–1584.

Mora, A., Comejo J., Revilla, E., Hermosin, M.C. (1996) Persistence and degradation of carbofuran in Spanish soil suspensions. *Chemosphere* 32, 1585–1598.

Morrill, L.G., Mahilum, B.C., Mohiuddin, S.H. (1982) *Organic Compounds in Soils*. Ann Arbor Science Publishers, Ann Arbor, Michigan.

Mortimer, M.R., Connell, D.W. (1995) A model of the environmental fate of chloro-hydrocarbon contaminants associated with Sydney sewage discharge. *Chemosphere* 30, 2021–2038.

Mudami, A.R., Hassett, J.P. (1988) Photochemical activity of mirex associated with dissolved organic matter. *Chemosphere* 17, 1133–1146.

Muir, D.C.G., Hobdem, B.R., Servos, M.R. (1994) Bioconcentration of pyrethroid insecticides and DDT by rainbow trout: Uptake, depuration, and effect of dissolved organic carbon. *Aquatic Toxicol.* 29, 223–240.

Muir, D.C.G., Rawn, G.P., Townsend, B.E., Lockhart, W.L. (1985) Bioconcentration of cypermethrein, deltamethrin, fenvalerate and permethrin by *Chironomus tentans* larvae in sediment and water. *Environ. Toxicol. Chem*. 4, 51–61.

Muir, D.C.G., Teixeira, C, Wania, F. (2004) Empirical and modeling evidence of regional atmospheric transport of current-use pesticides. *Environ. Toxicol. Chem*. 23, 2421–2432.

Muir, D.C.G., Townsend, B.E., Lockhart, W.L. (1983) Bioavailability of six organic chemicals to *Chironomus tentans* larvae in sediment and water. *Environ. Toxicol. Chem*. 2, 269–281.

Müller, M.A., Buser, H.-R. (1995) Environmental behavior of acetamide pesticide stereoisomers. 2. Sereo- and enantioselective degradation in sewage sludge and soil. *Environ. Sci. Technol*. 29, 2031–2037.

Müller, J.F., Hawker, D.W., Connell, D.W. (1994) Calculation of bioconcentration factors of persistent hydrophobic compounds in the air/vegetation system. *Chemosphere* 29, 623–640.

Müller, M., Klein, W. (1992) Comparative evaluation of methods predicting water solubility for organic compounds. *Chemosphere* 25, 769–782.

Müller, M., Kördel, W. (1996) Comparison screening methods for the estimation of adsorption coefficients on soils. *Chemosphere* 32, 2495–2504.

Mundy, R.L., Bowman, M.C., Farmer, J.H., Haley, T.J. (1978) Quantitative structure-activity study of a series of substituted O,O-dimethyl O-(*p*-nitrophenyl) phosphorothionates and O-analogues. *Arch. Toxicol*. 41, 111–123.

Murphy, T.J., Mullin, M.D., Meyer, J.A. (1987) Equilibration of polychlorinated biphenyls and toxaphene with air and water. *Environ. Sci. Technol*. 21, 155–162.

Nakagawa, Y., Izumi, K., Oikawa, N., Kurozumi, A., Iwamura, H., Fujita, T. (1991) Quantitative structure-activity relationships of benzoylphenylurea larvicides. VII. *Pestic. Biochem. Physiol*. 40, 12–26.

Nakamura, M., Suzuki, T., Amano, K., Yamada, S. (2001) Relation of sorption behavior of agricultural chemicals in solid-phase extraction with their *n*-octanol/water partition coefficients evaluated by high-performance liquid chromatography (HPLC). *Anal. Chim. Acta* 428, 219–226.

Nash, R.G. (1974) In: *Pesticides in Soil and Water.* Guenzi, W.D., Ed., Soil Sci. Soc. of America, Madison, Wis.

Nash, R.G. (1980) Dissipation rate of pesticides from soils. In: CREAMS: A field scale model for chemical, runoff, and erosion from agricultural management systems. Vol. 3, Knisel, W.G., Editor, pp. 560–594, USDA Conserv. Res. Rep. 26, U.S. Government Printing Office, Washington, DC.

Nash, R.G. (1983a) Comparative volatilization and dissipation rates of several pesticides from soil. *J. Agric. Food Chem*. 31, 210–217.

Nash, R.G. (1983b) Determining environmental fate of pesticides with microagroecosystems. *Res. Rev*. 85, 199–215.

Nash, R.G. (1988) Chapter 5. Dissipation from soil. In: *Environmental Chemistry of Herbicides.* Volume I, Grover, R., Editor, pp. 131–169, CRC Press, Inc., Boca Raton, Florida.

Nash, R.G. (1989) Models for estimating pesticide dissipation from soil and vapor decline in air. *Chemosphere* 18, 2375–2381.

Nash, R.G., Harris, W.G. (1977) Toxaphene and 1,1,1-trichloro-2,2-bis(*p*-chlorophenyl)ethane (DDT) losses from cotton in an agroecosystem chamber. *J. Agric. Food Chem*. 25, 336.

Nash, R.G., Woolson, E.A. (1967) Persistence of chlorinated hydrocarbon insecticides. *Science* 157, 924–927.

Neary, D.G., Bush, P.B., Michael, J.L. (1993) Fate, dissipation and environmental effects of pesticides in southern forests: A review of a decade of research progress. *Environ. Toxicol. Chem*. 12, 411–428.

Neely, W.B. (1978) Personal communication. Dow Chemical Company, Midland, Michigan.

Neely, W.B. (1980) Chapter 20. A method for selecting the most appropriate environmental experiments on a new chemical. In: *Dynamics, Exposure and Hazard Assessment of Toxic Chemicals.* Haque, R., Ed., pp. 287–196, Ann Arbor Science Publishers, Ann Arbor, Michigan.

Neely, W.B., Blau, G.E. (1977) The use of laboratory data to predict the distribution of chlorpyrifos in a fish pond. In: *Pesticides in Aquatic Environments.* Khan, M.A.Q., Editor, Plenum Press, New York.

Neely, W.B., Blau, G.E. (1985) Chapter 1. Introduction to Environmental exposure from chemicals. In: *Environmental Exposure from Chemicals.* Neely, W.B., Blau, G.E., Editors, pp. 1–12, CRC Press, Boca Raton, Florida.

Neely, W.B., Blau, G.E., Eds. (1985) *Environmental Exposure from Chemicals.* CRC Press, Boca Raton, Florida.

Neely, W.B., Branson, D.R., Blau, G.E. (1974) Partition coefficient to measure bioconcentration potential of organic chemicals in fish. *Environ. Sci. Technol.* 8, 1113–1115.

Nendza, M. (1991) Predictive QSAR models estimating ecotoxic hazard of phenylureas: Aquatic toxicity. *Chemosphere* 23, 497–506.

Nendza, M., Seydel, J.K. (1988) Quantitative structure-toxicity relationship for ecotoxicologically relevant biotest systems and chemicals. *Chemosphere* 17, 1585–1602.

Neudorf, S., Khan, M.A.Q. (1975) Pick-up and metabolism of DDT, dieldrin and photodieldrin by fresh water algae (*Ankistrodesmus*) and a micro-crustacean (*Daphnia pulex*). *Bull. Environ. Contam. Toxicol*. 13, 443–450.

Neumüller, O.A. (1974) *Römpp's Chemie-Lexikon.* p. 2538, Frank'sche Verlagsbuchhandlung, Stuttgart.

Ngabe, B., Bidleman, T.F., Falconer, R.L. (1993) Base hydrolysis of α- and γ-hexachlorocyclohexanes. *Environ. Sci. Technol*. 27, 1930–1933.

NIEHS (1975) National Institute of Environmental Health Services Grant No. ES 00040–10 Annual Progress Report.

Niimi, A.J. (1987) Biological half-life of chemicals in fishes. *Rev. Environ. Contam. Toxicol.* 99, 1–46.

Niimi, A.J., Cho, C.Y. (1983) Laboratory and field analysis of pentachlorophenol (PCP) accumulation by salmonids. *Water Res*. 17, 1791–1795.

Niimi, A.J., Palazzo, V. (1985) Temperature effect on the elimination of pentachlorophenol, hexachlorobenzene and mirex by rainbow trout (*Salmo gairdneri*). *Water Res*. 19(2), 205–207.

Nirmalakhandan, N.N., Speece, R.E. (1988) QSAR model for predicting Henry's law constant. *Environ. Sci. Technol.* 22, 1349–1357.

Nishimura, K., Fujita, T. (1983) Quantitative structure-activity relationships of DDT and its related compounds. *Nippon Noyaku Gakkaishi* 8, 69–81.

Noegrohati, S., Hammers, W.E. (1992) Regression models for octanol-water partition coefficients, and for bioconcentration in fish. *Toxicol. Environ. Chem.* 34, 155–173.

Norstrom, R.J., Clark, T.P., Jeffrey, D.A., Won, H.T., Gilman, A.P. (1986) Dynamics of organochlorine compounds in herring gulls (*Larus argentatus*): I. Distribution and clearance of [^{14}C]DDE in free-living herring gulls *(Larus argentatus*). *Environ. Toxicol. Chem.* 5, 41–48.

NRC (1974) Chlordane; Its effects on Canadian ecosystems and its chemistry. NRCC No. 14094, National Research Council, Ottawa, Canada.

O'Brien, R.D. (1975) Nonenzymic effects of pesticides on membranes. In: *Environmental Dynamics of Pesticides*. Haque, R., Freed, V.H., Editors, pp. 331–342, Plenum Press, New York.

OECD (1981) *OECD Guidelines for Testing of Chemicals*. Section 1: Physical-Chemical Properties. Organization for Economic Co-operation and Development. OECD, Paris.

Oliver, B.G. (1987) Biouptake of chlorinated hydrocarbons from laboratory-spiked and field sediments by oligochaete worms. *Environ. Sci. Technol.* 21, 785–790.

Oliver, B.G., Charlton, M.N. (1984) Chlorinated organic contaminants on settling particulates in the Niagara River vicinity of Lake Ontario. *Environ. Sci. Technol*. 18, 903–908.

Oliver, B.G., Charlton, M.N., Durham, R.W. (1989) Distribution, redistribution, and geochronology of polychlorinated biphenyl congeners and other chlorinated hydrocarbons in Lake Ontario sediments. *Environ. Sci. Technol*. 23, 200–208.

Oliver, B.G., Niimi, A.J. (1985) Bioconcentration factors of some halogenated organics for rainbow trout: Limitations in their use for prediction of environmental residues. *Environ. Sci. Technol.* 19, 842–849.

Oliver, B.G., Niimi, A.J. (1988) Tropodynamic analysis of polychlorinated biphenyl congeners and other chlorinated hydrocarbons in the Lake Ontario ecosystems. *Environ. Sci. Technol.* 22, 388–397.

Othman, M.A., Antonious, G.F., Khattab, M.M., Abdel-All, A., Khamis, A.E. (1987) Residues of dimethioate and methomyl on tomato and cabbage in relation to their effect on quality-related properties. *Environ. Toxicol. Chem.* 6, 947–952.

Ou, L.-T., Rao, P.S.C. (1986) Degradation and metabolism of oxamyl and phenamiphos in soils. *J. Environ. Sci. Health* B21, 25–40.

Ou, L.T., Sture, K., Edvardsson, V., Suresh, P., Rao, C. (1985) Aerobic and anaerobic degradation of aldicarb in soils. *J. Agric. Food Chem.* 33, 72–78.

Oubina, A., Ferrer, I, Gascon, J., Barcelo, D. (1996) Disappearance of aerially applied fenitrothion in rice crop waters. *Environ. Sci. Technol.* 30, 3551–3557.

Pait, A.W., De Souza, A.E., Farrow, D.R.G. (1992) *Agricultural Pesticide Use in Coastal Areas: A National Summary*. National Oceanic and Atmospheric Administration, Rockville, Maryland.

Paraiba, L.C., Carrasco, J.M., Bru, R. (1999) Level IV Fugacity model by a continuous time control system. *Chemosphere* 38, 1763–1775.

Paris, D.F., Lewis, D.L. (1976) Accumulation of methoxychlor by microorganisms. *Bull. Environ. Contam. Toxicol.* 15, 24–32.

Paris, D.F., Lewis, D.L., Barnett, J.T. (1977) Bioconcentration of toxaphene by microorganisms. *Bull. Environ. Contam. Toxicol.* 17, 564–573.

Paris, D.F., Lewis, D.L., Barnett, J.T., Baughman, G.L. (1975a) Microbial Degradation and Accumulation of Pesticides in Aquatic Systems. Report No. U.S.EPA-660/3–75–007, US EPA, Athens, Georgia.

Paris, D.F., Lewis, D.L., Wolfe, N.L. (1975b) Rates of degradation of malathion by bacteria isolated from aquatic system. *Environ. Sci. Technol.* 9, 135–138.

Paris, D.F., Steen, W.C., Baughman, G.L. (1978) Prediction of microbial transformation of pesticides in natural waters. (unpublished), presented before the American Chemical Society, Division of Pesticide Chemistry, Anaheim, Calif., Environmental Research Laboratory, U.S. EPA, Athens, Georgia.

Paris, D.F., Steen, W.C., Baughman, G.L., Barnett, J.T. (1981) Second-order model to predict microbial degradation of organic compounds in natural waters. *Appl. Environ. Microbiol.* 41, 603–609.

Park, K.S., Bruce, W.N. (1968) The determination of the water solubility of aldrin, dieldrin, heptachlor and heptachlor epoxide. *J. Econ. Entomol.* 61(3), 770–774.

Park, S.S., Erstfeld, K.M. (1997) A numerical kinetic model for bioaccumulation of organic chemicals in sediment-water system. *Chemosphere* 34, 419–427.

Parrish, P.R. (1974) Aroclor 1254, DDT and DDD, and dieldrin: Accumulation and loss by American oysters (*Crassostrea virginica)* exposed continuously for 56 weeks. *Proc. Natl. Shellfish Assoc.* 64, 7.

Parrish, P.R., Dyar, E.E., Enos, J.M., Wilson, W.G. (1978) Chronic toxicity of chlordane, trifluralin, and pentachlorophenol to sheepshead minnows (*Cyprinodon variegatus*). *EPA Ecol. Res. Ser.* EPA-600/3–78–010. U.S. EPA, Gulf Breeze, Florida.

Parrish, P.R., Dyar, E.E., Lindberg, M.A., Shanika, C.M., Enos, J.M. (1977) Chronic toxicity of methoxychlor, malathion and carbofuran to sheepshead minnows (*Cyprinodon variegatus*). NTIS PB-272101.

Parrish, P.R., Schimmel, S.C., Hansen, D.J., Patrick, J.M., Jr., Forester, J. (1976) Chlordane: Effects on several estuarine organisms. *J. Toxicol. Environ. Health* 1, 485.

Paschke, A., Schüürmann, G. (1998) Octanol/water-partitioning of four HCH isomer at 5, 25, and 45°C. *Fresenius Environ. Bull.* 7, 25–263.

Pasarela, N.R., Brown, R.G., Shaffer, C.B. (1962) Insecticide residues in meat and milk. Feeding of malathion to cattle; residue analyses of milk and tissue. *J. Agric. Food Chem.* 10, 7–9.

Passivirta, J., Sinkonen, S., Mikkelson, P., Rantio, T., Wania, F. (1999) Estimation of vapor pressures, solubilities and Henry's law constants of selected persistent organic pollutants as functions of temperature. *Chemosphere* 39, 811–832.

Paterson, S., Mackay, D. (1985) The fugacity concept in environmental modelling. In: *The Handbook of Environmental Chemistry.* Vol. 2, Part C, Hutzinger, O., Ed., pp. 121–140, Springer-Verlag, Heidelberg, Germany.

Paterson, S., Mackay, D., Bacci, E., Calamari, D. (1991) Correlation of the equilibrium and kinetics of leaf-air exchange of hydrophobic organic chemicals. *Environ. Sci. Technol.* 25, 866–871.

Pavlou, S.P., Weston, D.P. (1983, 1984) Initial Evaluation of Alternatives for Development of Sediment Related Criteria for Toxic Contaminants in Marine Waters (Puget Sound), Phase I and II. EPA Contract No. 68–01–6388, US EPA.

Perrin, D.D. (1989) *pK_a Prediction for Organic Acids and Bases.* Chapman & Hall, New York.

Platford, R.F. (1981) The environmental significance of surface films. II. Enhanced partitioning of lindane in thin films of octanol on the surface of water. *Chemosphere* 10(7), 719–722.

Platford, R.F. (1982) Pesticide partitioning in artificial surface films. *J. Great Lakes Res.* 8, 307–309.

Platford, R.F. (1983) The octanol-water partitioning of some hydrophobic and hydrophilic compounds. *Chemosphere* 12, 1107–1111.

Platford, R F., Carey, J.H., Hale, E.J. (1982) The environmental significance of surface films: Part 1. Octanol-water partition coefficients for DDT and hexachlorobenzene. *Environ. Pollution* (series B), 125–128.

Plato, C. (1972) Differential scanning calorimetry as a general method for determining the purity and heat of fusion of high purity organic chemicals. Application to 64 compounds. *Anal. Chem.* 44, 1531–1534.

Plato, C., Glasgow, A.R., Jr. (1969) Differential scanning calorimetry as a general method for determining the purity and heat of fusion of high purity organic chemicals. Application to 95 compounds. *Anal. Chem.* 41, 330–336.

Pontolillo, J., Eganhouse, R.P. (2001) *The Search for Reliable Aqueous Solubility (S_W) and Octanol-Water Partition Coefficient (K_{OW}) Data for Hydrophobic Organic Compounds: DDD and DDE as a Case Study.* U.S. Geological Survey, Water Resources Investigations Report 01-4201, Reston, VA.

Porter, P.E. (1964a) Aldrin. In: *Analytical Methods for Pesticides, Plant Growth Regulators and Food Additives.* Vol. 2, Zweig, G., Editor, p. 1–, Academic Press, New York.

Porter, P.E. (1964b) Dieldrin. In: *Analytical Methods for Pesticides, Plant Growth Regulators and Food Additives.* Vol. 2, Zweig, G., Editor, pp. 143–163, Academic Press, New York.

Portier, R.J. (1985) In: *ASTM STP 865.* (Validat. Predict. Lab Methods Assess. Fate Eff. Contam. Aquat. Ecosyst.), pp. 14–30.

Potter, J.C., Marxmiller, R.L., Barber, G.F., Young, R., Loefller, J.E., Burton, W.B., Dixon, L.D. (1974) Total ^{14}C residues and dieldrin residues in milk and tissues of cows fed dieldrin-^{14}C. *J. Agric. Food Chem.* 22, 889–899.

Quaife, M.L., Winbush, J.S., Fitzhugh, O.G. (1967) Survey of quantitative relations between ingestion and storage of aldrin and dieldrin in animals and man. *Fed. Cosmet. Toxicol.* 5, 39–50.

Quellette, R.P., King, J.A. (1977) *Chemical Week. Pesticide Register.* McGraw-Hill, New York.

Racke, K.D. (1993) Environmental fate of chlorpyrifos. *Rev. Environ. Contam. Toxicol.* 131, 1–150.

Racke, K.D., Steele, K.P., Yoder, R.M., Dick, W.A., Avidov, E. (1996) Factors affecting the hydrolytic degradation of chlorpyrifos in soil. *J. Agric. Food Chem.* 44, 1582–1592.

Radelleff, R.D., Bushland, R.C., Claborn, H.V. (1952) *Insects: The Yearbook of Agriculture.* U.S. Dept. of Agriculture, Washington DC.

Ramamoorthy, S. (1985) Competition of fate processes in the bioconcentration of lindane. *Bull. Environ. Contam. Toxicol.* 34, 349–358.

Rao, P.S.C., Davidson, J.M. (1979) Adsorption and movement of selected pesticides at high concentrations in soils. *Water Res.* 13, 375–380.

Rao, P.S.C., Davidson, J.M. (1980) Estimation of pesticide retention and transformation parameters required in nonpoint source pollutant models. In: *Environmetal Impact of Nonpoint Pollution.* Overcash, M.R., Davidson, J.M., Editors, Ann Arbor Science Publishers, Ann Arbor, Michigan.

Rao, P.S.C., Davidson, J.M. (1982) Retention and Transformation of Selected Pesticides and Phosphorus in Soil Water System: A Critical Review. U.S. EPA-600/S3-82-060.

Rao, P.S.C. et al. (1984) Degradation and sorption of aldicarb and metolachlor in Dougherty Plains soils. Progress report to U.S. EPA of EPA Co-operative Agreement CR-810464.

Reich, A.R., Perkins, J.L., Cutter, G. (1986) DDT contamination of a North Alabama aquatic ecosystem. *Environ. Toxicol. Chem.* 5, 725–736.

Reinert, R.E. (1967) The accumulation of deldrin in an algal (*Scenedesmus obliquus),* daphnia (*Daphnia magna*), guppy (*Lebistes reticulatus*) food chain. *Diss. Abstr.* 28, 2210-B.

Reinert, R.E. (1972) The accumulation of deldrin in an alga (*Scenedesmus obliquus),* daphnia (*Daphnia magna*), guppy (*Lebistes reticulatus*). *J. Fish Res. Board Can.* 29, 1413–1418.

Reish, D.J., Kauwling, T.J., Mearns, A.J., Oshida, P.S., Rossi, S.S., Wilkes, F.G., Ray, M.J. (1978) Marine and estuarine pollution. *J. Water Pollut. Control Fed.* 50, 1424–1469.

Renberg, L. (1981) Gas chromatographic determination of chlorophenols in environmental samples. *National Swedish Environment Protection Board Report* 1410, 135pp.

Renberg, L., Sundström, G. (1979) Prediction of bioconcentration potential of organic compounds using partition coefficients derived from reversed phase thin layer chromatography. *Chemosphere* 7, 449–459.

Renberg, L., Sundström, G., Rosen-Olofsson, S. (1985) The determination of partition coefficients of organic compounds in technical products and waste waters for the estimation of their bioaccumulation potential using reversed phase thin layer chromatography. *Toxicol. Environ. Chem.* 10, 333–349.

Renner, G. (1990) Gas chromatographic studies of chlorinated phenols, chlorinated anisoles, and chlorinated phenylacetates. *Toxicol. Environ. Chem.* 27, 217–224.

Rice, C.P., Chernyak, S.M., Hapeman, C.J., Bilboulian, S. (1997a) Air-water distribution of the endosulfan isomers. *J. Environ. Qual*. 26, 1101–1106.

Rice, C.P., Chernyak, S.M., McConnell, L.L. (1997b) Henry's law constants for pesticides measured as a function of temperature and salinity. *J. Agric. Food Chem.* 45, 2291–2298.

Richards, A.G., Cutkomp, L.K. (1946) Correlation between the possession of a chitinous cuticle and sensitivity to DDT. *Biol. Bull.* 90, 97–108.

Richards, R.P., Baker, D.B. (1993) Pesticide concentration patterns in agricultural drainage networks in the Lake Erie basin. *Environ. Toxicol. Chem*. 12, 13–26.

Richardson, G., Qadri, S.U. (1986) Tissue distribution of ^{14}C-labeled residues of aminocarb in brownhead (*Ictalurus nebulosus Le Sueur)* following acute exposure. *Ecotoxicol. Environ. Saf.* 12, 180–186.

Richardson, L.T., Miller, D.M. (1960) Fungitoxicity of chlorinated hydrocarbon insecticides in relation to water solubility and vapor pressure. *Can. J. Botany* 38, 163–175.

Roark, R.C. (1951) A digest of information on chlordane. U.S. Dept. of Agriculture, Bureau Entomol. and Plant Quarantine E-817. 132 pp.

Robeck, G.G., Dostal, K.K., Cohen, J.M., Dreissal, J.F. (1965) Effectiveness of water treatment processes in pesticide removal. *J. Am. Water Works Assn.* 57, 181–200.

Roberts, J.R., De Frietas, A.S.W., Gidney, M.A.J. (1977) Influence of lipid pool size on bioaccumulation of the insecticide chlordane by northern redhorse suckers (*Moxostoma macrolepidotum*). *J. Fish Res. Board Can*. 34, 89.

Robinson, J., Roberts, M., Baldwin, M., Walker, A.I.T. (1969) Pharmacokinetics of HEOD (dieldrin) in the rat. *Fed. Cosmet. Toxicol*. 7, 317–332.

Rordorf, B.F. (1989) Unpublished data, private communication.

Rose, F L., McIntire, C.D. (1970) Accumulation of dieldrin by benthic algae in laboratory streams. *Hydrobiologia* 35, 481.

Rothman, A.M. (1980) Low vapor pressure determination by the radiotracer transpiration method. *J. Agric. Food Chem.* 28, 1225–1228.

Ruelle, P., Kesselring, U.W. (1997) Aqueous solubility prediction of environmentally important chemicals from the mobile order thermodynamics. *Chemosphere* 34(2), 275–298.

Ruzicka, J.H., Thomson, J., Wheals, B.B. (1967) The gas chromatographic determination of organophosphorous pesticides. Part II. A comparative study of hydrolysis rates. *J. Chromatogr.* 31, 37–47.

Ryan, J.A., Bell, R.M., Davidson, J.M., O'Connor, G.A. (1988) Plant uptake of non-ionic organic chemicals from soils. *Chemosphere* 17, 2299–2322.

Saarikoski, J., Viluksela, M. (1982) Relation between physicochemical properties of phenols and their toxicity and accumulation in fish. *Ecotoxicol. Environ. Saf.* 6, 501–512.

Saarikoski, J., Lindström, R., Tyynelä, M., Viluksela, M. (1986) Factors affecting the absorption of phenolics and carboxylic acids in the guppy (*Poecilia reticulata). Ecotoxicol. Environ. Saf.* 11, 158–173.

Sabljic, A. (1984) Prediction of the nature and strength of soil sorption of organic pollutants by molecular topology. *J. Agric. Food Chem.* 32, 243–246.

Sabljic, A. (1987a) On the prediction of soil sorption coefficients of organic pollutants from molecular structure: Application of molecular topology model. *Environ. Sci. Technol.* 21, 358–366.

Sabljic, A. (1987b) Nonempirical modeling of environmental distribution and toxicity of major organic pollutants. In: *QSAR in Environmental Toxicology*-II. Kaiser, K.L.E., Editor, pp. 309–322, D. Reidel Publ. Co., Dordrecht, The Netherlands.

Sabljic, A., Güsten, H., Verhaar, H., Hermens, J. (1995) QSAR modelling of soil sorption. Improvements and systematics of log K_{OC} vs. log K_{OW} correlations. *Chemosphere* 31, 4489–4514.

Saha, J.G. (1969) Significance of organochlorine insecticide residues in fresh plants as possible contaminants and beef products. *Res. Rev.* 26, 89–126.

Sahsuvar, L., Helm, P.A., Jantunen, L.M., Bidleman, T.F. (2003) Henry's law constants for α-, β-, and γ-hexachlorocyclohexanes (HCHs) as a function of temperature and revised estimates of gas exchange in Arctic regions. *Atmos. Environ*. 37, 983–992.

Saito, S., Tanoue, A., Matsuo, M. (1992) Applicability of the i/o-characters to a quantitative description of bioconcentration of organic chemicals in fish. *Chemosphere* 24(1), 81–87.

Saito, S., Koyasu, J., Yoshida, K., Shigeoka, T., Koike, S. (1993) Cytotoxicity of 109 chemicals to goldfish GFS cells and relationships with 1-octanol/water partition coefficients. *Chemosphere* 26, 1015–1028.

Saleh, F.Y., Dickson, K.L., Rodgers, Jr. J.H. (1982) Fate of lindane in the aquatic environment: Rate constants of physical and chemical processes. *Environ. Toxicol. Chem.* 1, 289–297.

Samanidou, V., Fytianos, K., Pfister, G., Bahadir, M. (1988) Photochemical decomposition of waters of Northern Greece. *Sci. Total Environ.* 76, 85–92.

Sanborn, J.R., Metcalf, W.N.B., Bruce, W.N., Lu, P.Y. (1976) The fate of chlordane and toxaphene in a terrestrial-aquatic model ecosystem. *Environ. Entomol.* 5(3), 533–538.

Sancho, E., Ferrando, M.D., Andreu, E., Gamon, M. (1993) Bioconcentration and excretion of diazinon by eel. *Bull. Environ. Contam. Toxicol.* 50, 578–585.

Sanders, P.F., Jones, K.C., Hamilton-Taylor, J. (1993) A simple method to assess the susceptibility of polynuclear aromatic hydrocarbons to photolytic decomposition. *Atmos. Environ.* 27A, 139–144.

Sanders, P.F., Seiber, J.N. (1984) Organophosphorus pesticides volatilization. Model soil pits and evaporation ponds. In: *Treatment and Disposal of Pesticide Wastes*. Krueger, R.F., Seiber, J.N. Editors, Am. Chem. Soc. Sym. Series 259, 279–295.

Sangster, J. (1993) LOGKOW Databank, Sangster Research Laboratory, Montreal, Quebec.

Sattar, M.A. (1990) Fate of organophosphorus pesticides in soils. *Chemosphere* 20, 387–396.

Schauberger, C.W., Wildman, R.B. (1977) Accumulation of aldrin and dieldrin by blue-green algae and related effects on photosynthetic pigments. *Bull. Environ. Contam. Toxicol.* 17, 534–541.

Schimmel, S.C., Patrick, Jr., J.M., Forester, J. (1976) Heptachlor: Uptake, depuration, retention, and metabolism by spot (*Leiostromus xanthurus*). *J. Toxicol. Environ. Health* 2, 169.

Schimmel, S.C., Patrick, Jr., J.M., Forester, J. (1977) Toxicity and bioconcentration of BHC and lindane in selected estuarine animals. *Arch. Environ. Contam. Toxicol.* 6, 355–363.

Schimmel, S.C., Garnas, R.L., Patrick, Jr., J.M., Moore, J.C. (1983) Acute toxicity, bioconcentration, and persistence of AC 222, 705, benthiocarb, chlorpyrifos, fenvalerate, methyl parathion, and permethrin in the estuarine environment. *J. Agric. Food Chem.* 31, 104–113.

Schellenberg, K., Leuenberger, C., Schwarzenbach, R.P. (1984) Sorption of chlorinated phenols by natural sediments and aquifer materials. *Environ. Sci. Technol.* 18, 652–657.

Schmidt-Bleek, F., Haberland, W., Klein, A.W., Caroli, S. (1982) Steps toward environmental hazard assessment of new chemicals (including a hazard ranking scheme, based upon directive 78/831/EEC). *Chemosphere* 11, 383–415.

Schnoor, J.L. (1992) 1, Chemical fate and transport in the environment. In: *Fate of Pesticides and Chemicals in the Environment.* Schnoor, J.L., Editor, pp. 1–24, John Wiley & Sons, New York.

Schnoor, J.L., Editor (1992) *Fate of Pesticides and Chemicals in the Environment.* John Wiley & Sons, New York.

Schnoor, J.L., McAvoy, D.C. (1981) Pesticide transport and bioconcentration model. *J. Environ. Eng. Div.* (*Am. Soc. Civ. Eng.*) 107(EE6), 1229–1246.

Schnoor, J.L., Sato, C., McKechnie, D., Sahoo, D. (1987) Processes, Coefficients, and Models for Simulating Toxic Organics and Heavy Metals in Surface Waters. EPA 600/3–87–015. US EPA, Athens, Georgia.

Schomburg, C.J., Glotfelty, D.E., Seiber, J.N. (1991) Pesticide occurrence and distribution in fog collected near Monterey, California. *Environ. Sci. Technol.* 25, 155–160.

Schreitmüller, J., Ballschmiter, K. (1995) Air-water equilibrium of hexachlorocyclohexanes and chloromethoxy-benzenes in North and South Atlantic. *Environ. Sci. Technol.* 29, 207–215.

Scow, K.M. (1982) Rate of biodegradation. In: *Handbook of Chemical Property Estimation Methods.* Lyman, W.J., Rechl, W.F., Rosenblatt, D.H., Editors, pp. 9–1 to 9–84, McGraw-Hill, New York.

Seguchi, K., Asaka, S. (1981) Intake and excretion of diazinon in freshwater fishes. *Bull. Environ. Contam. Toxicol.* 27, 244–249.

Seiber, J.N. (1987) Solubility, partition coefficient and bioconcentration factor. In: *Fate of Pesticides in the Environment.* Biggar, J.W., Seiber, J.N., Editors, publication 3320 of the Agricultural Experiment Station, Division of Agriculture and Nature Resources, University of California, Oakland, California. pp. 53–59.

Seiber, J.N., Catahan, M P., Barril, C.R. (1978) Loss of carbofuran from rice paddy water: Chemical and physical factors. *J. Environ. Sci. Health* B13, 131–148.

Seiber, J.N., Madden, S.C., McChesney, M.M., Winterlin, W.N. (1979) Toxaphene dissipation from treated cotton field environments: Component residual behaviour on leaves and in air, soil, and sediments determined by capillary gas chromatography. *J. Agric. Food Chem.* 27, 284.

Seiber, J.N., McChesney, M.M. (1987) Measurement and computer model simulation of the volatilization flux of molinate and methyl parathion from a flooded rice field. Final Report to Department of Food and Agriculture, Sacramento, California.

Seiber, J.N., McChesney, M.M., Woodrow, J.E. (1989) Airborne residues resulting from use of methyl parathion, molinate and thiobencarb on rice in the Sacramento Valley, California. *Environ. Toxicol. Chem.* 8, 577–588.

Seiber, J.N., Woodrow, J.E., Sanders, P.F. (1981) Estimation of ambient vapor pressures of pesticides from gas chromatographic retention data. Abstract, 183rd Am. Chem. Soc. Meeting, New York.

Sethunathan, N., MacRae, I.C. (1969) Persistence and biodegradation of diazinon in submerged soils. *J. Agric. Food Chem.* 17(2), 221–225.

Sharom, M.S., Miles, J.R.W., Harris, C.R., McEwen, F L. (1980) Persistence of 12 insecticides in water. *Water Res.* 14, 1089–1093.

Sharom, M., Miles, J.R.W., Harris, C R., McEwen, F.L. (1980) Behaviour of 12 insecticides in soil and aqueous suspensions of soil and sediment. *Water Res.* 14, 1095–1100.

Shen, L., Wania, F. (2005) Compilation, evaluation, and selection of physical-chemical property data for organochlorine pesticides. *J. Chem. Eng. Data* vol. pp. 50, 740–768.

Shigeoka, T., Yamagata, T., Minoda, T., Yamauchi, F. (1988) Acute toxicity and hatching inhibition of chlorophenol to Japanese medaka, *Oryzias latipes*, and structure-activity relationships. *Jpn. J. Toxicol. Environ. Health* 34, 343–349.

Shoeib, M., Harner, T. (2002) Using measured octanol-air partition coefficients to explain environmental partitioning of organochlorine pesticides. *Environ. Toxicol. Chem.* 21, 984–990.

Sicbaldi, F., Finizio, A. (1993) K_{OW} estimation by combination of RP-HPLC and molecular indexes for a heterogeneous set of pesticide. In: *Proceedings IX Symposium Pesticide Chemistry, Mobility and Degradation of Xenobiotics.* 11–13, Oct 1993, Piacenza, Italy.

Siebers, J., Gottschild, D., Nolting, H.-G. (1994) Pesticides in precipitation in Northern Germany. *Chemosphere* 28(8), 1559–1570.

Siebers, J., Mattusch, P. (1996) Determination of airborne residues in greenhouses after application of pesticides. *Chemosphere* 33(8), 1597–1607.

Sillén, L.G., Martell, A.E. (1971) *Stability Constants of Metal-Ion Complexes.* Supplement No. 1, Spec. Publ. No. 25, The Chemical Society, London, England.

Simpson, C.D., Wilcock, R.J., Smith, T.J., Wilkins, A.L., Langdon, A.G. (1995) Determination of octanol-water partition coefficients for the major components of technical chlordane. *Bull. Environ. Contam. Toxicol.* 55, 149–153.

Skea, J.C., Simonin, H.J., Symula, J. (1981) Accumulation and retention of mirex by brook trout fed a contaminated diet. *Bull. Environ. Contam. Toxicol.* 27, 79–83.

Slade, R.E. (1945) The γ-isomer of hexachlorocyclohexane (Gammexane). An insecticide with outstanding properties. *Chem. Ind.* 40, 314–319.

Slater, R.M., Spedding, D.J. (1981) Transport of dieldrin between air and water. *Arch. Environ. Contam. Toxicol.* 10, 25–33.

Smelt, J.H., Dekker, A., Leistra, M. (1979) *Neth. J. Agric. Sci.* 27, 191–198.

Smelt, J.H., Dekker, A., Leistra, M., Houx, N.W.H. (1983) Conversion from carbamoyloximes in soil samples from above and below the soil water table. *Pest. Sci.* 14, 173–181.

Smelt, J.H., Leistra, M., Houx, N.W.H., Dekker, A. (1978) Conversion rates of aldicarb and its oxidation products in soils. III. Aldicarb. *Pest. Sci.* 9, 293–300.

Smith, A.D., Bharath, A., Mallard, C., Orr, D., McCarty, L.S., Ozbum, G.W. (1990) Bioconcentration kinetics of some chlorinated benzenes and chlorinated phenols in American flagfish, *Jordanella floridae* (Goode and Bean). *Chemosphere* 20, 379–386.

Smith, J.H., Mabey, W.R., Bahonos, N., Holt, B.R., Lee, S.S., Chou, T.W., Venberger, D., Mill, T. (1978) Environmental pathways of selected chemicals in freshwater systems: Part II. Laboratory Studies. Interagency Energy-Environmental Research Program Report. EPA-600/7–78–074. Environmental Research Laboratory Office of Research and Development. U.S. EPA, Athens, Georgia.

Smith, P.D., Brockway, D.L., Stancil, F.E., Jr. (1987) Effect of hardness, alkalinity and pH on toxicity of pentachlorophenol to *Selenastrum capricornutum* (printz). *Environ. Toxicol. Chem.* 6, 891–900.

Söderström, M., Wachtmeister, C.A., Förlin, L. (1994) Analysis of chlorophenolics from bleach Kraft Mill effluents (BKME) in bile of perch (*Perca fluviatilis*) from the Baltic Sea and development of an analytical procedure also measuring chlorocatechols. *Chemosphere* 28, 1701–1719.

Somasundaram, L., Coats, J.R., Racke, K.D. (1991) Mobility of pesticides and their hydrolysis metabolites in soil. *Environ. Toxicol. Chem.* 10, 185–194.

Soon, L.G., Hock, O.S. (1987) Environmental problems of pesticide usage in Malaysian rice-fields. In: *Management of Pests and Pesticides.* Tait, J., Napompeth, B., Editors, pp. 10–21, Westview, London, United Kingdom.

Sotomatsu, T., Nakagawa, Y., Fujita, T. (1987) Quantitative structure-activity studies of benzoylphenylurea larvicides. IV. Benzoyl ortho substituent effects and molecular conformation. *Pestic. Biochem. Physiol.* 27, 156–164.

Spain, J.C., Pritchard, P., Bourquin, A.W. (1980) Effects of adaptation on biodegradation rates in sediment water cores from estuarine and freshwater environments. *Appl. Environ. Microbiol.* 40, 726–734.

Spehar, R.L., Tanner, D.K., Nordling, B.R. (1983) Toxicity of the synthetic pyrethroids, permethrin and AC 222, 705 and their accumulation in early life stages of fathead minnows and snails. *Aquatic Toxicol.* 3, 171–182.

Spencer, E.Y. (1976) Vapor pressure and vapor loss. In: *A Literature Survey of Bench-mark Pesticides.* Medical Center, Dept. of Medical and Public Affairs, Science Communication Division, The George Washington University, Washington, DC.

Spencer, E.Y., Editor (1982) *Guide to the Chemicals Used in Crop Protection.* 7th Edition, Research Branch Agriculture Canada, Ontario, Canada.

Spencer, J.R., Hermandez, B.Z., Schneider, F.A., Gonzales, M., Begum, S., Krieger, R.I. (1992) Seasonal mevinphos degradation on row crops in Monterey county, 1990. *Chemosphere* 24, 773–777.

Spencer, W.F. (1975) Movement of DDT and its derivatives into the atmosphere. *Res. Rev.* 59, 91–117.

Spencer, W.F., Cliath, M.M. (1968) Vapor density of dieldrin. *Environ. Sci. Technol.* 3, 670–674.

Spencer, W F., Cliath, M.M. (1970) Vapor density and apparent vapor pressure of lindane (γ BHC). *J. Agric. Food Chem.* 18(3), 529–530.

Spencer, W.F., Cliath, M.M. (1972) Volatility of DDT and related compounds. *J. Agric. Food Chem.* 20, 645–649.

Spencer, W.F., Shoup, T.D., Cliath, M.M., Farmer, W.J., Haque, R. (1979) Vapor pressure and relative volatility of ethyl and methyl parathion. *J. Agric. Food Chem.* 27, 273–278.

Spiller, D. (1961) A digest of available information on insecticide malathion. *Adv. Pest. Control Res.* 4, 249.

SRI International (1980) Interim Report on Task No. 11, Contract No. 68–01–3867, U.S. EPA Monitoring and Data Support Div., Office of Water Regulations and Standards, Washington, DC.

Statham, C.N., Melancon, Jr., M.J., Leck, J.L. (1976) Bioconcentration of xenobiotics in trout bile: A proposed monitoring aid for some water borne chemicals. *Science* 193, 680–681.

Staudinger, J., Roberts, P.V. (1996) A critical review of Henry's law constants for environmental application. *Crit. Rev. Environ. Sci. Technol.* 26, 205–297.

Staudinger, J., Roberts, P.V. (2001) A critical compilation of Henry's law constant temperature dependence relations for organic compounds in dilute aqueous solutions. *Chemosphere* 44, 561–576.

Stehly, G.R., Hayton, W.L. (1990) Effect of pH on the accumulation kinetics of penta-chlorophenol in goldfish. *Arch. Environ. Contam. Toxicol.* 19, 464–470.

Stephen, H., Stephen, T. (1963) *Solubilities of Inorganic and Organic Compounds.* Vols. I and II, MacMillan Co., New York.

Stephenson, R.M., Malanowski, A. (1987) *Handbook of the Thermodynamics of Organic Compounds.* Elsevier, N.Y.

Stephenson, R.R. (1982) Aquatic toxicity of cypermethrin. I. Acute toxicity to some freshwater fish and invertebrates in laboratory tests. *Aquatic Toxicology* 2, 175–185.

Stewart, D.K.R., Chisholm, D. (1971) Long term persistence of BHC, DDT and chlordane in a sandy loam clay. *Can. J. Soil Sci.* 61, 379–383.

Sugiura, K., Aoki, M., Kaneko, S., Daisaku, I., Komatsu, Y., Shibuya, H., Suzuki, H., Goto, M. (1984) Fate of 2,4,6-trichlorophenol, pentachlorophenol, *p*-chlorobiphenyl, and hexachlorobenzene in an outdoor experimental pond: Comparison between observations and predictions based on laboratory data. *Arch. Environ. Contam. Toxicol.* 13, 745–758.

Sugiura, K., Washino, T., Hattori, M., Sato, E., Goto, M. (1979) Accumulation of organo-chlorines in fishes-Difference of accumulation factors by fishes. *Chemosphere* 8(6), 359–364.

Sukop, M., Cogger, C.G. (1992) Adsorption of carbofuran, metalaxyl, and simazine: K_{OC} evaluation and relation to soil transport. *J. Environ. Sci. Health* B27(5), 565–590.

Sun, H., Xu, J., Yang, S., Liu, G., Dai, S. (2004) Plant uptake of aldicarb from contaminated soil and it enhanced degradation in the rhizosphere. *Chemosphere* 54, 569–574.

Suntio, L.R., Shiu, W.Y., Mackay, D., Seiber, J.N., Glotfelty, D. (1988) Critical review of Henry's law constants. *Rev. Environ. Contam. Toxicol.* 103, 1–59.

Sutherland, G.L., Giang, P.A., Archer, T.E. (1980) In: *Analytical Methods for Pesticides and Plant Growth Regulators.* Vol. 11, Zweig, G., Editor, pp. 487–505, Academic Press, New York.

Svenson, S., Björndal, H. (1988) A convenient test method for photochemical transformation of pollutants in the aquatic environment. *Chemosphere* 17, 2397–2405.

Swann, R.L., Laskowski, D.A., McCall, P.J., Vander, Kuy K., Dishburger, H.J. (1983) A rapid method for estimation of the environmental parameters octanol/water partition coefficient, soil sorption constant, water to air ratio, and water solubility. *Res. Rev.* 85, 17–28.

Swoboda, A.R., Thomas, G.W. (1968) Movement of parathion in soil columns. *J. Agric. Food Chem.* 16, 923–927.

Szeto, S.Y., MacCarthy, H.R., Oloffs, P.C., Shepherd, R.F. (1979) The fate of acephate and carbaryl in water. *J. Environ. Sci. Health*. B14, 635–654.

Szeto, S.Y., Vernon, R.S., Brown, M.J. (1983) Degradation of disulfoton in soil and its translocation into asparagus. *J. Agric. Food Chem.* 31, 217–220.

Tafuri, F., Businelli, M., Scarponi, L., Marucchini, C.J. (1977) Decline and movement of AG chlordane in soil and its residues in alfalfa. *J. Agric. Food Chem*. 25, 353–356.

Takase, I., Oyama, H. (1985) Uptake and bioconcentration of disulfoton and its oxidation compounds in carp, *Cyprinus carpio L. Nippon Noyaku Gakkaishi* 10, 47–53.

Takimoto, Y., Miyamoto, J. (1976) Studies on the accumulation and metabolism of sumithion in fish. *J. Pest. Sci.* 1, 261–271.

Takimoto, Y., Ohshima, M., Miyamoto, J. (1987) Comparative metabolism of fenitrothion in aquatic organisms. I. Metabolism in the euryhaline fish, *Oryzalias latipes* and *Mugil cephalus*. *Ecotox. Environ. Saf.* 13, 104–117.

Takimoto, Y., Ohshima, M., Yamada, H., Miyamoto, J. (1984) Fate of fenitrothion in several developmental stages of the killifish (*Oryzalias latipes*). *Arch. Environ. Contam. Toxicol.* 13, 579–587.

Taylor, A.W., Glotfelty, D.E. (1988) Evaporation from soils and crops. In: *Environmental Chemistry of Herbicides.* Vol. I, Grover, R., Editor, pp. 89–130, CRC Press, Boca Raton, Florida.

Taylor, A.W., Spencer, W.F. (1990) Volatilization and vapor transport processes. In: *Pesticides in the Soil Environment: Processes, Impacts, and Modeling.* Cheng, H.H., Editor, pp. 213–269, Soil Science Society of America, Madison, Wisconsin.

Tejada, A.W. (1995) Pesticide residues in foods and the environment as a consequence of crop protection. *Philipp. J. Agric.* 78, 63–79.

Tejada, A.W., Magallona, E.D. (1985) Fate of carbosulfan in a rice paddy environment. *Philipp. Entomol.* 6, 255–273.

Tejada, A.W., Varca, L.M., Ocampo, P., Bajet, C.M., Magallona, E.D. (1993) Fate and residues of pesticides in rice production. *Int. J. Pest. Manage.* 39, 281–287.

Terada, H., Kosuge, Y., Murayama, W., Nakaya, N., Nunogaki, Y., Nunogaki, K.-I. (1987) Correlation of hydrophobic parameters of organic compounds determined by centrifugal partition chromatography with partition coefficients between octanol and water. *J. Chromatogr.* 400, 343–351.

Thibodeaux, L.J. (1979) *Chemodynamics.* John Wiley & Sons, New York.

Thomann, R.V. (1989) Bioaccumulation model of organic chemical distribution in aquatic food chains. *Environ. Sci. Technol.* 23, 699–707.

Thomas, R.G. (1982) Chapter 15: Volatilization from water, and Chapter 16: Volatilization from soil. In: *Handbook of Chemical Property Estimation Methods.* Lyman, W.J., Rechl, W.F., Rosenblatt, D.H., Editors, McGraw-Hill, New York.

Thor (1989) from Medchem Release 3.54, Daylight Chemical Information Systems, Claremont, California.

Tomlin, C. (1994) *The Pesticide Manual (A World Compendium).* 10th Ed., Incorporating the Agrochemicals Handbook. The British Crop Protection Council, Surrey, UK and The Royal Society of Chemistry, Cambridge, U.K.

Toyota, H., Kuwahara, M. (1967) The study on production of PCP chemical fertilizer and its effect as herbicide and fertilizer, the solubility in water of PCP in PCP chemical fertilizer. *Nippon Dojohiryogaku Zasshi* 38, 93–97.

Trapp, St., Pussemier, L. (1991) Model calculations and measurements of uptake and translocation of carbamates by bean plants. *Chemosphere* 22, 327–339.

Tratnyek, P.G., Hoigné, J. (1991) Oxidation of substituted phenols in the environment: A QSAR analysis of rate constants for reaction with singlet oxygen. *Environ. Sci. Technol.* 25, 626–631.

Travis, C.C., Arms, A.D. (1988) Bioconcentration of organics in beef, milk, and vegetation. *Environ. Sci. Technol.* 22, 271–274.

Trotter, D.M., Kent, R.A., Wong, M.P. (1991) Aquatic fate and effect of carbofuran. *Critical Reviews in Environ. Control* 21(2), 137–176.

Trujillo, D.A., Ray, L.E., Murray, H.E., Giam, C.S. (1982) Bioaccumulation of penta-chlorophenol by killifish (*Fundulus similus*). *Chemosphere* 11, 25–31.

Tsuda, T., Aoki, S., Inoue, T., Kojima, M. (1995) Accumulation and excretion of diazinon, fenthion and fenitrothion by killifish: Comparison of individual and mixed pesticides. *Water Res.* 29, 455–458.

Tsuda, T., Aoki, S., Kojima, M., Fujita, T. (1992) Pesticides in water and fish from rivers flowing into Lake Biwa (II). *Chemosphere* 24, 1523–1531.

Tsuda, T., Aoki, S., Kojima, M., Fujita, T. (1992) Accumulation and excretion of organo-phosphorus pesticides by willow shiner. *Chemosphere* 25(12), 1945–1951.

Tsuda, T., Aoki, S., Kojima, M., Fujita, T. (1993) Accumulation and excretion of organo-phosphorus pesticides by carp *Cyprinus carpio. Comp. Biochem. Physiol.* 104C(2), 275–278.

Tsuda, T., Aoki, S., Kojima, M., Harada, H. (1989) Bioconcentration and excretion of diazinon, IBP, malathion and fenitrothion by willow shiner. *Toxicol. Environ. Chem.* 24, 185–190.

Tsuzuki, M., (2000) Thermodynamic estimation of vapor pressure fo organophosphorus pesticides. *Environ. Toxiccol. Chem.* 19, 1717–2000.

Tsuzuki, M. (2001) Vapor pressures of carboxylic acid esters including pyrethroids: measurement and estimation from molecular structure. *Chemosphere* 45, 729–736.

Tucker, W.A., Lyman, W.J., Preston, A.L. (1983) Estimation of the dry deposition velocity and scavenging ratio for organic chemicals. In: *Precipitation Scavenging, Dry Deposition, and Resuspension.* Pruppacher, et al., Editors, pp. 1242–1256, Elsevier Science Publishing Co., New York.

Ugland, K., Lundanes, E., Greibrok, T., Bjoseth, A. (1981) Determination of chlorinated phenols by high-performance liquid chromatography. *J. Chromatogr.* 213, 83–90.

Ulmann, E. (1972) Lindane, Monograph of an Insecticide. Verlag K. Schillinger-Freiburg in Breisgau. p.16.

USDA (1989) Final environmental impact statement, vegetation management in the Piedmont and Coastal Plain. Southern Region Management Bulletin R8-MB-23, USDA Forest Service, Atlanta, Georgia.

USEPA (1984) Review of In-place Treatment for Contaminated Surface Soils. Vol. 1 and 2, U.S. EPA 540/2–84–003. U.S. EPA, Cincinnati, Ohio.

Valsaraj, K.T., Thibodeaux, L.J., Lu, X.-Y. (1991) Studies in batch and continuous solvent sublation. III. Solubility of pentachlorophenol in alcohol-water mixtures and its effects on solvent sublation. *Sep. Sci. Technol.* 26(4), 529–538.

Van Gestel, C.A.M., Ma, W.-C. (1988) Toxicity and bioaccumulation of chlorophenols in earthworms, in relation to bioavailability in soil. *Ecotoxicol. Environ. Saf.* 16, 289–297.

Veith, G.D., Austin, N.M., Morris, R.T. (1979a) A rapid method for estimation log P for organic chemicals. *Water Res.* 13, 43–47.

Veith, G.D., Defoe, D.L., Bergstedt, B.V. (1979b) Measuring and estimating the bioconcentration factor of chemicals in fish. *J. Fish Res. Board Can.* 26, 1040–1048.

Veith, G.D., Kosian, P. (1983) Estimating bioconcentration potential from octanol/water partition coefficients. In: *Physical Behavior of PCBs in the Great Lakes.* Mackay, D., Paterson, S., Eosemreocj. S.J., Simmons, M.S., Editors, Chapter 15, pp. 269–282, Ann Arbor Science, Ann Arbor, Michigan.

Veith, G.D., Macek, K.J., Petrocelli, S.R., Caroll, J. (1980) An evaluation of using partition coefficient and water solubilities to estimate bioconcentration factors for organic chemicals in fish. In: *Aquatic Toxicology.* ASTM STP 707, Eaton, J.G., Parrish, P.R., Hendricks, A.C., Editors, pp. 116–129, American Society for Testing and Materials, Philadelphia, Pennsylvania.

Veith, G.D., Morris, R.T. (1978) A Rapid Method for Estimating Log P for Organic Chemists. U.S. Environmental Protection Agency, ERL, Duluth, Minnesota.

Verschueren, K. (1977) *Handbook of Environmental Data on Organic Chemicals.* Van Nostrand Reinhold, New York.

Verschueren, K. (1983) *Handbook of Environmental Data on Organic Chemicals.* 2nd Edition, Van Nostrand Reinhold, New York.

Vigano, L., Galassi, S., Gatto, M. (1992) Factors affecting the bioconcentration of hexachlorocyclohexanes in early life stages of *Oncorhynchus mykiss*. *Environ. Toxicol. Chem.* 11, 535–540.

Voerman, S., Besemer, A.F.H. (1975) Persistence of dieldrin, lindane, and DDT in a light sandy soil and their uptake by grass. *Bull. Environ. Contam. Toxicol*. 13, 501–505.

Voerman, S., Tammes, P.M.L. (1969) Adsorption and desorption of lindane and dieldrin by yeast. *Bull. Environ. Contam. Toxicol*. 4, 271.

von Rümker, R., Horay, F. (1972) *Basic Information on Thirty-five Pesticide Chemicals. Pesticide Manual*. Part II, U.S. Agency for International Development.

Walsh, A.H., Ribelin, W.E. (1973) In: *The Pathology of Fish.* Ribelin, W.E., Migaki, G., Editors, University of Wisconsin Press, Madison, Wisconsin.

Walker, A.I., Stevenson, D.E., Robinson, J., Thorpe, E., Roberts, M. (1969) *Toxicol. Appl. Pharmacol*. 15, 345–373.

Walker, W.W., Cripe, C.R., Pritchard, P.H., Bourquin, A.W. (1988) Biological and abiotic degradation of xenobiotic compounds in *in vitro* esturine water and sediment/water system. *Chemosphere* 17, 2255–2270.

Walker, W.W., Stojanovic, B.J. (1973) Microbial versus chemical degradation of malathion in soil. *J. Environ. Qual*. 2, 229–232.

Wang, T.C., Hoffman, M.E. (1991) Degradation of organophosphorus pesticides in coastal water. *J. Assoc. Off. Anal. Chem.* 74(5), 883–886.

Wang, X., Harada, S., Watanabe, M., Koshikawa, H., Geyer, P.R. (1996) Modelling the bioconcentration of hydrophobic organic organisms. *Chemosphere* 32, 1783–1793.

Wania, F., Mackay, D. (1993) Global fractionation and cold condensation of low volatility organochlorine compounds in polar regions. *Ambio* 22, 10–18.

Wania, F., Mackay, D. (1993) Modelling the global distribution of toxaphene: A discussion of feasibility and desirability. *Chemosphere* 27, 2079–2094.

Wania, F., Mackay, D. (1996) Tracking the distribution of persistent organic pollutants. *Environ. Sci. Technol*. 30, 390A–396A.

Wania, F., Shiu, W.Y., Mackay, D. (1994) Measurements of the vapor pressure of several low-volatility organochlorine chemicals at low temperatures with a gas saturation method. *J. Chem. Eng. Data* 39, 572–577.

Wanner, O., Egli, T., Fleischmann, T., Lanz, K., Reichert, P., Schwazenbach, R.P. (1989) Behavior of the insecticides disulfolton and thiometon in the Rhine River: A chemodynamic study. *Environ. Sci. Technol*. 23, 1232–1242.

Ward, T.E. (1985) Characterizing the aerobic and anaerobic microbial activities in surface and subsurface soils. *Environ. Toxicol. Chem.* 4, 727–737.

Warner, H.P., Cohen, J.M., Ireland, J.C. (1980) Determination of Henry's Law Constants of Selected Priority Pollutants. *MERL,* Cincinnati, Ohio.

Warner, H.P., Cohen, J.M., Ireland, J.C. (1987) Determination of Henry's Law Constants of Selected Priority Pollutants. EPA/600/D-87/229; NTIS PB87–212684. U.S. Environmental Protection Agency, Cincinnati, Ohio.

Warner, H.P., Cohen, J.M., Ireland, J.C. (1980) In-house report of U.S. EPA, Municipal Environmental Research Laboratory, Wastewater Research Division, Cincinnati, Ohio.

Watanabe, I., Tatsukawa, R. (1989) Anthropogenic brominated aromatics in the Japanese environment. In: *Proceedings: Workshop on Brominated Aromatic Flame Retardants*. pp. 63–70. Skokloster, Sweden, 24–26 October, 1989.

Wauchope, R.D. (1978) The pesticide content of surface water draining from agricultural fields- A review. *J. Environ. Quality.* 7(4), 459–472.

Wauchope, R.D. (1989) *ARS/SCS Pesticide Properties Database*. Version 1.9, preprint, August, 1989.

Wauchope, R.D., Buttler, T.M., Hornsby, A.G., Augustijn-Beckers, P.W.M., Burt, J.P. (1992) The SCS/ARS/CES Pesticide Properties Database for Environmental Decision-Making. *Rev. Environ. Contam. Toxicol*. 123, 1–164.

Way, M.J., Scopes, N.E A. (1968) Studies on the persistence and effects on soil fauna and some soil-applied systemic insecticides. *Ann. Appl. Biol*. 62, 199–214.

Weast, R.C., Ed. (1972–73) *Handbook of Chemistry and Physics.* 53rd edition, CRC Press, Cleveland, Ohio.

Weast, R.C., Ed. (1976–77) *Handbook of Chemistry and Physics.* 57th edition, CRC Press, Cleveland, Ohio.

Weber, J.B., Shea, P.J., Strek, H.J. (1980) An evaluation of nonpoint sources of pesticide pollution in runoff. In: *Environmental Impact of Nonpoint Source Pollution.* Overcash, M., Davidson, J., Editors, Ann Arbor Science Publishers, Ann Arbor, Michigan.

Weber, K. (1976) Degradation of parathion in seawater. *Water Res*. 10, 237–241.

Webster, G.R.B., Friesen, K.J., Sarna, L.P., Muir, D.C.G. (1985) Environmental fate modelling of chlorodioxins: determination of physical constants. *Chemosphere* 14, 689–622.

Wei, D., Zhang, A., Wu, C., Han, S., Wang, L. (2001) Progressive study and robustness test of QSAR model based on quantum chemical parameters for predicting BCF of selected polychlorinated organic compounds (PCOCs). *Chemosphere* 44, 1421–1428.

Weil, V.G., Dure, G., Quentin, K.L. (1974) Solubility in water of insecticide chlorinated hydrocarbons and polychlorinated biphenyls in view of water pollution. *Z. Wasser Abwasser Forsch* 7(6), 169–175.

Weinberger, P., Greenhalgh, R. (1983) Review of ecotoxicity of matacil in freshwater environment: chemical and phytobiological impact studies. In: *Aquatic Toxicology*, Nriagu, J.O., Ed., pp. 437–438, Wiley-Interscience, New York.

Weisgerber, I., Kohli, J., Kaul, R., Klein, W., Korte, F. (1974) Fate of aldrin-^{14}C in maize, wheat, and soils under outdoor conditions. *J. Agric. Food Chem*. 22, 609–612.

Wells, D., Grayson, B.T., Langner, E. (1986) Vapor pressure of permethrin. *Pest. Sci.* 17, 473–476.

Westall, J.C., Leuenberger, C., Swarzenbach, R.P. (1985) Influence of pH and ionic strength on the aqueous-nonaqueous distribution of chlorinated phenols. *Environ. Sci. Technol.* 19, 193–198.

Westcott, J.W., Bidleman, T.F. (1981) Determination of polychlorinated biphenyl vapor pressures by capillary gas chromatography. *J. Chromatogr.* 210, 331–336.

Westcott, J.W., Simon, C.G., Bidleman, T.F. (1981) Determination of polychlorinated biphenyl vapor pressures by a semimicro gas saturation method. *Environ. Sci. Technol.* 15, 1375–1378.

Wheatley, G.A., Hardman, J.A. (1968) Organochlorine insecticide residues in earthworms from arable soils. *J. Sci. Food Chem. Agric.* 19, 219–225.

Whiting, F.M., Brown, W.H., Stull, J.W. (1973) Pesticide residues in milk and in tissues following long, low 2,2-bis(*p*-chlorophenyl)-1,1,1-trichloroethane intake. *J. Dairy Sci.* 56, 1324.

Wilcock, R.J., Smith, T.J., Pridmore, R.D., Thrush, S.F., Cummings, V.J., Hewitt, J.E. (1993) Bioaccumulation and elimination of chlordane by selected intertidal benthic fauna. *Environ. Toxicol. Chem.* 12, 733–742.

Williams, E.F. (1951) Properties of O,O-diethyl O-*p*-nitrophenyl thiophosphate and *O,O*-diethyl *O-p*-nitrophenyl phosphate. *Ind Eng. Chem.* 43, 950–954.

Williams, P.P. (1977) Metabolism of synthetic organic pesticides by anaerobic microorganisms. *Res. Rev.* 66, 63.

Willis, G.H., Hamilton, R.A. (1973) Agricultural chemicals in surface runoff, ground water, and soil: 1. Emdrin. *J. Environ. Qual.* 2, 463.

Willis, G.H., McDowell, L.L. (1982) Pesticides in agricultural runoff and their effects on downstream water quality. *Environ. Toxicol. Chem.* 1, 267–279.

Willis, G.H., McDowell, L.L. (1987) Pesticide persistence on foliage. *Rev. Environ. Contam. Toxicol.* 100, 23–73.

Willis, G.H., McDowell, L.L., Smith, S., Southwick, L.M., Lemon, E.R. (1980) Toxaphene volatilization from a mature cotton canopy. *Agron. J.* 72, 627.

Willis, G.H., Parr, J.F., Smith, S. (1971) Volatilization of soil-applied DDT and DDD from flooded and nonflooded plots. *Pest. Monit. J.* 4, 204.

Wilson, A.J. (1963) Chemical assays. In: *Annual Report of the Bureau of Commercial Fisheries*, U.S. Bureau of Commercial Fisheries Circ. #247. Biology Lab., Gulf Breeze, Florida.

Wilson, K.A., Cook, R.M. (1972) Metabolism of xenobiotics in remnants. IV. Storage and excretion of HEOD in Holstein cows. *J. Agric. Food Chem.* 20, 391–394.

Windholz, M., Editor (1983) *The Merck Index. An Encyclopedia of Chemicals, Drugs and Biologicals.* 11th Edition, Merck and Co., Rahway, New Jersey.

Winer, A.M., Atkinson, R. (1990) Chapter 9, Atmospheric reaction pathways and lifetimes for organophosphorous compounds. In: *Long Range Transport of Pesticides.* Kurtz, D.A., Ed., Lewis Publ., Ann Arbor, MI.

Winget, P., Cramer, C.J., Truhlar, D.G. (2000) Prediction of soil sorption coefficients using a universal solvation model. *Environ. Sci. Technol.* 34, 4733–4740.

Wolfdietrich, E., Editor (1965) *Handbuch der Insektizidkunde*. Veb Verlag Volk und Gesundheit, Berlin.

Wolfe, N.L. (1980) Organophosphate and organophosphorothionate esters: Application of linear free energy relationships to estimate hydrolysis rate constants for use in environmental fate assessment. *Chemosphere* 9, 571–579.

Wolfe, N.L., Kitchens, B.E., Macalady, D.L., Grundl, T.J. (1986) Physical and chemical factors that influence the anaerobic degradation of methyl parathion in sediment systems. *Environ. Toxicol. Chem.* 5, 1019–1026.

Wolfe, N.L., Zepp, R.G., Gordon, T.A., Baughman, G.L., Cline, D.M. (1977) Kinetics of chemical degradation of malathion in water. *Environ. Sci. Technol.* 11, 88–93.

Wolfe, N.L., Zepp, R.G., Paris, D.F. (1978) Carbaryl, propham, and chloropropham: A comparison of the rates of hydrolysis and photolysis with the rate of biolysis. *Water Res.* 12, 565.

Wolfe, N.L., Zepp, R.G., Paris, D.F. (1978) Use of structure-reactivity relationships to estimate hydrolytic persistence of carbamate pesticides. *Water Res.* 12, 561–563.

Wolfe, N.L., Zepp, R.G., Paris, D.F., Baughman, G.L., Hollis, R.C. (1977) Methoxychlor and DDT degradation in water: Rates and products. *Environ. Sci. Technol.* 11, 1077–1081.

Wolfe, N.L., Zepp, R.G., Baughman, G.L., Fincher, R.C., Gordon, T.A. (1976) Chemical and Photochemical Transformation of Selected Pesticides in Aquatic Environments. EPA-600/3–76–067. US EPA, Athens, GA.

Wollerton, C., Husband, R. (1988) *Water Solubility, Vapour Pressure, octanol-Water Partition Coefficient and Henry's Law Constant*; Zeneca Report Series RJ06998 pp. 321; Blacknell: Berkshire, UK.

Wong, A.S., Crosby, D.B. (1978) Photolysis of pentachlorophenol in water. In: *Pentachlorophenol: Chemistry, Pharmacology, and Environmental Toxicology.* Rao, K.R., Editor, pp. 19–25, Plenum Press, New York.

Wong, A.S., Crosby, D.B. (1981) Photodecomposition of pentachlorophenol in water. *J. Agric. Food Chem.* 29, 125–130.

Woolford, M.H., Jr. (1975) American Cyanamid Co. Letter to W.F. Spencer, Sept. 3, 1975.

Worthing, C.R., Editor (1979) The Pesticide Manual (A World Compendium). 6th edition. The British Crop Protection Council, Suffolk, England.

Worthing, C.R., Walker, S.B., Editors (1983) *The Pesticide Manual (A World Compendium).* 7th edition, The British Crop Protection Council, Croydon, England.

Worthing, C.R., Walker, S.B., Editors (1987) *The Pesticide Manual (A World Compendium).* 8th edition, The British Crop Protection Council, Croydon, England.

Worthing, C.R., Hance, R. Editors (1991) *The Pesticide Manual (A World Compendium).* 9th edition, The British Crop Protection Council, Surrey, England.

Wszolek, P.C., Lein, D.H., Lisk, D.J. (1980) Excretion of fenvalerate insecticide in the milk of dairy cows. *Bull. Environ. Contam. Toxicol.* 24, 296.

Xiao, Hang, Li, N., Wania, F. (2004) Compilation, evaluation, and selection of physical-chemical property data for α-, β-, and γ-hexachlorocyclohexane. *J. Chem. Eng. Data* 49, 173–185.

Xie, T.M. (1983) Determination of trace amounts of chlorophenols and chloroguaiacols in sediment. *Chemosphere* 12, 1183–1191.

Xie, T.M., Abrahamsson, K., Fogelqvist, E., Josefsson, B. (1986) Distribution of chlorophenols in a marine environment. *Environ. Sci. Technol.* 20, 457–463.

Xie, T.M., Dyrssen, D. (1984) Simultaneous determination of partition coefficients and acidity constants of chlorinated phenols and guaiacols by gas chromatography. *Anal. Chem. Acta* 160, 21–30.

Xu, F., Liang, X.-M., Su, F., Zhang, Z., Lin, B.-C., Wu, W.-Z., Yediler, A., Kettrup, A. (1999) A column method for determination of soil organic partition coefficients of eight pesticides. *Chemosphere* 39, 787–794.

Yalkowsky, S.H., Banerjee, S. (1992) *Aqueous Solubility. Methods of Estimation for Organic Compounds.* Marcel Dekker, New York.

Yao, C.C.D., Haag, W.R. (1991) Rate constants for direct reactions of ozone with several drinking water contaminants. *Water Res.* 25, 761–773.

Yaron, B., Heuer, B., Birk, Y. (1974) Kinetics of azinphosmethyl losses in the soil environment. *J. Agric. Food Chem.* 22(3), 439–441.

Yin, C., Hassett, J.P. (1986) Gas partition approach for laboratory and field studies of mirex fugacity in water. *Environ. Sci. Technol.* 20, 1213–1217.

Yoshida, K., Shigeoka, T., Yamauchi, F. (1983) Non-steady state equilibrium model for the preliminary prediction of the fate of chemicals in the environment. *Ecotoxicol. Environ. Saf.* 7, 179–190.

Yoshida, K., Shigeoka, T., Yamauchi, F. (1983) Relationship between mole fraction and *n*-octanol/water partition coefficient. *Ecotoxicol. Environ. Saf.* 7, 558–565.

Yoshioka, Y., Mizuno, T., Ose, Y., Sato, T. (1986) The estimation for toxicity of chemicals on fish by physico-chemical properties. *Chemosphere* 15, 195–203.

Zamy, C., Mazellier, P., Legube, B. (2004) Phototransformation of selected organophosphorus pesticides in dilute aqueous solutions. *Water Res.* 38, 2305–2314.

Zaroogian, G.E., Hertshe, J.F., Johnson, M. (1985) Estimation of bioconcentration in marine species using structure-activity models. *Environ. Toxicol. Chem.* 4, 3–12.

Zepp, R.G., Baughman, G.L. (1978) Prediction of photochemical transformation of pollutants in the aquatic environment. In: *Aquatic Pollutants: Transformation and Biological Effects.* Hutzinger, O., Van Lelyveld, I.H., Zoeteman, B.C.J., Editors, pp. 237–164, Pergamon Press, Oxford, England.

Zepp, R.G., Baughman, G.L., Schlotzhauer, P.F. (1981) Comparison of photochemical behavior of various humic substances in water: I. Sunlight induced reactions of aquatic pollutants photosensitized by humic substances. *Chemosphere* 10, 109–117.

Zepp, R.G., Schlotzhauer, P F. (1983) Influence of algae on photolysis rates of chemicals in water. *Environ. Sci. Technol.* 17, 462–468.

Zepp, R.G., Wolfe, N.L., Gordon, J.A., Fincher, R.C. (1976) Light-induced transformation of methoxychlor in aquatic systems. *J. Agric. Food Chem.* 24, 727–733.

Zimmerli, B., Marek, B. (1974) Modellversuche zur kontamination von lebensmitteln mit pestiziden via gasphase. *Mitt Gebiete Lebensm Hyg.* 65, 55–64.

Zitko, V., McLeese, D.W. (1980) Canadian Technical Report, Fish Aquatic Science No. 985, Dec. 1980.

Zoeteman, B.C.J., de Greef, E., Brinkmann, F.J.J. (1981) Persistency of organic contaminants in ground water. Lessons learned from soil pollution incidents in the Netherlands. *Sci. Total Environ.* 21, 187–202.

Zoeteman, B.C.J., Harmsen, K., Linders, J.B.H.J., Morra, C.F.H., Slooff, W. (1980) Persistent organic pollutants in river water and ground water of the Netherlands. *Chemosphere* 9, 231–249.

19 Fungicides

CONTENTS

19.1 List of Chemicals and Data Compilations (by Functional Group)

Alanine Derivatives:

Amides:

Carbamates:

Chlorobenzenes:

Imidazoles:

Phosphorothioates:

Quinones:

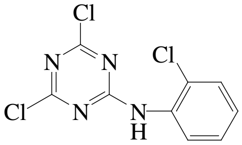
Thioimides:

Triazoles:

Miscellaneous:

19.1 LIST OF CHEMICALS AND DATA COMPILATIONS

19.1.1 ANILAZINE



Common Name: Anilazine
Synonym: Botrysan, Direz, Dyrene, Kemate, Triasyn, triazine, Zinochlor
Chemical Name: 2-chloro-*N*-(4,6-dichloro-1,3,5-triazin-2-yl)aniline; 2,4-dichloro-6-(*o*-chloro-anilino)-*s*-triazine; 4,6-dichloro-*N*-(2-chlorophenyl)-1,3,5-triazin-2-amine
Uses: as fungicide to control early and late blights of potatoes and tomatoes; anthracnose in cucurbits; leaf spot diseases in many crops; glume blotch of wheat; also used on vegetables, ornaments, berry fruits, melons, coffee and tobacco, etc.
CAS Registry No: 101-05-3
Molecular Formula: $C_9H_5Cl_3N_4$
Molecular Weight: 275.522
Melting Point (°C):

160	(Lide 2003)

Boiling Point (°C):
Density (g/cm^3 at 20°C): 1.80 (Hartley & Kidd 1987; Tomlin 1994)
Molar Volume (cm^3/mol):

252.8	(calculated-Le Bas method at normal boiling point)
153.1	(calculated-density)

Dissociation Constant pK_a:
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
Entropy of Fusion, ΔS_{fus} (J/mol K):
Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F: 0.0474 (mp at 160°C)

Water Solubility (g/m^3 or mg/L at 25°C or as indicated):

8.00	(20°C, Hartley & Kidd 1987; Worthing & Hance 1991; Tomlin 1994; Milne 1995)
8.00	(20–25°C, selected, Wauchope et al. 1992; Hornsby et al. 1996)
8.00	(selected, Lohninger 1994)

Vapor Pressure (Pa at 25°C or as indicated):

negligible	(20°C, Hartley & Kidd 1987)
8.20×10^{-7}	(20°C, Worthing & Hance 1991; Tomlin 1994)
8.26×10^{-7}	(20–25°C, selected, Wauchope et al. 1992; Hornsby et al. 1996)

Henry's Law Constant (Pa·m^3/mol at 25°C or as indicated):

2.82×10^{-5}	(20°C, calculated-P/C, this work)

Octanol/Water Partition Coefficient, log K_{OW}:

4.39	(calculated, Chiou 1981)
3.79	(calculated-CLOGP program, Biagi et al. 1991)
3.01	(20°C, Worthing & Hance 1991; Tomlin 1994)
3.88	(RP-HPLC-RT correlation, Saito et al. 1993)
1.91	(at pH 7, Milne 1995)
3.00	(selected, Hansch et al. 1995)

Bioconcentration Factor, log BCF:

2.28	(calculated-S as per Kenaga 1980, this work)

Sorption Partition Coefficient, log K_{OC}:

3.00 (20–25°C, estimated, Wauchope et al. 1992; Hornsby et al. 1996)
3.00 (estimated-chemical structure, Lohninger 1994)
3.14 (calculated-S as per Kenaga 1980, this work)
3.00, 2.53, 3.30 (soil, quoted obs.; estimated-class-specific model, estimated-general model using molecular descriptors, Gramatica et al. 2000)

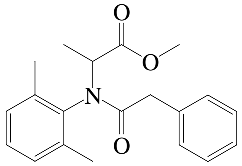
Environmental Fate Rate Constants, k, or Half-Lives, $t_{1/2}$:

Hydrolysis: stable in neutral and slightly acidic media, $t_{1/2}$ = 730 h at pH 4, $t_{1/2}$ = 790 h at pH 7, $t_{1/2}$ = 22 h at pH 9, 22°C (Tomlin 1994).

Half-Lives in the Environment:

Air:
Surface water:
Groundwater:
Sediment:
Soil: $t_{1/2}$ ~ 12 h in damp soil (Hartley & Kidd 1987; Tomlin 1994);
field $t_{1/2}$ = 1 d (20–25°C, selected, Wauchope et al. 1992; Hornsby et al. 1996).
Biota:

19.1.2 BENALAXYL



Common Name: Benalaxyl
Synonym: Galben, M 9834, Tairel
Chemical Name: methyl *N*-phenylacetyl-*N*-2,6-xylyl-*DL*-alaninate; methyl *N*-(2,6-dimethylphenyl)-*N*-(phenylacetyl)-*DL*-alaninate
CAS Registry No: 71626-11-4
Uses: as fungicide to control late blights of potatoes and tomatoes; downy mildews of hops, vines, lettuce, onions, soybeans and other crops; many diseases in flowers and ornamentals; and often used in combination with other fungicides, etc.
Molecular Formula: $C_{20}H_{23}NO_3$
Molecular Weight: 325.402
Melting Point (°C):

79	(Lide 2003)

Boiling Point (°C):
Density (g/cm^3 at 20°C):

1.27	(25°C, Hartley & Kidd 1987; Milne 1995)

Molar Volume (cm^3/mol):

390.8	(calculated-Le Bas method at normal boiling point)
256.2	(calculated-density)

Dissociation Constant pK_a:
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
Entropy of Fusion, ΔS_{fus} (J/mol K):
Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F: 0.295 (mp at 79°C)

Water Solubility (g/m^3 or mg/L at 25°C):

37.0	(Hartley & Kidd 1987; Worthing & Hance 1991; Tomlin 1994; Milne 1995)
37.0	(20–25°C, Augustijn-Beckers et al. 1994; Hornsby et al. 1996)

Vapor Pressure (Pa at 25°C or as indicated):

6.7×10^{-4}	(Hartley & Kidd 1987; Worthing & Hance 1991; Tomlin 1994)
1.33×10^{-3}	(20–25°C, Augustijn-Beckers et al. 1994; Hornsby et al. 1996)

Henry's Law Constant (Pa·m^3/mol):

0.0117	(calculated-P/C, this work)

Octanol/Water Partition Coefficient, log K_{OW}:

3.40	(Worthing & Hance 1991; Milne 1995)
3.40	(Tomlin 1994)
3.40	(selected, Hansch et al. 1995)
3.24	(RP-HPLC-RT correlation using short ODP column, Donovan & Pescatore 2002)

Bioconcentration Factor, log BCF:

1.91	(calculated-S as per Kenaga 1980, this work)

Sorption Partition Coefficient, log K_{OC}:

3.44–3.86	(soil, Tomlin 1994)
3.00	(soil, estimated, Augustin-Beckers et al. 1994; Hornsby et al. 1996)

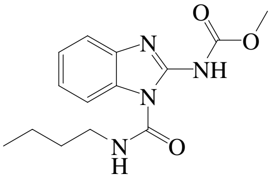
Environmental Fate Rate Constants, k, or Half-Lives, $t_{1/2}$:

Hydrolysis: $t_{1/2}$ = 86 d at pH 9, 25°C, but stable in aqueous solutions at pH 4–9 (Tomlin 1994).

Half-Lives in the Environment:

Air:
Surface water:
Groundwater:
Sediment:
Soil: $t_{1/2}$ = 20–71 d in soil (Tomlin 1994);
field $t_{1/2}$ = 30 d (Augustijn-Beckers et al. 1994; Hornsby et al. 1996).
Biota:

19.1.3 BENOMYL



Common Name: Benomyl
Synonym: Arilate, BBC, Benex, Benlate, Benosan, Fibenzo, Fundazol
Chemical Name: methyl *N*-(1-butylcarbamoyl-2-benzimidazole)carbamate; methyl 1-(butyl-carbamoyl)benzimidazol-2-ylcarbamate; methyl 1-[(butylamino)carbonyl]-1*H*-benz-imidazol-2-ylcarbamate
Uses: as fungicide to control a wide range of diseases of fruit, nuts, vegetables, mushrooms, field crops, ornamentals, turf and trees; also provides secondary acaricidal control, principally as an ovicide, etc.
CAS Registry No: 17804-35-2
Molecular Formula: $C_{14}H_{18}N_4O_3$
Molecular Weight: 290.318
Melting Point (°C):
140 (dec., Tomlin 1994)
dec (Lide 2003)
Boiling Point (°C):
Density (g/cm^3 at 20°C):
Molar Volume (cm^3/mol):
320.0 (calculated-Le Bas method at normal boiling point)
Dissociation Constant pK_a:
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
Entropy of Fusion, ΔS_{fus} (J/mol K):
Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F: 0.0744 (mp at 140°C)

Water Solubility (g/m^3 or mg/L at 25°C or as indicated):
3.8 (Austin et al. 1976; quoted, Kenaga 1980; Howard 1991)
18.2, 4.0, 3.6, 2.8, 3.0, 1.9, 1.8, 8.8, 4.5 (pH 1, 3, 5,7, 8, 9, 10, 11, 12, room temperature, shake flask-HPLC/UV, Singh & Chiba 1985)
2.8 (shake flask-HPLC/UV at pH 7, Singh & Chiba 1985; quoted, Howard 1991)
2.0 (Hartley & Kidd 1987; Milne 1995)
4.0 (pH 3–10, Worthing & Hance 1991)
2.0 (20–25°C, selected, Wauchope et al. 1992; Hornsby et al. 1996)
2.0 (stable only at pH 7, Montgomery 1993)
4.0 (selected, Lohninger 1994)
4.0 (pH 3–10, very soluble at pH 1, decomposes at pH 13, Tomlin 1994)

Vapor Pressure (Pa at 25°C or as indicated):
$< 1.00 \times 10^{-5}$ (20°C, Hartley & Kidd 1987)
$< 1.33 \times 10^{-8}$ (20–25°C, selected, Wauchope et al. 1992; Hornsby et al. 1996)
$< 4.90 \times 10^{-6}$ (Tomlin 1994)

Henry's Law Constant ($Pa \cdot m^3/mol$ at 25°C):
$< 1.93 \times 10^{-6}$ (calculated-P/C)

Octanol/Water Partition Coefficient, log K_{OW}:
2.12 (20°C, shake flask-UV, Austin & Briggs 1976)
2.42 (Rao & Davidson 1982; Hansch & Leo 1985; 1987)
3.11 (Garten & Trabalka 1983; Travis & Arms 1988)
2.12 (Hansch & Leo 1985)

2.42	(Sangster 1993)
1.40–3.11	(Montgomery 1993)
2.12	(recommended, Hansch et al. 1995)
1.33	(RP-HPLC-RT correlation using short ODP column, Donovan & Pescatore 2002)

Bioconcentration Factor, log BCF:

2.46	(estimated-S, Kenaga 1980; quoted, Howard 1991)
–0.47	(vegetation, Popov & Sboeva 1974; Jalali & Anderson 1976)

Sorption Partition Coefficient, log K_{OC}:

3.32	(estimated-S, Kenaga 1980; quoted, Howard 1991)
3.28	(soil, 20–25°C, selected, Wauchope et al. 1992; Hornsby et al. 1996)
3.28	(soil, calculated, Montgomery 1993)
3.28	(selected, Lohninger 1994)
3.28	(soil, Tomlin 1994)
2.71	(soil, calculated-MCI $^1\chi$, Sabljic et al. 1995)
2.73, 1.92	(soil, estimated-class-specific model, estimated-general model using molecular descriptors, Gramatica et al. 2000)

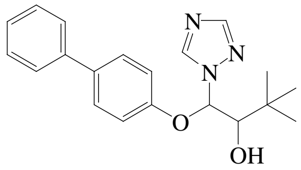
Environmental Fate Rate Constants, k, or Half-Lives, $t_{1/2}$:

Volatilization:
Photolysis:
Oxidation: photooxidation $t_{1/2}$ = 1.6 h in air, based on estimated rate constant for the vapor-phase reaction with hydroxyl radicals in air (Atkinson 1987; quoted, Howard 1991).
Hydrolysis: very significant in water with $t_{1/2}$ < 1 wk (Howard 1991).
Biodegradation:
Biotransformation:
Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants:

Half-Lives in the Environment:

Air: estimated $t_{1/2}$ ~ 1.6 h, based on the vapor-phase reaction with hydroxyl radicals in air (Atkinson 1987; quoted, Howard 1991).
Surface water: $t_{1/2}$ = 2 h (Tomlin 1994).
Groundwater:
Sediment:
Soil: degradation occurred within 15 d in unsterilized soil (Hine et al. 1969);
$t_{1/2}$ = 6–12 months (Hartley & Kidd 1987);
field $t_{1/2}$ = 67 d (20–25°C, selected, Wauchope et al. 1992; Hornsby et al. 1996);
$t_{1/2}$ = 19 h in soil (Tomlin 1994).
Biota: $t_{1/2}$ = 3–7 d on foliage (quoted, Montgomery 1993).

19.1.4 BITERTANOL



Common Name: Bitertanol

Synonym: Baycor, Baymat, Biloxazol, Sibutol

Chemical Name: 1-(biphenyl-4-yloxy)-3,3-dimethyl-1-(1*H*-1,2,4-triazol-1-yl)butan-2-ol; β-([1,1′-biphenyl]-4-yloxy)-α-(1,1-dimethylethyl)-1*H*-1,2,4-triazole-1-ethanol

Uses: as fungicide to control scab on apples and pears; rusts and powdery mildews on ornamentals; black spot on roses; and leaf spot and other diseases of vegetables, cucurbits, cereals, deciduous fruit, bananas, groundnuts, soy beans, etc.

CAS Registry No: 70585-38-5 (diastereoisomer A), 55179-31-2 (diastereoisomer B)

Molecular Formula: $C_{20}H_{23}N_3O_2$

Molecular Weight: 337.415

Melting Point (°C):
139.8 (diastereoisomer A, Hartley & Kidd 1987)
146.3 (diastereoisomer B, Hartley & Kidd 1987)
118.0 (eutectic mixture of the two diastereoisomers, Hartley & Kidd 1987; Worthing & Hance 1991)
136.7 (diastereoisomer A, Worthing & Hance 1991; Tomlin 1994)
145.2 (diastereoisomer B, Worthing & Hance 1991; Tomlin 1994)

Boiling Point (°C):

Density (g/cm^3 at 20°C):

Molar Volume (cm^3/mol):
399.7 (calculated-Le Bas method at normal boiling point)

Dissociation Constant pK_a:

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

Entropy of Fusion, ΔS_{fus} (J/mol K):

Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F: 0.122 (eutectic mixture, mp at 118° C)

Water Solubility (g/m^3 or mg/L at 25°C or as indicated):
5.0 (20°C, eutectic mixture; Hartley & Kidd 1987; Worthing & Hance 1991)
2.9 (20°C, diastereoisomer A, Worthing & Hance 1991; Tomlin 1994)
1.6 (20°C, diastereoisomer B, Worthing & Hance 1991; Tomlin 1994)

Vapor Pressure (Pa at 25°C or as indicated):
1.0×10^{-6} (20°C, Hartley & Kidd 1987)
0.0038 (100°C, diastereoisomer A, Worthing & Hance 1991)
0.0032 (100°C, diastereoisomer B, Worthing & Hance 1991)
2.2×10^{-10} (20°C, diastereoisomer A, Tomlin 1994)
2.5×10^{-10} (20°C, diastereoisomer B, Tomlin 1994)

Henry's Law Constant (Pa·m^3/mol at 25°C or as indicated):
8.45×10^{-5} (20°C, eutectic mixture, calculated-P/C, this work)

Octanol/Water Partition Coefficient, log K_{OW}:
4.10 (20°C, diastereoisomer A, Worthing & Hance 1991; Tomlin 1994)
4.40 (20°C, diastereoisomer B, Worthing & Hance 1991; Tomlin 1994)
4.16 (Schreiber & Schönherr 1992)
4.16 (selected, Hansch et al. 1995)

Bioconcentration Factor, log BCF:

2.40	(20°C, eutectic mixture, calculated-S as per Kenaga 1980, this work)

Sorption Partition Coefficient, log K_{OC}:

2.25	(20°C, eutectic mixture, calculated-S as per Kenaga 1980, this work)

Environmental Fate Rate Constants, k, or Half-Lives, $t_{½}$:

Volatilization:

Photolysis:

Oxidation:

Hydrolysis: stable in neutral, acidic and alkaline media, hydrolytic $t_{½}$ > 1 yr at 25°C and pH 4, 7 and 9 (Tomlin 1994).

Biodegradation: degradation in soil is rapid (Tomlin 1994).

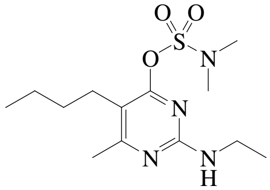
Biotransformation:

Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants:

Half-Lives in the Environment:

Surface water: environmental $t_{½}$ = 1 month to 1 yr (Tomlin 1994).

19.1.5 BUPIRIMATE



Common Name: Bupirimate
Synonym: Nimrod, PP 588
Chemical Name: 5-butyl-2-ethylamino-6-methylpyrimidin-4-yl dimethylsulfamate; 5-butyl-2-(ethylamino)-6-methyl-4-pyrimidinyl dimethylsulfamate
Uses: as fungicide to control powdery mildews of apples and pears, stone fruit, strawberries, gooseberries, vines, roses and other ornamentals, cucurbits, hops, beet, and other crops, etc.
CAS Registry No: 41483-43-6
Molecular Formula: $C_{13}H_{24}N_4O_3S$
Molecular Weight: 316.419

Melting Point (°C):

50–51	(Hartley & Kidd 1987; Worthing & Hance 1991; Tomlin 1994)

Boiling Point (°C):
Density (g/cm³ at 20°C):

Molar Volume (cm³/mol):

368.9	(calculated-Le Bas method at normal boiling point, this work)

Dissociation Constant pK_a:
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
Entropy of Fusion, ΔS_{fus} (J/mol K):
Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F:

Water Solubility (g/m³ or mg/L at 25°C):

22.0	(Martin & Worthing 1977)
22.0	(Hartley & Kidd 1987; Worthing & Hance 1991; Tomlin 1994)
23.0	(at pH 5.2, Worthing & Hance 1991)

Vapor Pressure (Pa at 25°C or as indicated):

6.7×10^{-5}	(20°C, Hartley & Kidd 1987; Worthing & Hance 1991)
1.0×10^{-4}	(Tomlin 1994)

Henry's Law Constant (Pa·m³/mol at 25°C):

9.64×10^{-3}	(calculated-P/C, this work)

Octanol/Water Partition Coefficient, log K_{OW}:

2.70	(shake flask, pH 7, Stevens et al. 1988)
3.70	(Worthing & Hance 1991)
3.90	(Tomlin 1994)
2.70	(selected, Sangster 1993; Hansch et al. 1995)

Bioconcentration Factor, log BCF:

2.02	(calculated-S, Kenaga 1980)
2.56	(calculated-K_{OW} as per Kenaga 1980, this work)

Sorption Partition Coefficient, log K_{OC}:

2.90	(calculated-S, Kenaga 1980)

Environmental Fate Rate Constants, k, or Half-Lives, $t_{1/2}$:

Volatilization:

Photolysis: rapidly decomposed by ultraviolet irradiation in aqueous solutions (Tomlin 1994).

Oxidation:

Hydrolysis: stable in dilute alkalis, but readily hydrolyzed by dilute acids (Tomlin 1994).

Biodegradation:

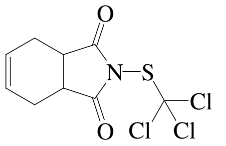
Biotransformation:

Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants:

Half-Lives in the Environment:

Soil: $t_{1/2}$ = 35–90 d for nonsterile flooded or non-flooded soil, pH 5.1 to pH 7.3 (Tomlin 1994).

19.1.6 CAPTAN



Common Name: Captan

Synonym: Aacaptan, Amercide, Captab, Captaf, Captane, Captex, Flit 406, Glyodex 37-22, Malipur, Merpan, Orthocide, Pillarcap, Vondcaptan

Chemical Name: *N*-(trichloromethylthio)cyclohex-4-ene-1,2-dicarboximide; 1,2,3,6-tetrahydro-*N*-(trichloromethylthio)phthalimide; 3a,4,7,7a-tetrahydro-[(trichloromethyl)thio]-1*H*-isoindole-1,3(2*H*)-dione

CAS Registry No: 133-06-2

Uses: as fungicide to control a wide range of fungal diseases; also used as seed treatment on maize, ornamentals, vegetables, oilseed rape, and other crops.

Molecular Formula: $C_9H_8Cl_3NO_2S$

Molecular Weight: 300.590

Melting Point (°C):

178	(Hartley & Kidd 1987; Howard 1991; Worthing & Hance 1991; Tomlin 1994; Milne 1995)
172.5	(Lide 2003)

Boiling Point (°C):

Density (g/cm^3 at 20°C):

1.74	(Hartley & Kidd 1987; Tomlin 1994; Milne 1995)

Molar Volume (cm^3/mol):

250.5	(calculated-Le Bas method at normal boiling point)
172.8	(calculated-density)

Dissociation Constant pK$_a$:

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

44.35	(DSC method, Plato 1972)

Entropy of Fusion, ΔS_{fus} (J/mol K):

Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F: 0.0357 (mp at 172.5°C)

Water Solubility (g/m^3 or mg/L at 25°C or as indicated):

8.70	(colorimetric, Burchfield 1959)
< 0.5	(Martin & Worthing 1977)
0.50	(Briggs 1981)
3.30	(Hartley & Kidd 1987; Worthing & Hance 1991; Tomlin 1994)
0.50	(20°C, selected, Suntio et al. 1988; quoted, Howard 1991; Majewski & Capel 1995)
5.10	(20–25°C, selected, Wauchope et al. 1992; Hornsby et al. 1996)
1.44	(calculated, Patil 1994)

Vapor Pressure (Pa at 25°C or as indicated):

< 0.0013	(Khan 1980)
< 0.0013	(Hartley & Kidd 1987; Worthing & Hance 1991; Tomlin 1994)
0.0010	(20°C, selected, Suntio et al. 1988; quoted, Howard 1991; Majewski & Capel 1995)
1.1×10^{-5}	(20–25°C, selected, Wauchope et al. 1992; Hornsby et al. 1996)

Henry's Law Constant (Pa·m^3/mol at 25°C or as indicated):

0.60	(20°C, calculated-P/C, Suntio et al. 1988)

Octanol/Water Partition Coefficient, log K_{OW}:

2.35	(Leo et al. 1971)
1.52	(Rao & Davidson 1980)
2.54	(shake flask-UV, Lord et al. 1980; Briggs 1981)
2.35	(Hansch & Leo 1985)
2.79	(Worthing & Hance 1991; Milne 1995)
2.35	(RP-HPLC-RT correlation, Saito et al. 1993)
2.60	(RP-HPLC-RT correlation, Sicbaldi & Finizio 1993)
2.35	(recommended, Sangster 1993)
2.35	(recommended, Hansch et al. 1995)
2.60	(RP-HPLC-RT correlation, Finizio et al. 1997)

Bioconcentration Factor, log BCF:

> 2.96	(estimated-S, Kenaga 1980a; quoted, Howard 1991)
2.67	(earthworms, Lord et al. 1980)
1.30	(activated sludge, Freitag et al. 1984, 1985)
1.30	(algae, Freitag et al. 1984,85)
1.00	(golden ide, Freitag et al. 1985)
1.56	(regression-log K_{OW}, Hansch & Leo 1985)

Sorption Partition Coefficient, log K_{OC}:

2.30	(soil, converted from K_{OM} multiplied by 1.724, Briggs 1981)
2.29	(Lyman et al. 1982; quoted, Howard 1991)
1.52	(estimated, Jury et al. 1987)
1.52	(screening model calculations, Jury et al. 1987b)
2.30	(soil, quoted exptl., Meylan et al. 1992)
2.94	(soil, calculated-MCI χ and fragments contribution, Meylan et al. 1992)
2.30	(soil, 20–25°C, selected, Wauchope et al. 1992; Hornsby et al. 1996)
2.30	(selected, Lohninger 1994)
2.30	(soil, quoted or calculated-MCI $^1\chi$, Sabljic et al. 1995)

Environmental Fate Rate Constants, k, or Half-Lives, $t_{½}$:

Volatilization:

Photolysis: photolysis $t_{½}$ = 37 min in isopropanol, $t_{½}$ = 420 min in cyclohexene and $t_{½}$ = 380 min in cyclohexane by UV-irradiation ($\lambda > 280$ nm): (Schwack & Flößer-Müller 1990).

Oxidation: photooxidation $t_{½}$ = 3.2–32 h in air, based on estimated rate constant for the vapor-phase reaction with hydroxyl radicals in air (Atkinson 1987; quoted, Howard et al. 1991)

Hydrolysis: pseudo-first-order hydrolysis $t_{½}$ = 0.1 d (Burchfield 1959; quoted, Freed 1976);

$t_{½}$ = 1.8 h, based on first-order rate constant $k = 6.5 \times 10^{-3}$ s^{-1} at pH 7.1 and 28°C (Wolfe et al. 1976; quoted, Howard et al. 1991);

$t_{½}$ = 10.3 h, based on first-order rate constant $k = 1.87 \times 10^{-5} \cdot s^{-1}$ at pH 5.2 and 28°C (Wolfe et al. 1976; quoted, Howard et al. 1991);

$t_{½}$ = 10.5 minutes, based on first-order rate constant $k = 1.10 \times 10^{-3} \cdot s^{-1}$ at pH 8.3 and 28°C (Wolfe et al. 1976; quoted, Howard et al. 1991);

$t_{½}$ = 170 min in a river water sample at pH 7 and 28°C (Wolfe et al. 1976; quoted, Howard 1991);

over rate constant $k = 6.5 \times 10^{-5}$ s^{-1} with $t_{½}$ = 3 h at 25°C and pH 7 (Mabey & Mill 1978)

$t_{½}$ = 7 h in Lake Superior water at pH 7.6 and 12°C, $t_{½}$ = 1 h at pH 7.6 and 25°C, $t_{½}$ = 40 h at pH 6.7 and 12°C, and $t_{½}$ = 8 h at pH 6.7 and 23°C (Wolfe et al. 1976; quoted, Howard 1991).

Biodegradation: unacclimated aqueous aerobic degradation $t_{½}$ = 48–1440 h, based on unacclimated and acclimated soil grab sample data (Agnihotri 1970; Foschi et al. 1970; quoted, Howard et al. 1991); unacclimated aqueous anaerobic degradation $t_{½}$ = 192–5760 h, based on unacclimated aqueous aerobic half-life (Howard et al. 1991);

rate constant $k = 0.231$ d^{-1} with a biodegradation $t_{½}$ = 3 d in soil (Rao & Davidson 1980).

Biotransformation:

Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants:

Half-Lives in the Environment:

Air: $t_{1/2}$ = 2.6 h and 1.4 h for the vapor-phase reaction with photochemically produced hydroxyl radicals and ozone (Atkinson 1985; quoted, Howard 1991);

photooxidation $t_{1/2}$ = 3.2–32 h in air, based on estimated rate constant for the vapor-phase reaction with hydroxyl radicals in air (Atkinson 1987; quoted, Howard et al. 1991);

atmospheric transformation lifetime was estimated to be < 1 d (Kelly et al. 1994).

Surface water: hydrolysis $t_{1/2}$ = 170 min in a river water sample at pH 7 and 28°C (Wolfe et al. 1976; quoted, Howard 1991);

$t_{1/2}$ = 7 h in Lake Superior water at pH 7.6 and 12°C, $t_{1/2}$ = 1 h at pH 7.6 and 25°C, $t_{1/2}$ = 40 h at pH 6.7 and 12°C, and $t_{1/2}$ = 8 h at pH 6.7 and 23°C (Wolfe et al. 1976; quoted, Howard 1991).

Groundwater: $t_{1/2}$ = 10.5 min at pH 8.3 to $t_{1/2}$ = 10.3 h at pH 5.2, based on first-order hydrolysis rate constants in surface waters (Wolfe et al. 1976; quoted, Howard et al. 1991).

Sediment:

Soil: $t_{1/2}$ = 48–1440 h, based on unacclimated and acclimated soil grab sample data (Agnihotri 1970; Foschi et al. 1970; quoted, Howard et al. 1991);

rate constant k = 0.231 d^{-1} with a biodegradation $t_{1/2}$ = 3 d (Rao & Davidson 1980);

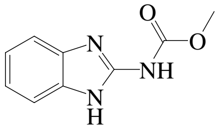
$t_{1/2}$ = 2.5 d in soil (Halfon et al. 1996);

field $t_{1/2}$ = 2.5 d (20–25°C, selected, Wauchope et al. 1992; Hornsby et al. 1996);

$t_{1/2}$ = 1 d at pH 7.2 (Tomlin 1994).

Biota: biochemical $t_{1/2}$ = 3 d from screening model calculations (Jury et al. 1987b).

19.1.7 CARBENDAZIM



Common Name: Carbendazim
Synonym: Bavistin, BCM, BMK, Carbendazime, Carbendazol, Carbendazym, G 665, Kemdazin, Mecarzole
Chemical Name: carbamic acid, methyl 1*H*-benzimidazol-2-yl, methyl ester; methyl benzimidazole-2-ylcarbamate; methyl 1*H*-benzimidazol-2-ylcarbamate
Uses: as fungicide for control of a wide range of fungal diseases in cereals, fruit, vines, hops, ornamentals, vegetables, rice coffee, cotton, mushrooms, and other crops; also used by trunk injection to give some control of Dutch elm disease.
CAS Registry No: 10605-21-7
Molecular Formula: $C_9H_9N_3O_2$
Molecular Weight: 191.186
Melting Point (°C):
302–307 (with dec., Hartley & Kidd 1987; Worthing & Hance 1991; Tomlin 1994; Milne 1995)
300 (dec, Lide 2003)
Boiling Point (°C):
Density (g/cm^3 at 20°C):
1.45 (Hartley & Kidd 1987; Tomlin 1994; Milne 1995)

Molar Volume (cm^3/mol):
194.8 (calculated-Le Bas method at normal boiling point)
131.9 (calculated-density)

Dissociation Constant pK$_a$:
4.48 (Austin & Briggs 1976)
4.24 (Sangster 1993)
4.20 (Tomlin 1994)
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
Entropy of Fusion, ΔS_{fus} (J/mol K):
Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F: 0.002 (mp at 300°C)

Water Solubility (g/m^3 or mg/L at 25°C or as indicated):
8.0 (24°C at pH 7, Hartley & Kidd 1987; Worthing & Hance 1991; Milne 1995)
29, 8.0, 7.0 (24°C, at pH 4, 7, 8, Tomlin 1994)
8.0 (20–25°C at pH 7, selected, Augustijn-Beckers et al. 1994; Hornsby et al. 1996)

Vapor Pressure (Pa at 25°C or as indicated):
6.50×10^{-8} (20°C, Hartley & Kidd 1987)
$< 9.0 \times 10^{-5}$ (20°C, Worthing & Hance 1991)
9.0×10^{-5}, 1.5×10^{-4}, 0.0013 (20, 25, 50°C, quoted, Tomlin 1994)
$< 1.0 \times 10^{-7}$ (20°C, quoted, Tomlin 1994)
6.50×10^{-8} (20–25°C, selected, Augustijn-Beckers et al. 1994; Hornsby et al. 1996)

Henry's Law Constant (Pa·m^3/mol at 25°C):
1.55×10^{-6} (calculated-P/C, this work)

Octanol/Water Partition Coefficient, log K_{OW}:
1.52 (shake flask, Austin & Briggs 1976)
1.40 (shake flask-UV, Lord et al. 1980)
1.34 (shake flask at pH 5, Barak et al. 1983)

1.56 (Worthing & Hance 1991; Milne 1995)
1.43 (recommended, Sangster 1993)
1.38, 1.505, 1.49 (pH 5, 7, 9, Tomlin 1994)
1.56, 1.77 (pH 6, 7, Tomlin 1994)
1.52 (recommended, Hansch et al. 1995)
1.80 (Pomona-database, Müller & Kördel 1996)
1.35 (RP-HPLC-RT correlation using short ODP column, Donovan & Pescatore 2002)

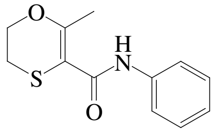
Bioconcentration Factor, log BCF:
2.28 (calculated-S, Kenaga 1980)
1.57 (earthworms, Lord et al. 1980; quoted, Connell & Markwell 1990)

Sorption Partition Coefficient, log K_{OC}:
3.14 (soil, calculated-S, Kenaga 1980)
2.35 (soil, HPLC-screening method, mean value of different stationary and mobile phases, Kördel et al. 1993, 1995)
2.30–2.40 (soil, Tomlin 1994)
2.35 (soil, calculated-MCI $^1\chi$, Sabljic et al. 1995)
2.69 (soil, 20–25°C at pH 7, selected, Augustijn-Beckers et al. 1994; Hornsby et al. 1996)
2.35; 2.25 (HPLC-screening method; calculated-PCKOC fragment method, Müller & Kördel 1996)
4.00, 2.09, 2.41, 2.28, 2.83 (first generation Eurosoils ES-1, ES-2, ES-3, ES-4, ES-5, shake flask/batch equilibrium-HPLC/UV, Gawlik et al. 1998)
2.318, 2.346, 2.091, 2.198 (second generation Eurosoils ES-2, ES-3, ES-4, ES-5, shake flask/batch equilibrium-HPLC/UV and HPLC-k′ correlation, Gawlik et al. 2000)

Environmental Fate Rate Constants, k, or Half-Lives, $t_{½}$:
Hydrolysis: $t_{½}$ > 35 d (pH 5 and 7 at 22°C, Worthing & Hance 1991);
slowly decomposed in alkaline solution, $t_{½}$ > 350 d at pH 5, 7, 124 d at pH 9 (Tomlin 1994).

Half-Lives in the Environment:
Air:
Surface water: $t_{½}$ = 2 and 25 months in water under aerobic and anaerobic conditions, respectively (Tomlin 1994).
Groundwater:
Sediment:
Soil: $t_{½}$ = 8–32 d under outdoor conditions, decomposes with $t_{½}$ = 6–12 months on bare soil, $t_{½}$ = 3 to 6 months on turf (Tomlin 1994);
field $t_{½}$ = 120 d (20–25°C, selected, Augustijn-Beckers et al. 1994; Hornsby et al. 1996).
Biota:

19.1.8 CARBOXIN



Common Name: Carboxin
Synonym: Carbathiin, D 735, Kemikar, Kisvax, Vitavax
Chemical Name: 5,6-dihydro-2-methyl-1,4-oxathi-ine-3-carboxanilide; 2,3-dihydro-6-methyl-5-phenylcarbamoyl-1,4-oxathi-ine
CAS Registry No: 5234-68-4
Uses: as fungicide in seed treatment for control of seed diseases of barley, wheat, oats, rice, groundnuts, soybeans, cotton, vegetables, maize, and other crops, etc.
Molecular Formula: $C_{12}H_{13}NO_2S$
Molecular Weight: 235.302
Melting Point (°C):

91.5–92.5	(Spencer 1982; Harley & Kidd 1987; Worthing & Hance 1991; Tomlin 1994)
98.0–100	(dimorphic, Spencer 1982; Hartley & Kidd 1987; Worthing & Hance 1991; Tomlin 1994)
94	(Lide 2003)

Boiling Point (°C):
Density (g/cm³ at 20°C):

1.30	(Worthing & Hance 1991; Montgomery 1993; Tomlin 1994)

Molar Volume (cm³/mol):

246.6	(calculated-Le Bas method at normal boiling point)
173.0	(calculated-density)

Dissociation Constant pK_a:
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

22.175	(DSC method, Plato 1972)

Entropy of Fusion, ΔS_{fus} (J/mol K):
Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F: 0.210 (mp at 94°C)

Water Solubility (g/m³ or mg/L at 25°C or as indicated):

170	(Martin & Worthing 1977)
170	(Spencer 1982; Hartley & Kidd 1987; Montgomery 1993; Milne 1995)
199	(Worthing & Hance 1991; Tomlin 1994)
215	(calculated-group contribution fragmentation method, Kühne et al. 1995)
195	(20–25°C, selected, Wauchope et al. 1992; Hornsby et al. 1996)
195	(selected, Lohninger 1994)

Vapor Pressure (Pa at 25°C or as indicated):

$< 1.0 \times 10^{-3}$	(20°C, Hartley & Kidd 1987)
2.5×10^{-5}	(Worthing & Hance 1991; Tomlin 1994)
1.3×10^{-5}	(20–25°C, selected, Wauchope et al. 1992; Hornsby et al. 1996)
2.5×10^{-5}	(20°C, Montgomery 1993)

Henry's Law Constant (Pa·m³/mol at 25°C):

3.45×10^{-5}	(calculated-P/C, Montgomery 1993)
1.57×10^{-5}	(calculated-P/C, this work)

Octanol/Water Partition Coefficient, log K_{OW}:

2.17	(Worthing & Hance 1991; Montgomery 1993; Milne 1995)
2.18	(Tomlin 1994)
2.14	(selected, Hansch et al. 1995)
2.60	(RP-HPLC-RT correlation using short ODP column, Donovan & Pescatore 2002)

Bioconcentration Factor, log BCF:

1.53	(calculated-S, Kenaga 1980)

Sorption Partition Coefficient, log K_{OC}:

2.41	(soil, calculated-S, Kenaga 1980)
2.41	(soil, 20–25°C, selected, Wauchope et al. 1992; Hornsby et al. 1996)
2.41	(calculated, Montgomery 1993)
2.41	(estimated-chemical structure, Lohninger 1994)
2.57	(soil, Tomlin 1994)

Environmental Fate Rate Constants, or Half-Lives, $t_{½}$:

Volatilization:

Photolysis: $t_{½} < 3$ h when exposed to light in aqueous solutions at pH 7 (Tomlin 1994).

Oxidation:

Hydrolysis: hydrolysis $t_{½} < 3$ d when exposed to light (Montgomery 1993).

Biodegradation:

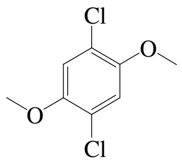
Biotransformation:

Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants:

Half-Lives in the Environment:

Soil: $t_{½} \sim 24$ h (Worthing & Hance 1991; quoted, Montgomery 1993; Tomlin 1994);
field $t_{½} = 3$ d (20–25°C, selected, Wauchope et al. 1992; Hornsby et al. 1996).

19.1.9 CHLORONEB



Common Name: Chloroneb
Synonym: Demosan; Tersan SP
Chemical Name: 1,4-dichloro-2,5-dimethoxybenzene
CAS Registry No: 2675-77-6
Uses: as fungicide applied to soil or used as seed treatment for control of seedling diseases of beans, cotton, soybeans, and beet; also used for control of snow mold (*Typhula* spp.) and Pythium blight on turf grass.
Molecular Formula: $C_8H_8Cl_2O_2$
Molecular Weight: 207.055

Melting Point (°C):
134 (Lide 2003)
Boiling Point (°C):
268 (Spencer 1982; Hartley & Kidd 1987; Worthing & Hance 1991; Tomlin 1994; Milne 1995)
Density (g/cm^3 at 20°C):
1.66 (Spencer 1982)
Molar Volume (cm^3/mol):
200.4 (calculated-Le Bas method at normal boiling point)
124.8 (calculated-density)
Dissociation Constant pK_a:
Enthalpy of Vaporization, ΔH_V (kJ/mol):
71.91 (Rordorf 1989)
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
30.54 (DSC method, Plato & Glasgow 1969)
29.1 (Rordorf 1989)
Entropy of Fusion, ΔS_{fus} (J/mol K):
72.0 (Rordorf 1989)
Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F: 0.0852 (mp at 134°C)

Water Solubility (g/m^3 or mg/L at 25°C or as indicated):
8 (Martin & Worthing 1977; Spencer 1982)
8 (Hartley & Kidd 1987; Worthing & Hance 1991; Tomlin 1994; Milne 1995)
8 (20–25°C, selected, Wauchope et al. 1992; Hornsby et al. 1996)

Vapor Pressure (Pa at 25°C or as indicated and reported temperature dependence equations):
0.40 (Spencer 1982)
0.40 (Hartley & Kidd 1987; Worthing & Hance 1991; Tomlin 1994)
0.017, 0.43, 6.90, 77.0, 630 (25, 50, 70, 100, 125°C, gas saturation-GC, Rordorf 1989)
$\log (P_S/Pa) = 16.452 - 5436/(T/K)$; measured range 32.5–135°C (solid, gas saturation-GC, Rordorf 1989)
$\log (P_L/Pa) = 12.303 - 3757.8/(T/K)$; measured range 136–151°C (liquid, gas saturation-GC, Rordorf 1989)
0.40 (20–25°C, selected, Wauchope et al. 1992; Hornsby et al. 1996)

Henry's Law Constant (Pa·m^3/mol):

Octanol/Water Partition Coefficient, log K_{OW}:

Bioconcentration Factor, log BCF:

Sorption Partition Coefficient, log K_{OC}:

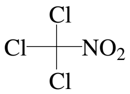
3.06	(soil, Hamaker & Thompson 1972)
3.10	(soil, quoted exptl., Meylan et al. 1992)
2.36	(calculated-MCI χ and fragments contribution, Meylan et al. 1992)
3.22	(soil, 20–25°C, selected, Wauchope et al. 1992; Hornsby et al. 1996)
3.22	(selected, Lohninger 1994)

Environmental Fate Rate Constants, k, or Half-Lives, $t_{1/2}$:

Half-Lives in the Environment:

Soil: $t_{1/2}$ ~ 24 h (Worthing & Hance 1991);
field $t_{1/2}$ = 130 d (20–25°C, selected, Wauchope et al. 1992; Hornsby et al. 1996).

19.1.10 CHLOROPICRIN



$\mathrm{Cl_3C{-}NO_2}$

Common Name: Chloropicrin
Synonym: Acquinite, Nemax, Nitrochloroform, Picfume
Chemical Name: Trichloronitromethane
CAS Registry No: 76-06-2
Uses: fungicide/herbicide/insecticide/nematicide/rodenticide; used as a soil disinfectant for control of nematodes, soil insects, soil fungi, and weed seeds; also used for fumigation of stored grain to control insects and rodents, for glasshouse and mushroom-house fumigation, etc.
Molecular Formula: CCl_3NO_2
Molecular Weight: 164.376
Melting Point (°C):
–64.0 (Spencer 1982; Hartley & Kidd 1987; Tomlin 1994; Lide 2003)
Boiling Point (°C):
112.4 (Spencer 1982; Hartley & Kidd 1987; Tomlin 1994)
Density (g/cm^3 at 20°C):
1.65659, 1.64756 (20°C, 25°C, Dreisbach 1961)
1.656 (20°C, Spencer 1982; Tomlin 1994)
1.6558, 1.6483 (20°C, 25°C, Montgomery 1993)
Molar Volume (cm^3/mol):
113.9 (calculated-Le Bas method at normal boiling point)
99.3 (calculated-density)
Dissociation Constant pK_a:
Enthalpy of Vaporization, ΔH_V (kJ/mol):
39.40, 33.12 (25°C, bp, Dreisbach 1961)
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
11.68 (Dreisbach 1961)
Entropy of Fusion, ΔS_{fus} (J/mol K):
Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F: 1.0

Water Solubility (g/m^3 or mg/L at 25°C or as indicated):
2270 (Martin & Worthing 1977; Kenaga 1980; Montgomery 1993; Lohninger 1994)
2270 (0°C, Spencer 1982; quoted, Howard 1991; Tomlin 1994)
2270, 1620 (0, 25°C, Hartley & Kidd 1987)
2300 (Davies & Lee 1987)
1621 (Howard 1991)
2270 (20–25°C, selected, Wauchope et al. 1992; Hornsby et al. 1996)
1620 (Tomlin 1994)

Vapor Pressure (Pa at 25°C or as indicated and the reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section.):
3174* (gas saturation, measured range 0–35°C, Baxter et al. 1920)
$\log(P/\text{mmHg}) = 8.2424 - 2045.1/(273 + t/°C)$; temp range 0–35°C (gas saturation, Baxter et al. 1920)
2666* (20°C, summary of literature data, temp range –25.5 to 111.9°C, Stull 1947)
3324 (calculated by formula, Dreisbach 1961)
$\log(P/\text{mmHg}) = 7.03335 - 1369.70/(218.0 + t/°C)$, temp range 28–176°C, (Antoine eq. for liquid state, Dreisbach 1961)
760, 3173 (0, 25°C, Spencer 1982)
3200 (Hartley & Kidd 1987)
3173 (Howard 1991)
2253, 3173, 4400 (20, 25, 30°C, Montgomery 1993)

Henry's Law Constant (Pa·m^3/mol at 25°C):

208.0	(Kawamoto & Urano 1989)

Octanol/Water Partition Coefficient, log K_{OW}:

1.03	(HPLC-RT correlation, Kawamoto & Urano 1989)
2.09	(shake flask, Hansch & Leo 1987)
2.07	(Howard 1991)
1.03, 2.09	(Montgomery 1993)
2.09	(selected, Sangster 1993; Hansch et al. 1995)

Bioconcentration Factor, log BCF:

0.90	(calculated, Kenaga 1980; quoted, Howard 1991)

Sorption Partition Coefficient, log K_{OC}:

1.79	(calculated, Kenaga 1980)
1.91	(soil, correlated-Freundlich Isotherm, Kawamoto & Urano 1989)
1.79	(soil, Wauchope et al. 1992; Hornsby et al. 1996)
1.79	(selected, Lohninger 1994)

Environmental Fate Rate Constants, k, or Half-Lives, $t_{1/2}$:

Volatilization: $t_{1/2}$ = 4.3 h for evaporation from a body of water 1 m deep with a current of 1 m/s and a wind of 3 m/s (Howard 1991).

Photolysis: $t_{1/2}$ = 20 d in simulated atmosphere, $t_{1/2}$ = 3 d in aqueous solution with sunlight irradiation (Montgomery 1993).

Oxidation:

Hydrolysis:

stable in neutral aqueous solution and with a minimum $t_{1/2}$ = 11 yr (Howard 1991).

Biodegradation: rate constant k(aerobic) = 1.5 d^{-1} with $t_{1/2}$ = 0.46 d at 20°C by aerobic activated sludge and k(anaerobic) = 1.5 d^{-1} with $t_{1/2}$ = 0.46 d at 20°C by anaerobic microorganisms cultivated an artificial sewage (Kawamoto & Urano 1990)

k(anaerobic) = 12 d^{-1} and $t_{1/2}$ = 0.058 d (corrigendum, Kawamoto & Urano 1991)

Biotransformation:

Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants:

Half-Lives in the Environment:

Air: $t_{1/2}$ = 20 d by photodegradation (Howard 1991).

Surface water: biodegradation $t_{1/2}$ = 0.46 d at 20°C by aerobic activated sludge or anaerobic microorganisms (Kawamoto & Urano 1990)

volatilization $t_{1/2}$ = 4.3 h from a model river and photodegradation $t_{1/2}$ = 3 d in the surface layer of water (Howard 1991).

Groundwater:

Sediment:

Soil: field $t_{1/2}$ ~ 1 d (estimated, Wauchope et al. 1992; Hornsby et al. 1996).

Biota:

TABLE 19.1.10.1
Reported vapor pressures of chloropicrin at various temperatures and the coefficients for the vapor pressure equations

$\log P = A - B/(T/K)$ (1) $\ln P = A - B/(T/K)$ (1a)

$\log P = A - B/(C + t/°C)$ (2) $\ln P = A - B/(C + t/°C)$ (2a)

$\log P = A - B/(C + T/K)$ (3)

$\log P = A - B/(T/K) - C \cdot \log (T/K)$ (4)

Baxter et al. 1920		Stull 1947		Spencer 1982		Montgomery 1993	
gas saturation		summary of literature data		handbook		handbook	
t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa
–20	200	–25.5	133.3	0	760	20	2253
–19	226.6	–3.30	666.6	25	3173	25	3173
–18	253.3	7.80	1333			30	4400
0	760.3	20.0	2666	Dreisbach eq.2			
10	1383	33.8	5333	A	7.03335		
15	1843	42.3	7999	B	1369.7		
20	2441	53.8	13332	C	218		
25	3174	71.8	26664	temp range 28–176°C			
30	4146	91.8	53329				
35	5352	111.9	101325				
eq. 2	P/mmHg	mp/°C	–64				
A	8.2424						
B	2045.1						
C	273						

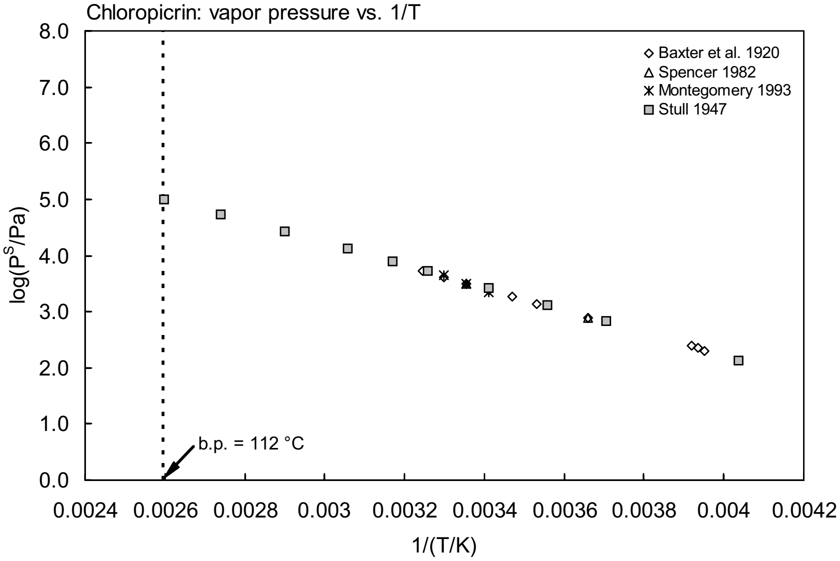
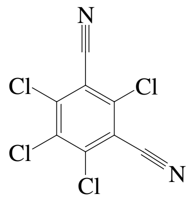


FIGURE 19.1.10.1 Logarithm of vapor pressure versus reciprocal temperature for chloropicrin.

19.1.11 CHLOROTHALONIL



Common Name: Chlorothalonil
Synonym: Bravo, chlorthalonil, Daconil, DAC 2787, Exotherm, Forturf, Nopcocide N 96, TPN
Chemical Name: tetrachloroisophthalonitrile; 2,4,5,6-tetrachloro-1,3-benzenedicarbonitrile; 2,4,5,6-tetrachloro-1,3-dicyanobenzene
CAS Registry No: 1897-45-6
Uses: fungicide, fumigant, soil insecticide
Molecular Formula: $C_8Cl_4N_2$
Molecular Weight: 265.911
Melting Point (°C):
250 (Lide 2003)
Boiling Point (°C):
350 (Hartley & Kidd 1987; Worthing & Hance 1991; Montgomery 1993; Tomlin 1994; Milne 1995)
Density (g/cm^3 at 20°C): 1.80 (Montgomery 1993; Tomlin 1994)
Molar Volume (cm^3/mol):
233.0 (calculated-Le Bas method at normal boiling point)
147.7 (calculated-density)
Dissociation Constant pK_a:
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
Entropy of Fusion, ΔS_{fus} (J/mol K):
Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F: 0.0062 (mp at 250°C)

Water Solubility (g/m^3 or mg/L at 25°C or as indicated):
0.60 (Martin & Worthing 1977; Kenaga 1980; Spencer 1982; Hartley & Kidd 1987; Worthing 1987, 1991)
0.30 (Davies & Lee 1987)
0.50 (calculated-group contribution fragmentation method, Kühne et al. 1995)
0.60 (20–25°C, selected, Wauchope et al. 1992; Hornsby et al. 1996)
0.90 (Tomlin 1994)

Vapor Pressure (Pa at 25°C or as indicated):
< 1.30 (40°C, Hartley & Kidd 1987; Worthing & Hance 1991)
232 (Worthing & Walker 1987; quoted, Majewski & Capel 1995)
0.133 (20–25°C, estimated, Wauchope et al. 1992; Hornsby et al. 1996)
1.3×10^{-3} (40°C, Montgomery 1993)
8.1×10^{-3} (selected, Brouwer et al. 1994)
7.6×10^{-5} (Tomlin 1994)

Henry's Law Constant (Pa·m^3/mol at 25°C or as indicated):
576 (calculated-P/C as per Worthing 1987, Majewski & Capel 1995)
0.0194 (20°C, Kawamoto & Urano 1989)
0.0151 (20°C, calculated-bond contribution method, Meylan & Howard 1991)
0.02 (Montgomery 1993)

Octanol/Water Partition Coefficient, log K_{OW}:
0.14 (screening model calculations, Jury et al. 1987b)

2.64 (HPLC-RT correlation, Kawamoto & Urano 1989)
2.64 (recommended, Sangster 1993)
2.89 (RP-HPLC-RT correlation, Saito et al. 1993)
2.90 (recommended, Hansch et al. 1995)
3.80 (RP-HPLC-RT correlation, Nakamura et al. 2001)

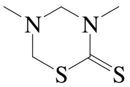
Bioconcentration Factor, log BCF:
1.92 (calculated-S, Kenaga 1980)
1.66 (calculated-K_{OW} as per Kenaga 1980, this work)

Sorption Partition Coefficient, log K_{OC}:
3.76 (soil, calculated, Kenaga 1980)
3.14 (soil, screening model calculations, Jury et al. 1987b)
3.14 (soil, Gustafson et al. 1989)
3.26 (soil, correlated-Freundlich Isotherm, Kawamoto & Urano 1989)
3.14 (soil, 20–25°C, selected, Wauchope et al. 1992; Hornsby et al. 1996)
2.76, 3.14 (soil, Montgomery 1993)
3.00 (sand, quoted, Montgomery 1993)
3.14 (estimated-chemical structure, Lohninger 1994)
3.20, 4.15 (sand, silt, Tomlin 1994)
3.26 (soil, calculated-MCI $^1\chi$, Sabljic et al. 1995)

Environmental Fate Rate Constants, or Half-Lives, $t_{1/2}$:
Volatilization:
Photolysis:
Oxidation:
Hydrolysis:
Biodegradation: biochemical $t_{1/2}$ = 70 d (Jury et al. 1987b);
first-order rate constants in biotic and abiotic shake-flask tests k = –0.0161 and –0.0155 d^{-1} in nonsterile sediment/estuarine water and k = –0.00574 d^{-1} in sterile sediment/estuarine water and k = –0.00355 and –0.00329 d^{-1} in nonsterile estuarine water and k = –0.00283 d^{-1} in sterile estuarine water both at Davis Bayou (Walker et al. 1988);
rate constant k(aerobic) = 1.7 d^{-1} with $t_{1/2}$ = 0.41 d at 20°C by aerobic activated sludge and k(anaerobic) = 1.7 d^{-1} with $t_{1/2}$ = 0.41 d at 20°C by anaerobic microorganisms cultivated an artificial sewage (Kawamoto & Urano 1990)
Biotransformation:
Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants:

Half-Lives in the Environment:
Air:
Surface water: biodegradation $t_{1/2}$ = 0.41 d at 20°C by aerobic activated sludge or anaerobic microorganisms cultivated by an artificial sewage (Kawamoto & Urano 1990)
Groundwater:
Sediment:
Soil: $t_{1/2}$ = 70 d from screening model calculations (Jury et al. 1987b);
$t_{1/2}$ ~ 1.5–3 months (Hartley & Kidd 1987; Worthing & Hance 1991);
soil $t_{1/2}$ = 68 d (Gustafson 1989);
field $t_{1/2}$ = 30 d (20–25°C, selected, Wauchope et al. 1992; Hornsby et al. 1996);
$t_{1/2}$ = 4.1 d and 1.5–3 months (Montgomery 1993);
$t_{1/2}$ = 5–35 d in aerobic and anaerobic soil studies and from a few hours to a few days in aerobic and anaerobic aquatic soil studies (Tomlin 1994).
Biota: biochemical $t_{1/2}$ = 70 d from screening model calculations (Jury et al. 1987b).

19.1.12 DAZOMET



Common Name: Dazomet
Synonym: tiazon, Mylone, Crag Fungicide 974, Salvo, Basamid, Fongosan
Chemical Name: 3,5-dimethyl-1,3,5-thiadiazinane-2-thione
Uses: soil fumigant, nematicide, fungicide, herbicide, insecticide
CAS Registry No: 533-74-4
Molecular Formula: $C_5H_{10}N_2S_2$
Molecular Weight: 162.276
Melting Point (°C):
106 (Lide 2003)
Boiling Point (°C):
Density (g/cm^3): 1.37 (Montgomery 1993; Tomlin 1994)
Acid Dissociation Constant, pK_a:
Molar Volume (cm^3/mol):
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
Entropy of Fusion, ΔS_{fus} (J/mol K):
Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F: 0.160 (mp at 106°C)

Water Solubility (g/m^3 or mg/L at 25°C or as indicated):

1200	(Spencer 1982)
3000	(20°C, Worthing & Walker 1983, 1987; Hartley & Kidd 1987; Montgomery 1993; Tomlin 1994)
2000	(Herbicide Handbook 1989, quoted, Augustijn-Beckers et al. 1994)
3000	(20–25°C, selected, Augustijn-Beckers et al. 1994; Hornsby et al. 1996)

Vapor Pressure (Pa at 25°C or as indicated):

3.7×10^{-4}	(20°C, Hartley & Kidd 1987; Worthing & Walker 1983, 1987; Montgomery 1993; Tomlin 1994)
4.0×10^{-4}, 3.73×10^{-4}	(20°C, quoted, Augustijn-Beckers et al. 1994)
4.0×10^{-4}	(20–25°C, selected, Augustijn-Beckers et al. 1994; Hornsby et al. 1996)

Henry's Law Constant (Pa·m^3/mol at 25°C or as indicated):

2.03	(20°C, calculated-P/C, Montgomery 1993)

Octanol/Water Partition Coefficient, log K_{OW}:

0.15	(Montgomery 1993)
1.40	(at pH 7, Tomlin 1994)

Octanol/Air Partition Coefficient, log K_{OA}:

Bioconcentration Factor, log BCF or log K_B:

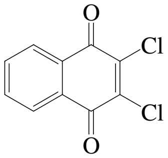
Sorption Partition Coefficient, log K_{OC}:

0.48	(calculated, Montgomery 1993)
–0.046 at pH 9, 0.778	(quoted values, Augustijn-Beckers et al. 1994)
1.0	(estimated, Augustijn-Beckers et al. 1994; Hornsby et al. 1996)

Environmental Fate Rate Constants, k, and Half-Lives, $t_{½}$:

Half-Lives in the Environment:
Soil: field $t_{½}$ = 7 d (Augustijn-Beckers et al. 1994; Hornsby et al. 1996).

19.1.13 DICHLONE



Common Name: Dichlone
Synonym: Algistat, Compound 604, Ent 3776, Phygon, Quintar, Sanquinon
Chemical Name: 2,3-dichloro-1,4-naphthoquinone; 2,3-dichloro-1,4-naphthalenedione
CAS Registry No: 117-80-6
Uses: fungicide/algicide; as fungicide for control of blossom blights, scab on apples and pears and brown spot on stone fruit, etc.; also used to control blue-green algae in ponds, lakes, and swimming pools.
Molecular Formula: $C_{10}H_4Cl_2O_2$
Molecular Weight: 227.044
Melting Point (°C):
195 (Lide 2003)
Boiling Point (°C):
275 (at 2 mmHg, Hartley & Kidd 1987; Howard 1991; Montgomery 1993)
Density (g/cm^3 at 20°C):
Molar Volume (cm^3/mol):
196.8 (calculated-Le Bas method at normal boiling point)
Dissociation Constant pK_a:
Enthalpy of Vaporization, ΔH_V (kJ/mol):
78.30 (Rordorf 1989)
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
27.0 (Rordorf 1989)
Entropy of Fusion, ΔS_{fus} (J/mol K):
58 (Rordorf 1989)
Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F: 0.0215 (mp at 195°C)

Water Solubility (g/m^3 or mg/L at 25°C as indicated):
0.10 (Kenaga 1980)
8.00 (20°C, Hodnett et al. 1983)
0.10 (Hartley & Kidd 1987; Worthing & Hance 1991; Tomlin 1994; Milne 1995)
1.00 (Montgomery 1993)
0.10 (20–25°C, selected, Augustijn-Beckers et al. 1994; Hornsby et al. 1996)

Vapor Pressure (Pa at 25°C or as indicated and reported temperature dependence):
3.30×10^{-4}, 8.80×10^{-3}, 0.15, 1.70, 14.0 (25, 50, 70, 100, 125°C, gas saturation-GC, Rordorf 1989)
$\log (P_S/\text{Pa}) = 14.965 - 5500.9/(T/K)$; measured range 40.4–191°C (solid, gas saturation-GC, Rordorf 1989)
$\log (P_L/\text{Pa}) = 13.396 - 4803.6/(T/K)$; measured range 40.4–191°C (liquid, gas saturation-GC, Rordorf 1989)
1.47×10^{-4} (calculated from S and Henry's law constant, Howard 1991)
10930 (20–25°C, estimated, Augustijn-Beckers et al. 1994; Hornsby et al. 1996)

Henry's Law Constant (Pa·m^3/mol at 25°C):
6.51×10^{-5} (Hine & Mookerjee 1975)

Octanol/Water Partition Coefficient, log K_{OW}:
3.16 (estimated, Hodnett et al. 1983)
5.62 (calculated, Montgomery 1993)

Bioconcentration Factor, log BCF:

3.35	(estimated-S, Kenaga 1980; quoted, Howard 1991)

Sorption Partition Coefficient, log K_{OC}:

4.19	(estimated-S, Kenaga 1980; quoted, Howard 1991)
4.00	(20–25°C, estimated, Augustijn-Beckers et al. 1994; Hornsby et al. 1996)
4.19	(calculated, Montgomery 1993)

Environmental Fate Rate Constants, k, or Half-Lives, $t_{½}$:

Volatilization:

Photolysis:

Oxidation: estimated photooxidation $t_{½}$ = 3.87 d in air, based on the vapor-phase reaction with hydroxyl radicals in air (Atkinson 1987; quoted, Howard 1991).

Hydrolysis: $t_{½}$ = 5 d at pH 7 (Howard 1991).

Biodegradation:

Biotransformation:

Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants:

Half-Lives in the Environment:

Air: estimated $t_{½}$ = 3.87 d, based on the vapor-phase reaction with hydroxyl radicals in air (Atkinson 1987; quoted, Howard 1991).

Surface water:

Groundwater:

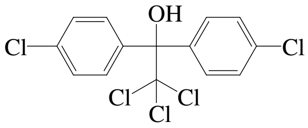
Sediment:

Soil: $t_{½}$ = 1 d in moist and slightly under three months in dry silt loam soil at pH 6.2–6.4 and 29°C, respectively (Burchfield 1959; quoted, Howard 1991);

field $t_{½}$ = 10 d (20–25°C, estimated, Augustijn-Beckers et al. 1994; Hornsby et al. 1996).

Biota:

19.1.14 DICOFOL



Common Name: Dicofol
Synonym: kelthane, kelthan
Chemical Name: 2,2,2-trichloro-1,1-bis(4-chlorophenyl)ethenol, 4-chloro-α-(4-chlorophenyl)-α-(trichloromethyl)-benzenemethanol
Uses: acaricide
CAS Registry No: 115-32-2
Molecular Formula: $C_{14}H_9Cl_5O$
Molecular Weight: 370.485
Melting Point (°C):
77.5 (Lide 2003)
Boiling Point (°C):
180 (0.1 mmHg, Hartley & Kidd 1987)
193 (360 mmHg, tech., Tomlin 1994)
Density (g/cm^3): 1.45 (Worthing & Walker 1987; Tomlin 1994)
Acid Dissociation Constant, pK_a:
Molar Volume (cm^3/mol):
Enthalpy of Vaporization, ΔH_V (kJ/mol):
104.0 (Rordorf 1989)
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
19.8 (Rordorf 1989)
Entropy of Fusion, ΔS_{fus} (J/mol K):
57 (Rordorf 1989)
Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F: 0.305 (mp at 77.5°C)

Water Solubility (g/m^3 or mg/L at 25°C or as indicated):
1.32 (generator column-GC/ECD, Weil et al. 1974)
1.20 (24°C, 99% purity, Verschueren 1983)
0.80 (20°C, in distilled water, Verschueren 1983)
0.80 (selected, Wauchope et al. 1992; Hornsby et al. 1996)
0.80 (Tomlin 1994)

Vapor Pressure (Pa at 25°C or as indicated and reported temperature dependence equations):
2.40×10^{-5}, 1.20×10^{-3}, 0.032, 0.56, 68.0 (25, 50, 70, 100, 125°C, gas saturation-GC, Rordorf 1989)
$\log (P_S/Pa) = 17.084 - 6470.1/(T/K)$; measured range 85.5–145°C (solid, gas saturation-GC, Rordorf 1989)
$\log (P_L/Pa) = 14.104 - 5354.8/(T/K)$; measured range 85.5–145°C (liquid, gas saturation-GC, Rordorf 1989)
5.33×10^{-5} (selected, Wauchope et al. 1992; Hornsby et al. 1996)
5.30×10^{-5} (tech., Tomlin 1994)

Henry's Law Constant (Pa·m^3/mol at 25°C):
5.66×10^{-5} (calculated-bond contribution method, Howard 1991)

Octanol/Water Partition Coefficient, log K_{OW}:
3.54 (Rao & Davidson 1980)
3.54 (Nigg et al. 1986)
4.28 (Tomlin 1994)
3.54 (Hansch & Leo 1987; quoted, Sangster 1993)

Octanol/Air Partition Coefficient, log K_{OA}:

Bioconcentration Factor, log BCF or log K_B:

4.18–4.27	(fathead minnow, Howard 1991)
3.98–4.16	(in presence of suspended clay, Howard 1991)
2.75, 3.54	(calculated-S, calculated-K_{OW}, Howard 1991)

Sorption Partition Coefficient, log K_{OC}:

3.60, 3,30	(estimated-S, calculated-K_{OW}, Howard 1991)
3.46–3.91	(range of reported data, Wauchope et al. 1992)
3.70	(soil, recommended, Wauchope et al. 1992; Hornsby et al. 1996)

3.92, 3.91, 3.79, 3.77 (sand, sandy loam, silty loam, clay loam, Tomlin 1994)

Environmental Fate Rate Constants, k, and Half-Lives, $t_{½}$:

Volatilization:

Photolysis: direct photolysis $t_{½}$ = 2.92 d in the atmosphere for reaction with OH radicals; $t_{½}$ = 6 d for exposure of thin film of dicofol to sunlight at 300 nm (Howard 1991).

Photooxidation:

Hydrolysis: $t_{½}$ = 60 min at pH 8.2 and 3 min at pH 10.2 with an initial concn of 0.4 mg/L (Verschueren 1983); stable to acids, but unstable in alkaline media, $t_{½}$ = 85 d at pH 5, 64–99 h at pH 7, 26 min at pH 9 (Tomlin 1994).

Biodegradation: degradation in anaerobic sewage to 4,4′-dichlorobenzophenone (DBP); 88–94% conversion to DBP for filtered river water, 47–56% for unfiltered river water of pH 7.5 in a 24-h expt. (Verschueren 1983); $t_{½}$ = 61 d and 16 d under aerobic and anaerobic conditions in silt loam (Tomlin 1994).

Biotransformation:

Bioconcentration and Uptake and Elimination Rate Constants (k_1 and k_2):

Half-Lives in the Environment:

Air: vapor phase $t_{½}$ ~ 2.92 s life in the atmosphere for reaction with OH radicals (estimated, Howard 1991)

Surface water: hydrolysis $t_{½}$ = 60 min at pH 8.2 and 3 min at pH 10.2 with an initial concn of 0.4 mg/L; degradation in anaerobic sewage to 4,4′-dichlorobenzophenone (DBP); 88–94% conversion to DBP for filtered river water, 47–56% for unfiltered river water of pH 7.5 in a 24-h expt. (Verschueren 1983)

aqueous photodegradation $t_{½}$ = 1–4 d at pH 5 in sensitized conditions and $t_{½}$ = 15–93 d in unsensitized conditions; stable to acids, but unstable in alkaline media, $t_{½}$ = 85 d at pH 5, 64–99 h at pH 7, 26 min at pH 9 (Tomlin 1994).

Ground water:

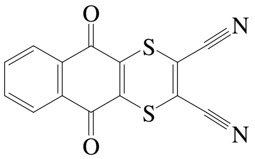
Sediment:

Soil: field $t_{½}$ = 45 d (Wauchope et al. 1992; Hornsby et al. 1996);

soil photodegradation $t_{½}$ = 30 d in silt loam, soil metabolism $t_{½}$ = 61 d under aerobic conditions and $t_{½}$ = 16 d under anaerobic conditions in silt loam; field dissipation $t_{½}$ = 60–100 d (Tomlin 1994).

Biota:

19.1.15 Dithianon



Common Name: Dithianon
Synonym: Delan, Delan-Col
Chemical Name: 2,3-dicyano-1,4-dithia-anthraquinone; 5,10-dihydro-5,10-dioxonaphtho[2,3-b]-*p*-dithin-2,3-dicarbonitrile
CAS Registry No: 3347-22-6
Uses: as fungicide for control of many foliar diseases.
Molecular Formula: $C_{14}H_4N_2O_2S_2$
Molecular Weight: 296.324
Melting Point (°C):
  220 (Lide 2003)
Boiling Point (°C):
Density (g/cm^3 at 20°C):
  1.580 (Tomlin 1994)
Molar Volume (cm^3/mol):
  264.0 (calculated-Le Bas method at normal boiling point)
  187.6 (calculated-density)
Dissociation Constant pK_a:
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
Entropy of Fusion, ΔS_{fus} (J/mol K):
Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F: 0.0122 (mp at 220°C)

Water Solubility (g/m^3 or mg/L at 25°C or as indicated):
  0.50 (20°C, Hartley & Kidd 1987; Worthing & Hance 1991; Tomlin 1994)

Vapor Pressure (Pa at 25°C):
  6.6×10^{-5} (Hartley & Kidd 1987; Worthing & Hance 1991; Tomlin 1994)

Henry's Law Constant (Pa·m^3/mol at 25°C):
  0.0391 (calculated-P/C, this work)

Octanol/Water Partition Coefficient, log K_{OW}:
  2.84 (Worthing & Hance 1991)
  3.20 (Tomlin 1994)
  2.84 (selected, Hansch et al. 1995)

Bioconcentration Factor, log BCF:
  2.96 (calculated-S per Kenaga 1980, this work)

Sorption Partition Coefficient, log K_{OC}:
  3.81 (soil, calculated-S per Kenaga 1980, this work)

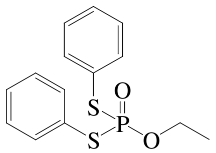
Environmental Fate Rate Constants, k, or Half-Lives, $t_{1/2}$:
  Volatilization:
  Photolysis: $t_{1/2}$ = 19 h when exposed to artificial sunlight in 0.1 mg/L aqueous solution (Tomlin 1994).
  Oxidation:
  Hydrolysis: $t_{1/2}$ = 12.2 h at pH 7 (Tomlin 1994).

Biodegradation:
Biotransformation:
Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants:

Half-Lives in the Environment:

Surface water: hydrolysis $t_{½}$ = 12.2 h at pH 7 and photolytic $t_{½}$ = 19 h when exposed to artificial sunlight in 0.1 mg/L aqueous solutions (Tomlin 1994).

19.1.16 EDIFENPHOS



Common Name: Edifenphos
Synonym: EDDP, Hinosan, edifenfos
Chemical Name: *O*-ethyl *S,S*-diphenyl phosphorodithioate
CAS Registry No: 17109-49-8
Uses: as fungicide for control of blast and blight diseases in rice, etc.
Molecular Formula: $C_{14}H_{15}O_2PS_2$
Molecular Weight: 310.371
Melting Point (°C):
–25 (Tomlin 1994)
Boiling Point (°C):
154 (at 0.01 mmHg, Hartley & Kidd 1987; Worthing & Hance 1991)
Density (g/cm^3 at 20°C):
1.230 (Hartley & Kidd 1987; Worthing & Hance 1991)
1.251 (Tomlin 1994)
Molar Volume (cm^3/mol):
250.5 (calculated from density)
Dissociation Constant pK_a:
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
Entropy of Fusion, ΔS_{fus} (J/mol K):
Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F: 1.0

Water Solubility (g/m^3 or mg/L at 25°C or as indicated):
56.0 (20°C, Hartley & Kidd 1987; Tomlin 1994)
insoluble (Worthing & Hance 1991)

Vapor Pressure (Pa at 25°C or as indicated):
0.013 (20°C, Hartley & Kidd 1987)
0.013 (20°C, Tomlin 1994)

Henry's Law Constant (Pa·m^3/mol at 25°C or as indicated):
0.0721 (20°C, calculated-P/C, this work)

Octanol/Water Partition Coefficient, log K_{OW}:
3.48 (RP-HPLC-RT correlation, Saito et al. 1993)
4.20 (RP-HPLC-RT correlation, Nakamura et al. 2001)

Bioconcentration Factor, log BCF:
1.81 (calculated-S as per Kenaga 1980, this work)

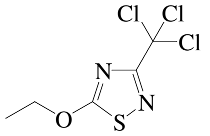
Sorption Partition Coefficient, log K_{OC}:
2.68 (calculated-S as per Kenaga 1980, this work)

Environmental Fate Rate Constants, k, or Half-Lives, $t_{1/2}$:
Hydrolysis: hydrolyzed by strong acids and alkalis, at 25°C, $t_{1/2}$ = 19 d at pH 7 and $t_{1/2}$ = 2 d at pH 9 (Tomlin 1994).

Half-Lives in the Environment:
Air:
Surface water: hydrolysis $t_{1/2}$ = 19 d at pH 7 and $t_{1/2}$ = 2 d at pH 9 (Tomlin 1994).

Groundwater:
Sediment:
Soil: half-life in soil in the range of few days to a few weeks (Tomlin 1994).
Biota:

19.1.17 ETRIDIAZOLE



Common Name: Etridiazole

Synonym: Aaterra, Banrot, Dwell, Echlomezol, ETCMTD, Ethazole, ETMT, Koban, MF-344, OM 2425, Pansoil, Terracoat, Terrazole, Truban

Chemical Name: 5-ethoxy-3-(trichloromethyl)-1,2,4-thiadiazole; ethyl 3-trichloromethyl-1,2,4-thiadiazolyl ether

Uses: as fungicide for control of *Phytophthora* and *Pythium* spp. in cotton, ornamentals, vegetables, groundnuts, cucurbits, tomatoes, and other crops; also used as a nitrification inhibitor in maize, cotton and wheat.

CAS Registry No: 2593-15-9

Molecular Formula: $C_5H_5Cl_3N_2OS$

Molecular Weight: 247.530

Melting Point (°C):
19.9 (Tomlin 1994; Milne 1995; Lide 2003)

Boiling Point (°C):
95.0 (at 1 mmHg, Hartley & Kidd 1987; Tomlin 1994; Milne 1995)

Density (g/cm^3 at 20°C):
1.503 (25°C, Hartley & Kidd 1987; Tomlin 1994)

Molar Volume (cm^3/mol):
219.0 (calculated-Le Bas method at normal boiling point)
164.7 (calculated-density)

Dissociation Constant pK$_a$:
2.77 (Tomlin 1994)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

Entropy of Fusion, ΔS_{fus} (J/mol K):

Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F: 1.0

Water Solubility (g/m^3 or mg/L at 25°C or as indicated):
50.0 (Hartley Kidd 1987; Worthing & Hance 1991; Milne 1995; selected, Lohninger 1994)
50.0 (20–25°C, selected, Wauchope et al. 1992; Hornsby et al. 1996)

Vapor Pressure (Pa at 25°C or as indicated):
0.013 (20°C, Hartley & Kidd 1987)
0.013 (rm. temp., Worthing & Hance 1991)
0.013 (20–25°C, selected, Wauchope et al. 1992; Hornsby et al. 1996)

Henry's Law Constant (Pa·m^3/mol at 25°C):
0.0644 (calculated-P/C, this work)

Octanol/Water Partition Coefficient, log K_{OW}:
2.48–2.60 (Worthing & Hance 1991; Milne 1995)
3.36 (Tomlin 1994)
2.55 (selected, Hansch et al. 1995)

Bioconcentration Factor, log BCF:
1.83 (calculated-S as per Kenaga 1980, this work)
1.22 (calculated-K_{OW} as per Kenaga 1980, this work)

Sorption Partition Coefficient, log K_{OC}:
0.725 (sandy soil, Worthing & Hance 1991)
0.149 (silt loam, Worthing & Hance 1991)

3.00 (soil, 20–25°C, estimated, Wauchope et al. 1992; Hornsby et al. 1996)
3.00 (selected, Lohninger 1994)

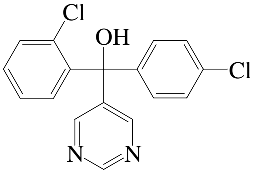
Environmental Fate Rate Constants, k, or Half-Lives, $t_{1/2}$:

Volatilization:
Photolysis:
Oxidation:
Hydrolysis: $t_{1/2}$ = 103 d at pH 6 (Worthing & Hance 1991);
$t_{1/2}$ = 12 d at pH 6, 45°C, $t_{1/2}$ = 103 d at pH 6, 25°C (Tomlin 1994).
Biodegradation: soil $t_{1/2}$ = 9.5 d under aerobic conditions and $t_{1/2}$ = 3 d under anaerobic conditions (Tomlin 1994).
Biotransformation:
Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants:

Half-Lives in the Environment:

Soil: $t_{1/2}$ = 9.5 d under aerobic, $t_{1/2}$ = 3 d under anaerobic conditions, field dissipation $t_{1/2}$ = 1 wk in sandy clay loam (Tomlin 1994);
field $t_{1/2}$ = 103 d (20–25°C, selected, Hornsby et al. 1996).

19.1.18 FENARIMOL



Common Name: Fenarimol

Synonym: Bloc, EL-222, Rimidin, Rubigan

Chemical Name: (±)-2,4′-dichloro-α-(pyrimidin-5-yl)benzhydryl alcohol; α-(2-chlorophenyl)-α-(4-chlorophenyl)-5-pyrimidinemethanol

CAS Registry No: 60168-88-9

Uses: as fungicide for control of powdery mildews in pome fruit, strawberries, vines, cucurbits, roses, and beet; also for control of scab on pome fruit, brown patch and snow mold of turf.

Molecular Formula: $C_{17}H_{12}Cl_2N_2O$

Molecular Weight: 331.195

Melting Point (°C):

118	(Lide 2003)

Boiling Point (°C):

Density (g/cm^3 at 20°C):

Molar Volume (cm^3/mol):

338.8	(calculated-Le Bas method at normal boiling point)

Dissociation Constant pK_a:

2.58	(Sangster 1993)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

Entropy of Fusion, ΔS_{fus} (J/mol K):

Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F: 0.122 (mp at 118°C)

Water Solubility (g/m^3 or mg/L at 25°C or as indicated):

13.7	(Martin & Worthing 1977)
13.7	(at pH 7, Hartley & Kidd 1987; Worthing & Hance 1991; Tomlin 1994; Milne 1995)
14.0	(20–25°C, selected, Wauchope et al. 1992; Hornsby et al. 1996)
14.0	(selected, Lohninger 1994)

Vapor Pressure (Pa at 25°C or as indicated):

$< 1.3 \times 10^{-5}$	(Hartley & Kidd 1987)
1.30×10^{-5}	(Worthing & Hance 1991)
2.93×10^{-5}	(20–25°C, selected, Wauchope et al. 1992; Hornsby et al. 1996)
6.5×10^{-5}	(vapor pressure balance, Tomlin 1994)

Henry's Law Constant (Pa·m^3/mol at 25°C or as indicated):

6.93×10^{-4}	(20–25°C, calculated-P/C, this work)

Octanol/Water Partition Coefficient, log K_{OW}:

0.67	(shake flask, at pH 5.3, Martin & Edgington 1981)
–1.59	(shake flask-UV at pH 5, Barak et al. 1983)
3.70	(Stevens et al. 1988)
3.60	(shake flask-HPLC, Bateman et al. 1990)
3.69	(pH 7, Worthing & Hance 1991; Tomlin 1994; Milne 1995)
3.60	(selected, Hansch et al. 1995)
3.61	(RP-HPLC-RT correlation using short ODP column, Donovan & Pescatore 2002)

Bioconcentration Factor, log BCF:

2.16	(calculated-S, Kenaga 1980)

Sorption Partition Coefficient, log K_{OC}:

3.01	(calculated-S, Kenaga 1980)
2.78	(soil, 20–25°C, selected, Wauchope et al. 1992; Hornsby et al. 1996)
0.176–1.08	(soil, Tomlin 1994)
2.78	(estimated-chemical structure, Lohninger 1994)

Environmental Fate Rate Constants, k, or Half-Lives, $t_{1/2}$:

Volatilization:

Photolysis: decomposed readily by sunlight (Tomlin 1994).

Oxidation:

Hydrolysis: $t_{1/2}$ = 28 d at 52°C and pH 3, 6 and 9 (Tomlin 1994).

Biodegradation: $t_{1/2}$ > 365 d under aerobic conditions in soil, and microbial degradation is accelerated by light (Tomlin 1994).

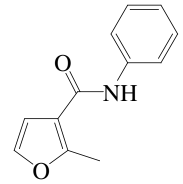
Biotransformation:

Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants:

Half-Lives in the Environment:

Soil: $t_{1/2}$ > 365 d under aerobic conditions in soil (28% sand, 14.7% clay, 57.3% silt and pH 6 (Tomlin 1994) field $t_{1/2}$ = 360 d (20–25°C, selected, Wauchope et al. 1992; Hornsby et al. 1996).

19.1.19 FENFURAM



Common Name: Fenfuram
Synonym: Panoram
Chemical Name: 2-methylfuran-3-carboxanilide; 2-methyl-3-furanilide; 2-methyl-N-phenyl-3-furancarboxamide
CAS Registry No: 24691-80-3
Uses: as fungicide for control of bunts and smuts (*Tilletie* and *Ustilago* spp.) in cereals, when applied as a seed treatment.
Molecular Formula: $C_{12}H_{11}NO_2$
Molecular Weight: 201.221
Melting Point (°C):
 109–110 (Worthing & Hance 1991)
Boiling Point (°C):
Density (g/cm^3 at 20°C):
 1.36 (Worthing & Hance 1991)
Molar Volume (cm^3/mol):
 217.1 (calculated-Le Bas method at normal boiling point)
 148.0 (calculated-density)
Dissociation Constant pK_a:
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
Entropy of Fusion, ΔS_{fus} (J/mol K):
Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F:

Water Solubility (g/m^3 or mg/L at 25°C or as indicated):
 100 (Martin & Worthing 1977; Kenaga 1980)
 100 (20°C, Hartley & Kidd 1987; Worthing & Hance 1991; Tomlin 1994)
 100 (20–25°C, selected, Hornsby et al. 1996)

Vapor Pressure (Pa at 25°C or as indicated):
 2.0×10^{-5} (20°C, Hartley & Kidd 1987)
 2.0×10^{-5} (extrapolated to 20°C, Worthing & Hance 1991; Tomlin 1994)
 2.0×10^{-5} (20–25°C, selected, Hornsby et al. 1996)

Henry's Law Constant (Pa·m^3/mol):

Octanol/Water Partition Coefficient, log K_{OW}:

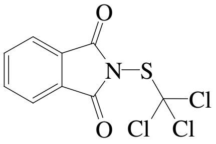
Bioconcentration Factor, log BCF:
 1.66 (calculated-S, Kenaga 1980)

Sorption Partition Coefficient, log K_{OC}:
 2.54 (calculated-S, Kenaga 1980)
 2.48 (20–25°C, estimated, Hornsby et al. 1996)

Environmental Fate Rate Constants, k, or Half-Lives, $t_{½}$:
 Hydrolysis: stable in neutral media, but hydrolyzed by strong acids and alkalis (Tomlin 1994).

Half-Lives in the Environment:
 Soil: $t_{½}$ ~ 42 d (Hartley & Kidd 1987; Tomlin 1994);
  field $t_{½}$ = 42 d (20–25°C, selected, Hornsby et al. 1996).

19.1.20 FOLPET



Common Name: Folpet
Synonym: ENT-26539, Faltan, Folpan, Folpel, Ftalan, Fungitrol, Orthophaltan, Phaltan, Spolacid, Thiophal, Vinicoll
Chemical Name: *N*-(trichloromethylthio)phthalimide; 2-[(trichloromethylthio]-1*H*-isoindole-1,3(2*H*)-dione
CAS Registry No: 133-07-3
Uses: fungicide for control of downy/powdery mildews, leaf spot diseases, etc.
Molecular Formula: $C_9H_4Cl_3NO_2S$
Molecular Weight: 296.558
Melting Point (°C):
177 (Worthing & Hance 1991; Tomlin 1994; Milne 1995; Lide 2003)
Boiling Point (°C):
Density (g/cm^3 at 20°C):
Molar Volume (cm^3/mol):
246.2 (calculated-Le Bas method at normal boiling point)
Dissociation Constant pK$_a$:
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
8.50 (DSC method, Plato 1972)
Entropy of Fusion, ΔS_{fus} (J/mol K):
Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F: 0.0323 (mp at 177°C)

Water Solubility (g/m^3 or mg/L at 25°C or as indicated):
1.0 (Martin & Worthing 1977)
1.0 (rm. temp., Hartley & Kidd 1987; Worthing & Hance 1991; Tomlin 1994; Milne 1995)

Vapor Pressure (Pa at 25°C or as indicated):
< 0.0013 (20°C, Hartley & Kidd 1987)
0.0013 (20°C, Worthing & Hance 1991; Tomlin 1994)

Henry's Law Constant (Pa·m^3/mol):

Octanol/Water Partition Coefficient, log K_{OW}:
3.63 (shake flask-UV, Briggs 1981)
2.85 (selected, Yoshioka et al. 1986)
2.85 (shake flask, log P database, Hansch & Leo 1987)
2.85 (recommended, Sangster 1993)
3.11 (Tomlin 1994)
2.85 (recommended, Hansch et al. 1995)

Bioconcentration Factor, log BCF:
1.91 (calculated-S, Kenaga 1980)
3.32 (earthworms, Lord et al. 1980)

Sorption Partition Coefficient, log K_{OC}:
1.78 (calculated-S, Kenaga 1980)
3.03 (reported as log K_{OM}, Briggs 1981)
3.27, 2.16 (soil, quoted exptl., calculated-fragment contribution method, Meylan et al. 1992)
3.27 (soil, calculated-MCI $^1\chi$, Sabljic et al. 1995)

Environmental Fate Rate Constants, k, or Half-Lives, $t_{½}$:

Volatilization:

Photolysis: $t_{½}$ = 101 min in isopropanol, $t_{½}$ = 144 min in cyclohexene and $t_{½}$ = 1620 min in cyclohexane by UV-irradiation ($\lambda > 280$ nm): (Schwack & Flößer-Müller 1990).

Oxidation:

Hydrolysis: hydrolyze at pH 7 with rates similar to captan, i.e., first-order rate constant $k = 6.5 \times 10^{-5}$ s^{-1} with $t_{½}$ = 2.96 h in a phosphate buffer solution at pH 7.07 and 28°C (Wolfe et al. 1976).

Biodegradation:

Biotransformation:

Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants:

Half-Lives in the Environment:

Air:

Surface water: $t_{½}$ = 4.3 d (Tomlin 1994).

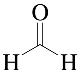
Groundwater:

Sediment:

Soil: $t_{½}$ = 4.3 d (Tomlin 1994).

Biota:

19.1.21 FORMALDEHYDE



Common Name: Formaldehyde
Synonym: formalin, methanal, oxomethane
Chemical Name: formaldehyde
Uses: fungicide/bactericide; used as soil sterilant in mushroom houses and other areas; also used as a silage preservative.
CAS Registry No: 50-00-0
Molecular Formula: HCHO
Molecular Weight: 30.026
Melting Point (°C):
–92 (Weast 1982–83; Dean 1985: Lide 2003)
Boiling Point (°C):
–19.1 (Lide 2003)
Density (g/cm^3):
0.815 (Weast 1982–83)
0.815 (–20°C, Verschueren 1983; Dean 1985)
Acid Dissociation Constant, pK_a:
Molar Volume (cm^3/mol):
29.6 (calculated-Le Bas method at normal boiling point)
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
Entropy of Fusion, ΔS_{fus} (J/mol K):
Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F: 1.0

Water Solubility (g/m^3 or mg/L at 25°C):
1,220,000 (Dean 1985)
very soluble, up to 55% (Howard 1989)

Vapor Pressure (Pa at 25°C or as indicated):
1333 (–88°C, Verschueren 1983)
451030 (> 1 atmospheric pressure, Howard 1989)

Henry's Law Constant (Pa·m^3/mol at 25°C):
0.0331 (Dong et al. 1986)
0.0169 (Gaffney et al. 1987)
0.0298 (gas stripping-HPLC, Zhou & Mopper 1990)

Octanol/Water Partition Coefficient, log K_{OW}:
–0.75 (calculated-f const. per Rekker 1977, Deneer et al. 1988)
0.00 (calculated, Verschueren 1983)
0.35 (Howard 1989)
0.35 (recommended, Sangster 1989, 1993)

Bioconcentration Factor, log BCF:
no bioconcentration in fish and shrimp observed (Howard 1989)

Sorption Partition Coefficient, log K_{OC}:
0.365 (estimated-S as per Kenaga 1980, this work)

Environmental Fate Rate Constants, k, and Half-Lives, $t_{1/2}$:
Volatilization:
Photolysis: sunlight photolysis $t_{1/2}$ = 1.25–6.0 h, based on measured gas-phase photolysis by simulated sunlight (Calvert et al. 1972; Su et al. 1979; quoted, Howard et al. 1991).

Oxidation: rate constant k = 3.2 × 10^{-16} cm^3 $molecule^{-1}$ s^{-1} for the vapor-phase reaction with NO_3 radicals in the atmosphere at (298 ± 1) K (Atkinson & Lloyd 1984; quoted, Carlier et al. 1986);

rate constant k = 4.50 × 10^{-14} cm^3 $molecule^{-1}$ s^{-1} for the vapor-phase reaction with HO_2 radicals in the atmosphere at 298 K (Baulch et al. 1984; quoted, Carlier et al. 1986);

rate constant k = 111.1 × 10^{-11} cm^3 $molecule^{-1}$ s^{-1} for the vapor-phase reaction with OH radicals in the atmosphere at 298 K (Baulch et al. 1984; quoted, Carlier et al. 1986);

atmospheric photooxidation $t_{1/2}$ = 7.13–71.3 h, based on measured rate constant for the vapor-phase reaction with OH radicals in air (Atkinson 1985; quoted, Howard et al. 1991);

aqueous photooxidation $t_{1/2}$ = 4,813–190,000 h, based on measured rate constant for the reaction with OH radicals in water (Dorfman & Adams 1973; quoted, Howard et al. 1991).

Hydrolysis: no hydrolyzable group (Howard et al. 1991).

Biodegradation: aqueous aerobic $t_{1/2}$ = 24–168 h, based on unacclimated aqueous aerobic biodegradation screening test data (Gellman & Heukelekian 1950; Heukelekian & Rand 1955; quoted, Howard et al. 1991); aqueous anaerobic $t_{1/2}$ = 96–672 h, based on unacclimated aqueous aerobic biodegradation half-life (Howard et al. 1991).

Biotransformation:

Bioconcentration Uptake (k_1) and Elimination (k_2) Rate Constants:

Half-Lives in the Environmental Compartments:

Air: photooxidation $t_{1/2}$ = 7.13–71.3 h, based on measured rate constant for the vapor-phase reaction with hydroxyl radicals in air (Atkinson 1985; quoted, Howard et al. 1991);

$t_{1/2}$ = 1.26–6.0 h, based on photolysis half-life in air (Howard et al. 1991).

Surface water: $t_{1/2}$ = 24–168 h, based on unacclimated aqueous aerobic biodegradation half-life (Howard et al. 1991).

Ground water: $t_{1/2}$ = 48–336 h, based on unacclimated aqueous aerobic biodegradation half-life (Howard et al. 1991).

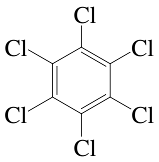
Sediment:

Soil: $t_{1/2}$ = 24–168 h, based on unacclimated aqueous aerobic biodegradation half-life (Howard et al. 1991).

Biota:

19.1.22 HEXACHLOROBENZENE

(See also Chapter 6. Chlorobenzenes and other Halogenated Mononuclear Aromatics)



Common Name: Hexachlorobenzene
Synonym: HCB, perchlorobenzene, anticarie, Bunt-cure, Bunt-no-more, Julin's carbon chloride
Chemical Name: hexachlorobenzene
Uses: as fungicide for seed treatment to control common bunt and dwarf bunt of wheat.
CAS Registry No: 118-74-1
Molecular Formula: C_6Cl_6
Molecular Weight: 284.782
Melting Point (°C):

230.0	(Weast 1982–83)
228.83	(Lide 2003)

Boiling Point (°C):

322	(sublime, Weast 1982–83)
325	(Lide 2003)

Density (g/cm^3):

1.5691	(23.6°C, Weast 1982–83; Horvath 1982)

Molar Volume (cm^3/mol):

181.5	(23.6°C, calculated-density, Weast 1972–73; Horvath 1982)
221.4	(calculated-Le Bas method at normal boiling point)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

28.744	(Tsonopoulos & Prausnitz 1971)
22.40	(Miller et al. 1984)

Entropy of Fusion, ΔS_{fus} (J/mol K):

57.32	(Tsonopoulos & Prausnitz 1971)
44.77	(Miller et al. 1984)

Fugacity Ratio (assuming ΔS_{fusion} = 56 J/mol K), F: 0.010 (mp at 228.83°C)

0.0090	(25°C, Miller et al. 1985)
0.0075, 0.0094	(20°C, 25°C, Suntio et al. 1988)

Water Solubility (g/m^3 or mg/L at 25°C):

0.005	(generator column-GC/ECD, Weil et al. 1974)
0.006	(shake flask-LSC/^{14}C, Lu & Metcalf 1975)
0.110	(shake flask-nephelometry, Hollifield 1979)
0.005	(shake flask-UV, Yalkowsky et al. 1979)
0.0034	(calculated-K_{OW}, Yalkowsky et al. 1979; Yalkowsky & Valvani 1980)
0.0035	(selected, Neely 1980)
0.036	(selected, Briggs 1981)
0.0039	(shake flask-GC, Könemann 1981)
0.0054	(generator column-GC/ECD, Hashimoto et al. 1982)
0.0012–0.014	(shake flask-GC/ECD, Hashimoto et al. 1982)
0.005	(recommended, Horvath 1982)
0.0051	(Deutsche Forschungsgemeinschaft 1983; Fischer et al. 1991)
0.0066	(selected, Yoshida et al. 1983b)
0.047	(generator column-GC/ECD, Miller et al. 1984; 1985)
0.0162	(calculated-UNIFAC activity coeff., Banerjee 1985)
0.005	(recommended, IUPAC 1985)

0.0146 (calculated-K_{OW} and HPLC-RT, Chin et al. 1986)
0.006–0.2 (calculated-K_{OW}, Anliker & Moser 1987)
0.00537 (calculated-UNIFAC activity coeff., Banerjee et al. 1990)

Vapor Pressure (Pa at 25°C or as indicated):

0.00028 (Sears & Hopke 1949)
0.0015 (Callahan et al. 1979)
0.0026 (selected, OECD 1979)
0.00145 (20°C, Kiltzer et al. 1979)
0.0023 (gas saturation-GC, Farmer et al. 1980)
0.0013 (selected, Neely 1980; Suntio et al. 1988; Nash 1989)
0.000453; 0.000167 (Klein et al. 1981)
0.00046 (evaporation rate, Dobbs & Cull 1982)
0.00121 (extrapolated, Antoine eq., Gückel et al. 1982)
0.0006 (20°C, evaporation rate & gravimetric, Gückel et al. 1982)
0.0024 (20°C, Deutsche Forschungsgemeinschaft 1983; Fischer et al. 1991)
0.00147 (selected, Yoshida et al. 1983b)
0.303; 0.159; 0.121 (supercooled liquid P_L, selected; GC-RT, Bidleman 1984)
0.0031 (selected, Mackay et al. 1985)
0.00147, 0.187 (20°C, selected, solid, supercooled liquid, Bidleman & Foreman 1987)
0.245 (selected, Suntio et al. 1988; quoted, Ballschmiter & Wittlinger 1991)
0.303, 0.127 (supercooled liquid, selected, Hinckley et al. 1990)
0.0023 (selected from Mackay et al. 1992, Mortimer & Connell 1995)
0.034; 0.141 (liquid P_L, GC-RT correlation; quoted lit., Donovan 1996)

Henry's Law Constant ($Pa\cdot m^3/mol$ at 25°C or as indicated):

68.2 (20°C, Callahan et al. 1979)
5.07 (calculated-P/C, Mackay & Shiu 1981)
131.3 (batch stripping, Atlas et al. 1982)
68.9 (20°C, calculated, Mabey et al. 1982)
12.16 (calculated-P/C, Calamari et al. 1983)
62.0 (calculated-P/C, Yoshida et al. 1983b)
139 (calculated-P/C, Bobra et al. 1985)
48.6 (20°C, batch stripping, Oliver 1985)
133, 115.9 (observed, calculated-QSAR, Nirmalakhandan & Speece 1988)
7.12 (20°C, calculated-P/C, Suntio et al. 1988)
11.0 (calculated, Nash 1989)
139.0 (calculated-P/C, Fischer et al. 1991)

Octanol/Water Partition Coefficient, log K_{OW}:

6.18 (Neely et al. 1974; selected, McKim et al. 1985)
4.13 (radioisotope tracer-^{14}C, Lu & Metcalf 1975)
6.51 (calculated-f const., Rekker 1977; quoted, Harnish et al. 1983)
6.18 (selected, Callahan et al. 1979; Neuhauser et al. 1985)
4.13 (Hansch & Leo 1979)
5.0, 6.27 (shake flask-GC, HPLC-k′ correlation, Könemann et al. 1979; selected, Figueroa & Simmons 1991)
6.44 (calculated-f constant, Könemann et al. 1979; Könemann 1981; selected, Opperhuizen 1986)
5.23 (HPLC-RT correlation, Veith et al. 1979a; selected, Mackay 1982; Freitag et al. 1985)
6.18 (HPLC-RT, Veith et al. 1979b; quoted, Veith & Kosian 1982; Ryan et al. 1988; Saito et al. 1992)
6.53 (calculated-f const., Yalkowsky et al. 1979,1983; Yalkowsky & Valvani 1980; Valvani & Yalkowsky 1980; selected, Miller et al. 1984)
5.23 (selected, Kenaga & Goring 1980; selected, Yoshida et al. 1983b)
5.44 (selected, Briggs 1981)
6.22 (HPLC-RT correlation, McDuffie 1981)

5.50 (shake flask-GC, Chiou et al. 1982; Chiou 1985; selected, Oliver & Niimi 1983; Oliver & Charlton 1984; Bobra et al. 1985; Hawker & Connell 1985; Oliver 1987a,b & c; Geyer et al. 1987; Suntio et al. 1988; Connell & Hawker 1988; Thomann 1989; Hawker 1990; Ballschmiter & Wittlinger 1991; Fischer et al. 1991)
5.66 (HPLC-RT correlation, Hammers et al. 1982)
5.40 (shake flask-GC, Watarai et al. 1982; quoted, Suntio et al. 1988)
6.13–6.27, 5.66 (range, mean, shake flask method, Eadsforth & Moser 1983)
6.27–6.48, 6.38 (range, mean, HPLC method, Eadsforth & Moser 1983)
5.0, 5.19 (selected, calculated, Kaiser 1983; Kaiser et al. 1984)
5.89 (selected, Calamari et al. 1983)
6.42 (calculated-f const., Veith et al. 1983)
5.23, 4.61 (selected, calculated-molar refraction, Yoshida et al. 1983)
5.47 (generator column-GC/ECD, Miller et al. 1984, 1985; Kerler & Schönherr 1988; Mackay & Paterson 1991)
5.75; 5.70–5.79 (quoted lit.; HPLC-RV correlation, Garst & Wilson 1984; Garst 1984)
5.20, 5.23, 5.44, 5.50, 5.55 (reported lit. values, Geyer et al. 1984)
5.47 (Sarna et al. 1984)
5.47, 6.86, 6.42 (selected, HPLC/MS, calculated-π const., Burkhard et al. 1985)
5.61 (selected, Mackay et al. 1985)
5.75 (selected OECD value, Brooke et al. 1986)
5.6, 5.9 (HPLC-RV correlation, Brooke et al. 1986)
6.51, 6.18 (selected, calculated-K_{OW} & HPLC-RT, Chin et al. 1986)
6.92 (HPLC-k′ correlation, De Kock & Lord 1987)
5.64 (HPLC-k′ correlation, Mailhot 1987)
5.45 (selected, Gobas et al. 1987, 1989; Travis & Arms 1988)
5.66 (correlated, Isnard & Lambert 1988, 1989)
5.47; 6.42, 6.55, 6.22, 5.34, 4.86, 4.75 (selected exptl.; calculated-π const., f const., HPLC-RT correlation, MW, MCI χ, TSA, Doucette & Andren 1988)
5.47; 5.37 (selected; calculated-V_I and solvatochromic parameters, Kamlet et al. 1988)
5.50 (shake flask-GC, Pereira et al. 1988)
5.31, 6.58 (selected, calculated-UNIFAC activity coeff., Banerjee & Howard 1988)
6.68 (calculated-f const., De Bruijn et al. 1989)
5.73 (shake flask/slow stirring-GC, De Bruijn et al. 1989; De Bruijn & Hermens 1990; quoted, Bintein & Devillers 1994; Sijm et al. 1995)
5.44 (recommended, Sangster 1993)
5.73 (recommended, Hansch et al. 1995)
6.42 (quoted Pomona-database, Müller & Kördel 1996)

Bioconcentration Factor, log BCF:

3.89 (rainbow trout, calculated-k_1/k_2, Neely et al. 1974)
3.09 (fish, Körte et al. 1978)
4.27, 3.73, 4.34 (fathead minnow, rainbow trout, green sunfish, Veith et al. 1979)
5.46 (guppy, lipid basis, Könemann & van Leeuwen 1980; selected, Chiou 1985)
4.27 (fish, Giam et al. 1980)
1.20 (rats, adipose tissue, Geyer et al. 1980)
3.93, 2.46 (fish, flowing water, static water, Kenaga & Goring 1980; Kenaga 1980a)
3.61, 2.45 (calculated from water solubility, K_{OC}, Kenaga 1980a)
4.39, 4.20 (algae, calculated, Geyer et al. 1981)
3.91 (fish, correlated, Mackay 1982)
4.27, 3.89 (fathead minnow, rainbow trout, selected, Bysshe 1982)
4.60 (guppy, calculated-MCI χ, Koch 1983)
4.08–4.30 (rainbow trout, Oliver & Niimi 1983)
5.16–5.37 (rainbow trout, lipid basis, Oliver & Niimi 1983; selected, Chiou 1985)
4.31 (calculated-K_{OW}, Calamari et al. 1983)
3.93 (calculated-K_{OW}, Yoshida et al. 1983b)

4.39, 3.36, 4.54 (algae, fish, activated sludge, Klein et al. 1984)
4.39, 3.83 (algae: exptl., calculated, Geyer et al. 1984; quoted, Wang et al. 1996)
4.27 (fathead minnow, 25°C, calculated, Davies & Dobbs 1984; Anliker & Moser 1987)
4.34, 3.74 (green sunfish, rainbow trout, 15°C, calculated, Davies & Dobbs 1984)
4.39, 3.36, 4.54 (algae, fish, sludge, Klein et al. 1984)
4.54 (activated sludge, Freitag et al. 1984; Halfon & Reggiani 1986)
4.39, 3.41, 4.54 (algae, fish, activated sludge, Freitag et al. 1985)
3.05 (fish, selected, Hawker & Connell 1986)
2.62–2.97 (human fat, lipid basis, Geyer et al. 1987)
2.44–2.79 (human fat, wet weight, Geyer et al. 1987)
4.41 (algae, Mailhot 1987)
4.34 (fathead minnow, Carlson & Kosian 1987)
4.38, 4.30 (worms, fish, Oliver 1987a)
3.48 (fish-normalized, Tadokoro & Tomita 1987)
4.19 (guppy, calculated, Gobas et al. 1987)
5.46 (guppy-lipid phase, calculated-K_{OW}, Gobas et al. 1987, 1989)
6.42, 6.71, 5.96, 5.98 (field data-lipid base: Atlantic croakers, blue crabs, spotted sea trout, blue catfish, Pereira et al. 1988)
–1.35 (beef, reported as biotransfer factor log B_b, Travis & Arms 1988)
–2.07 (milk, reported as biotransfer factor log B_m, Travis & Arms 1988)
–0.32 (vegetable, reported as biotransfer factor log B_v, Travis & Arms 1988)
5.30 (guppy-lipid phase, calculated-K_{OW}, Gobas et al. 1989)
3.90, 4.19 (fish, selected, Connell & Hawker 1988; Hawker 1990)
5.30 (guppy, correlated, Gobas et al. 1989)
3.53 (picea omorika, Reischl et al. 1989)
3.57 (fish, calculated, Figueroa & Simmons 1991)
4.37, 4.16 (rainbow trout, guppy, Saito et al. 1992)
4.27, 4.37 (fathead minnows, Saito et al. 1992)
4.25 (*Chlorella pyrenoidosa*, Sijm et al. 1995)
4.39, 3.18 (*Chlorella fusca, Myriophyllum spicatum*, Wang et al. 1996)

Sorption Partition Coefficient, log K_{OC}:
3.59 (Kenaga & Goring 1980; Kenaga 1980a; selected, Lyman 1982; Yoshida 1983b; Nash 1989)
4.45 (Kenaga 1980a)
4.44, 4.21, 3.59 (estimated-S, K_{OW}, BCF, Lyman 1982)
6.08 (calculated, Mabey et al. 1982)
3.59 (selected, Bysshe 1982; Lyman et al. 1982)
2.56 (shake flask-GC/ECD, Speyer soil, Freundlich isotherm, Rippen et al. 1982)
2.70 (shake flask-GC/ECD, Alfisol, Freundlich isotherm, Rippen et al. 1982)
4.58 (calculated-K_{OW}, Calamari et al. 1983)
5.90 (field data, Oliver & Charlton 1984)
4.90 (bottom sediment, Karickhoff & Morris 1985a)
5.10 (calculated-K_{OW}, Oliver & Charlton 1984)
5.2–6.7, 6.1 (suspended sediment, average, Oliver 1987c)
5.80 (algae > 50 μm, Oliver 1987c)
6.0–6.5, 6.3; 5.1 (Niagara River plume, range, mean; calculated-K_{OW}, Oliver 1987b)
4.77 (HPLC-k′, Hodson & Williams 1988)
4.70; 3.53 (HPLC-screening method; calculated-PCKOC fragment method, Müller & Kördel 1996)

Sorption Partition Coefficient, log K_{OM}:
4.25 (shake flask-GC, soil-organic matter, Briggs 1981)
5.50 (Niagara River-organic matter, Oliver & Charlton 1984)

Sorption Partition Coefficient, log K_P:

3.04–4.51 (sediment suspensions, Karickhoff & Morris 1985b; selected, Brusseau & Rao 1989)
5.11 (simulation of Oliver 1985, Brusseau & Rao 1989)

Half-Lives in the Environment:

Air: degradation rate constant of 0.0144 h^{-1} (Mackay et al. 1985; quoted, Mackay & Paterson 1991); 3753–37530 h, based on estimated photooxidation half-life (Atkinson 1987); 17000 h (selected from Mackay et al. 1992, Mortimer & Connell 1995).

Surface Water: 23256–50136 h, based on estimated unacclimated aqueous aerobic biodegradation half-life (Beck & Hansen 1974); 1.4–50 d estimated, 0.3–3 d for river water and 30–300 d for lakes, estimated from persistence (Zoeteman et al. 1980); 55000 h (selected from Mackay et al. 1992, Mortimer & Connell 1995).

Ground Water: 46512–100272 h, based on unacclimated aqueous aerobic biodegradation half-life (Beck & Hansen 1974); 30–300 d, estimated from persistence (Zoeteman et al. 1980).

Soil: 23256–50136 h, based on unacclimated aerobic soil grab sample data (Beck & Hansen, 1974); > 50 d (Ryan et al. 1988).

Sediment: 55000 h (selected from Mackay et al. 1992, Mortimer & Connell 1995).

Biota: half-life in rainbow trout, > 224 d (Niimi & Cho 1980); in subadult rainbow trout-calculated to be 210 d at 4°C, 80 d at 12°C and 70 d at 18°C (Niimi & Palazzo 1985); in worms at 8°C, 27 d (Oliver 1987a); picea omorika, 30 d (Reischl et al. 1989); 163 h, clearance from fish (Neely 1980).

Environmental Fate Rate Constants, k, or Half Lives, $t_{½}$:

Volatilization/Evaporation: 3.45×10^{-10} mol/m²·h (Gückel et al. 1982).

Photolysis:

Oxidation: rate constant in air, 1.44×10^{-2} h^{-1} (Brown et al. 1975; selected, Mackay et al. 1985); photooxidation half-life in air: 3753–37530 h, based on estimated rate constant for the vapor-phase reaction with hydroxyl radicals in air (Atkinson 1987).

Hydrolysis: not expected to be important, based on $k_h = 0$, observed after 13 d at pH 3, 7, 11 and 85°C (Ellington et al. 1987).

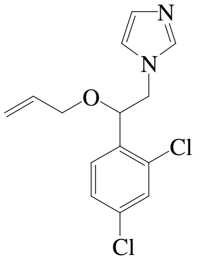
Biodegradation: aqueous aerobic biodegradation half-life: 23256–50136 h, based on unacclimated aerobic soil grab sample data (Beck & Hansen 1974); anaerobic aqueous biodegradation half-life: 93024–200544 h, based on estimated unacclimated aqueous aerobic biodegradation half-life (Beck & Hansen 1974) and degradation rate constant in soil, 1.9×10^{-5} h^{-1} (Beck & Hansen 1974; selected, Mackay et al. 1985; Mackay & Paterson 1991); not significant in an aerobic environment, and no significant degradation rate (Tabak et al. 1981; Mills et al. 1982).

Bioconcentration Uptake (k_1) and Elimination (k_2) Rate Constants:

k_1: 18.76 h^{-1} (trout muscle, Neely et al. 1974)
k_2: 0.00238 h^{-1} (trout muscle, Neely et al. 1974)
k_1: 10000 d^{-1} (guppy, Könemann & van Leeuwen 1980)
k_1: 22.5 h^{-1} (guppy, selected, Hawker & Connell 1985)
k_1: 18.8 h^{-1} (trout, selected, Hawker & Connell 1985)
k_1: 540.0 d^{-1} (fish, selected, Opperhuizen 1986)
k_2: 0.00510, 0.00818, 0.00640, 0.0047 d^{-1} (rainbow trout, calculated-fish mean body weight, Barber et al. 1988)
$1/k_2$: 420 h (trout, selected, Hawker & Connell 1985)
log k_1: 2.73 d^{-1} (fish, selected, Connell & Hawker 1988)
log k_1: 2.65 d^{-1} (fish, selected, Connell & Hawker 1988)
log $1/k_2$: 1.24 d^{-1}(fish, selected, Connell & Hawker 1988)
log k_2: –1.24 d^{-1} (fish, calculated-K_{OW}, Thomann 1989)
k_1: 0.049 h^{-1} (uptake of mayfly-sediment model II, Gobas et al. 1989b)
k_2: 0.023 h^{-1} (depuration of mayfly-sediment model II, Gobas et al. 1989b)
k_1 10489 h^{-1} (*Chlorella fusca*, Wang et al. 1996)
k_2: 0.424 h^{-1} (*Chlorella fusca*, Wang et al. 1996)

k_1: 6.558 h^{-1} (*Myriophyllum spicatum*, Wang et al. 1996)
k_2: 0.00429 h^{-1} (*Myriophyllum spicatum*, Wang et al. 1996)
Sediment Exchange Rate Constant:
0.026–1.2 d^{-1} (natural sediment, Karickhoff & Morris 1985).
Sediment Burial Rate Constant:
4.6×10^{-6} h^{-1} (Di Toro et al. 1981; selected, Mackay et al. 1985)
Stratospheric Diffusion Rate Constant:
1.7×10^{-6} h^{-1} (Mackay et al. 1985)

19.1.23 IMAZALIL



Common Name: Imazalil

Synonym: Bromazil, Deccozil, Enilconazole, Fecundal, Freshgard, Fungaflor, Fungazil, R 23979

Chemical Name: 1-(β-allyloxy-2,4-dichlorophenylethyl)imidazole; 1-[2-(2,4-dichlorophenyl)-2-(2-propenyloxy)ethyl]-1*H*-imidazole

CAS Registry No: 35554-44-0

Uses: as fungicide for control of a wide range of fungal diseases on fruit, vegetables, and ornamentals; also used as a seed dressing, for control of diseases of cereal and cotton, etc.

Molecular Formula: $C_{14}H_{14}Cl_2N_2O$

Molecular Weight: 297.129

Melting Point (°C):
50.0 (Hartley & Kidd 1987; Milne 1995; Lide 2003)

Boiling Point (°C):
> 340 (Worthing & Hance 1991; Tomlin 1994)
dec (Lide 2003)

Density (g/cm^3 at 20°C):
1.243 (23°C, Hartley & Kidd 1987; Worthing & Hance 1991; Milne 1995)
1.348 (26°C, Tomlin 1994)

Molar Volume (cm^3/mol):
318.8 (calculated-Le Bas method at normal boiling point)
239.1 (calculated-density)

Dissociation Constant pK_a:
6.53 (Worthing & Hance 1991)
7.47 (pK_b Tomlin 1994)

Enthalpy of Vaporization, ΔH_V (kJ/mol):
96.53 (Rordorf 1989)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
29.1 (Rordorf 1989)

Entropy of Fusion, ΔS_{fus} (J/mol K):
90 (Rordorf 1989)

Fugacity Ratio at 25°C (assuming $\Delta S_{fus} = 56$ J/mol K), F: 0.568 (mp at 50°C)

Water Solubility (g/m^3 or mg/L at 25°C or as indicated):
1400 (20°C, Hartley & Kidd 1987; Milne 1995)
180 (pH 7.6, Worthing & Hance 1991; Tomlin 1994)
1400 (20–25°C, selected, Augustijn-Beckers et al. 1994; Hornsby et al. 1996)

Vapor Pressure (Pa at 25°C or as indicated and reported temperature dependence equations.):
9.30×10^{-6} (20°C, Hartley & Kidd 1987)
1.60×10^{-4}, 8.0×10^{-3}, 0.230, 4.20, 53.0 (25, 50, 70, 100, 125°C, gas saturation-GC, Rordorf 1989)
$\log (P_S/Pa) = 18.21 - 6562.5/(T/K)$; measured range 53.–129°C (solid, gas saturation-GC, Rordorf 1989)
$\log (P_L/Pa) = 13.52 - 5042.4/(T/K)$; measured range 53.6–129°C (liquid, gas saturation-GC, Rordorf 1989)
1.60×10^{-4} (20°C, Worthing & Hance 1991)
1.58×10^{-4} (20°C, Tomlin 1994)
9.30×10^{-6} (20–25°C, selected, Augustijn-Beckers et al. 1994; Hornsby et al. 1996)

Henry's Law Constant (Pa·m^3/mol at 25°C or as indicated):

1.97×10^{-6}	(20–25°C, calculated-P/C, this work)

Octanol/Water Partition Coefficient, log K_{OW}:

3.82	(Worthing & Hance 1991; Milne 1995)
3.82	(pH 9.2, Tomlin 1994)
3.82	(recommended, Hansch et al. 1995)

Bioconcentration Factor, log BCF:

4.57	(calculated-S as per Kenaga 1980, this work)
2.70	(calculated-K_{OW} as per Kenaga 1980, this work)

Sorption Partition Coefficient, log K_{OC}:

2.26	(clay loam, Worthing & Hance 1991; Tomlin 1994)
2.32	(sandy loam, Worthing & Hance 1991; Tomlin 1994)
1.83	(sandy soil, Worthing & Hance 1991; Tomlin 1994)
3.60	(soil, 20–25°C, selected, Augustijn-Beckers et al. 1994; Hornsby et al. 1996)
3.73	(soil, calculated-MCI $^1\chi$, Sabljic et al. 1995)
3.73; 3.52	(soil, quoted obs.; estimated-general model using molecular descriptors, Gramatica et al. 2000)

Environmental Fate Rate Constants, k, or Half-Lives, $t_{1/2}$:

Volatilization:

Photolysis: stable to light under normal storage conditions (Tomlin 1994).

Oxidation:

Hydrolysis: very stable to hydrolysis in dilute acids and alkalis at room temperature (Tomlin 1994).

Biodegradation:

Biotransformation:

Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants:

Half-Lives in the Environment:

Soil: $t_{1/2}$ = 30–170 d (Tomlin 1994);
field $t_{1/2}$ = 150 d (20–25°C, selected, Augustijn-Beckers et al. 1994; Hornsby et al. 1996).

19.1.24 MANCOZEB

Common Name: Mancozeb
Synonym: dithane ultra, Dithane M45, Dithane SPC, Fore, Manzate, Manseb, Maezin, Nemispor, Penncozeb, Vondozeb, Zimanat, zine manganese ethylenebis[dithiocarbamate]
Chemical Name: manganese ethylenebis(dithiocarbamate) (polymeric) complex with zinc salt
CAS Registry No: 8018-01-7
Uses: fungicide
Molecular Formula: $(C_4H_6MnN_2S_4)_x(Zn)_y$
Molecular Weight:
Melting Point (°C):

192–194	(dec., Hartley & Kidd 1987; Montgomery 1993; Milne 1995)
192–204	(dec., Tomlin 1994)

Boiling Point (°C):
Density (g/cm^3 at 20°C):
Molar Volume (cm^3/mol):
Dissociation Constant pK_a:
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
Entropy of Fusion, ΔS_{fus} (J/mol K):
Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F:

Water Solubility (g/m^3 or mg/L at 25°C or as indicated):

insoluble	(Spencer 1982; Hartley & Kidd 1987; Milne 1995)
6–20	(Montgomery 1993)
6–20	(Tomlin 1994)
6.0	(20–25°C, selected, Wauchope et al. 1992; Hornsby et al. 1996)

Vapor Pressure (Pa at 25°C):

negligible	(Hartley & Kidd 1987; Tomlin 1994)
0	(selected, Wauchope et al. 1992; Hornsby et al. 1996)

Henry's Law Constant (Pa·m^3/mol at 25°C):

Octanol/Water Partition Coefficient, log K_{OW}:

3.12–3.70	(Montgomery 1993)

Octanol/Air Partition Coefficient, log K_{OA}:

Bioconcentration Factor, log BCF:

Sorption Partition Coefficient, log K_{OC}:

2.93–3.21	(soil, calculated, Montgomery 1993)
> 3.30	(soil, Wauchope et al. 1992; Hornsby et al. 1996)
> 3.30	(soil, Tomlin 1994)

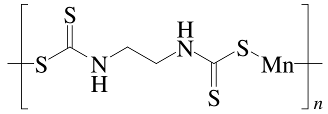
Environmental Fate Rate Constants, or Half-Lives:

Hydrolysis: unstable in acidic media (Hartley & Kidd 1987); $t_{1/2}$ = 20 d at pH 5, $t_{1/2}$ = 17 h at pH 7, $t_{1/2}$ = 34 h at pH 9 (Montgomery 1993; Tomlin 1994).

Half-Lives in the Environment:

Soil: field $t_{1/2}$ = 70 d (Wauchope et al. 1992; Hornsby et al. 1996);
$t_{1/2}$ ~. 6–15 d (Tomlin 1994).

19.1.25 MANEB



Common Name: Maneb
Synonym: MEB, Dithane, Bravo
Chemical Name: manganese ethylenebis(dithiocarbamate)
CAS Registry No: 12427-38-2
Uses: fungicide
Molecular Formula: $(C_4H_6MnN_2S_4)_x$
Molecular Weight: $(265.302)_x$
Melting Point (°C):

200	(dec, Lide 2003)

Boiling Point (°C):
Density (g/cm^3 at 20°C):

1.92	(Spencer 1982; Worthing & Walker 1983; Tomlin 1994)

Molar Volume (cm^3/mol):
Dissociation Constant pK_a:
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
Entropy of Fusion, ΔS_{fus} (J/mol K):
Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F:

Water Solubility (g/m^3 or mg/L at 25°C or as indicated):

slightly soluble (Spencer 1982)	
insoluble	(Worthing & Walker 1983; Hartley & Kidd 1987; Tomlin 1994; Milne 1995)
slight, 200, 6	(quoted, Wauchope et al. 1992)
6.0	(20–25°C, estimated and selected, Wauchope et al. 1992; Hornsby et al. 1996)

Vapor Pressure (Pa at 25°C or as indicated):

negligible	(20°C, Worthing 1983; Hartley & Kidd 1987; Tomlin 1994)
0	(selected, Wauchope et al. 1992; Hornsby et al. 1996)

Henry's Law Constant ($Pa \cdot m^3$/mol at 25°C):

Octanol/Water Partition Coefficient, log K_{OW}:

Octanol/Air Partition Coefficient, log K_{OA}:

Bioconcentration Factor, log BCF:

2.40	(activated sludge, Freitag et al. 1983)
2.40, 2.26, < 1.0	(activated sludge, algae, *Golden ide*, Freitag et al. 1985)

Sorption Partition Coefficient, log K_{OC}:

> 3.30	(soil, estimated, Wauchope et al. 1994; Hornsby et al. 1996)

Environmental Fate Rate Constants, k, or Half-Lives, $t_{½}$:
Volatilization:
Photolysis:
Oxidation:
Hydrolysis: rapidly hydrolyzed in acidic media (Hartley & Kidd 198);
$t_{½}$ < 24 h at pH 5.7 or 9 (Tomlin 1994).
Biodegradation:
Biotransformation:
Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants:

Half-Lives in the Environment:

Air: $t_{1/2}$ = 7–14 d, green house experiment in microagroecosystem chamber (Nash & Beall 1980).

Surface water: rapidly hydrolyzed in acidic media (Hartley & Kidd 1987).

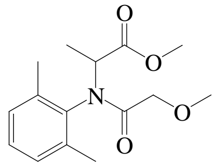
Groundwater:

Sediment:

Soil: $t_{1/2}$ = 36 d in soil (sandy loam with pH 6.7),
green house experiment in microagroecosystem chamber (Nash & Beall 1980);
$t_{1/2}$ ~ 25 d in loamy sand in dark, aerobic conditions (Tomlin 1994);
field $t_{1/2}$ ~ 70 d (estimated, Wauchope et al. 1992; Hornsby et al. 1996).

Biota: $t_{1/2}$ = 6.4 d for beans, $t_{1/2}$ = 7.4 d for tomatoes (Nash & Beall 1980);
$t_{1/2}$ = 14 d on tomato leaves, green house experiment in microagroecosystem chamber (Nash & Beall 1980);
$t_{1/2}$ = 10 d for tomato fruit, $t_{1/2}$ = 4.5 d for tomato leaves in the field, $t_{1/2}$ = 3 d for tomatoes and soybean leaves in microagroecosystem (Nash 1983).

19.1.26 METALAXYL



Common Name: Metalaxyl
Synonym: Apron, CGA 48988, Ridomil, Subdue
Chemical Name: methyl *N*-(2-methoxyacetyl)-*N*-(2,6-xylyl)-DL-alaninate; methyl-*N*-(2,6-dimethylphenyl)-*N*-(methoxyacetyl)-DL-alaninate
CAS Registry No: 57837-19-1
Uses: fungicide to control of foliar and soil-borne diseases caused by *Peronosporates* on a wide range of crops; also used to treat seeds, etc.
Molecular Formula: $C_{15}H_{21}NO_4$
Molecular Weight: 279.333
Melting Point (°C):
71 (Lide 2003)
Boiling Point (°C):
Density (g/cm^3 at 20°C):
1.21 (Hartley & Kidd 1987; Worthing & Hance 1991; Montgomery 1993)
Molar Volume (cm^3/mol):
328.2 (calculated-Le Bas method at normal boiling point)
230.9 (calculated-density)
Dissociation Constant pK_a: << 0 (Tomlin 1994)
Enthalpy of Vaporization, ΔH_V (kJ/mol):
89.73 (Rordorf 1989)
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
27.4 (Rordorf 1989)
Entropy of Fusion, ΔS_{fus} (J/mol K):
79 (Rordorf 1989)
Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F: 0.354 (mp at 71°C)

Water Solubility (g/m^3 or mg/L at 25°C or as indicated):
7100 (quoted, Burkhard & Guth 1981)
7000 (shake flask-HPLC, Ellgehausen et al. 1981)
7100 (20°C, Hartley & Kidd 1987; Worthing & Hance 1991; Montgomery 1993)
7000 (quoted-Yalkowsky & Dannenfelser 1994, Pinsuwan et al. 1995)
8400 (20–25°C, selected, Wauchope et al. 1992; Hornsby et al. 1996)
8400 (selected, Lohninger 1994)
8400 (22°C, Tomlin 1994)

Vapor Pressure (Pa at 25°C or as indicated and reported temperature dependence equations):
2.93×10^{-4} (20°C, volatilization rate, Burkhard & Guth 1981)
2.93×10^{-4} (20°C, Hartley & Kidd 1987; Worthing & Hance 1991)
7.50×10^{-4}, 2.90×10^{-2}, 0.67, 10.0, 110 (25, 50, 70, 100, 125°C, gas saturation-GC, Rordorf 1989)
$\log (P_S/Pa) = 17.423 - 4687.6/(T/K)$; measured range 32.7–69.7°C (solid, gas saturation-GC, Rordorf 1989)
$\log (P_L/Pa) = 13.243 - 4687.6/(T/K)$; measured range 72.3–130°C (liquid, gas saturation-GC, Rordorf 1989)
7.5×10^{-4} (20–25°C, selected, Wauchope et al. 1992; Hornsby et al. 1996)
2.93×10^{-4} (20°C, Montgomery 1993)
7.5×10^{-4} (Tomlin 1994)

Henry's Law Constant (Pa·m^3/mol at 25°C or as indicated):
1.155 (20°C, evaporation rate, Burkhard & Guth 1981)
2.48×10^{-5} (calculated-P/C, this work)

Octanol/Water Partition Coefficient, log K_{OW}:

1.65	(shake flask, Ellgehausen et al. 1980, 1981)
1.53	(shake flask, log P Database, Hansch & Leo 1987)
1.60	(shake flask at pH 7, Stevens et al. 1988)
1.70	(shake flask at pH 7, Baker et al. 1992)
1.59	(recommended value, Sangster 1993)
1.75	(Tomlin 1994)
1.693	(calculated-f const., Pinsuwan et al. 1995)
1.65	(recommended, Hansch et al. 1995)
1.40	(RP-HPLC-RT correlation using short ODP column, Donovan & Pescatore 2002)

Bioconcentration Factor, log BCF:

0.03	(*Daphnia magna,* wet wt. basis, Ellgehausen et al. 1980)

Sorption Partition Coefficient, log K_{OC}:

1.59	(av. of 3 soils, Sharom & Edgington 1982)
2.26	(av. of 7 soils, Carris 1983)
3.22	(av. of 12 soils, calculated-linearized Freundlich Isotherm, Sukop & Cogger 1992)
1.70	(soil, 20–25°C, estimated, Wauchope et al. 1992; Hornsby et al. 1996)
1.53–1.84	(soil, Montgomery 1993)
1.70	(estimated-chemical structure, Lohninger 1994)
1.57	(soil, calculated-MCI $^1\chi$, Sabljic et al. 1995)
1.57; 2.05	(soil, quoted obs.; estimated-general model using molecular descriptors, Gramatica et al. 2000)

Environmental Fate Rate Constants, k, or Half-Lives, $t_{½}$:

Volatilization: k(calc) = 0.71 ng cm^{-2} h^{-1} and k(measured) = 0.35 ng cm^{-2} h^{-1} from moist soils at 20°C (Burkhard & Guth 1981).

Photolysis: irradiated by UV at 290 nm in the presence of hydrogen peroxide and titanium dioxide, respectively, in aqueous solution resulted in 29% and 84% transformation in 2.5 h (Moza et al. 1994).

Oxidation:

Hydrolysis: stable in neutral and acidic media at room temp., calculated $t_{½} > 200$ d at 20°C and pH 1, $t_{½} = 115$ d at pH 9 and $t_{½} = 12$ d at pH 10 (Worthing & Hance 1991; Montgomery 1993; Tomlin 1994).

Biodegradation: overall degradation rate constant k = 0.0081 h^{-1} with $t_{½} = 85.5$ h in sewage sludge and k = 0.0217 d^{-1} with $t_{½} = 31.9$ d in garden soil (Müller & Buser 1995);

rate constant k = 0.060 d^{-1} for *R*-metalaxyl (fungicidally active) in soil expt incubated with *rac*-metalaxyl, k = 0.080 d^{-1} in soil expt incubated with *R*-metalaxyl; rate constant k = 0.015 d^{-1} for *S*-metalaxyl (fungicidally inactive) in soil expt incubated with *rac*-metalaxyl, k = 0.010/0.12 d^{-1} for in soil expt incubated with *S*-metalaxyl (Buser et al. 2002);

degradation rate constants for formulated racemic metalaxyl were found to be 0.039 d^{-1} with $t_{½} = 18$ d for German soil, k = 0.018 d^{-1} with $t_{½} = 38$ d for Cameroonian soil; for unformulated racemic metalaxyl rate constants were: k = 0.039 d^{-1} with $t_{½} = 18$ d for German soil, k = 0.019 d^{-1} with $t_{½} = 17$ d form Cameroonian soil; and for formulated R-metalaxyl rate constants were: k = 0.041 d^{-1} with $t_{½} = 17$ d for German soil, k = 0.018 d^{-1} with $t_{½} = 38$ d from Cameroonian soil. For soil incubated with metalaxyl enantiomers, R-metalaxyl degraded faster (k = 0.064 d^{-1}) than S-metalaxyl (k = 0.033 d^{-1}) in German soil when spiked with formulated racemic metalaxyl, while S-metalaxyl degraded faster (k = 0.026 d^{-1}) than R-metalaxyl (k = 0.014 d^{-1}) in Cameroonian soil when spiked with formulated racemic retalaxyl (Monkiedje et al. 2003).

Biotransformation:

Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants:

Half-Lives in the Environment:

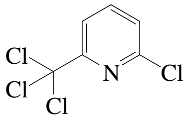
Soil: degradation $t_{½} = 39.5$ d in garden soil (Müller & Buser 1995);

field $t_{½} = 70$ d (20–25°C, selected, Wauchope et al. 1992; Hornsby et al. 1996);

residual activity in soil is about 70–90 d (Tomlin 1994);

degradation $t_{½} = 17$–38 d of the racemic mixture and enantiomers of metalaxyl in controlled incubation experiments in typical soils from Germany and Cameroon. (Monkiedje et al. 2003).

19.1.27 NITRAPYRIN



Common Name: Nitrapyrin
Synonym: N-Serve
Chemical Name: 2-chloro-6-(trichloromethyl)pyridine
CAS Registry No: 1929-82-4
Uses: bactericide
Molecular Formula: $C_6H_3Cl_4N$
Molecular Weight: 230.907
Melting Point (°C):

63	(Lide 2003)

Boiling Point (°C):
136–137.5/11 mmHg (Tomlin 1994)
Density (g/cm^3 at 25°C):

1.744	(Montgomery 1993)
1.579	(Tomlin 1994)

Molar Volume (cm^3/mol):
Dissociation Constant pK_a:
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
Entropy of Fusion, ΔS_{fus} (J/mol K):
Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F: 0.424 (mp at 63°C)

Water Solubility (g/m^3 or mg/L at 25°C or as indicated):

40	(quoted, Briggs 1981)
40	(22°C, Spencer 1982; Worthing & Walker 1983, 1987; Montgomery 1993; Tomlin 1994)
92; 54	(generator column-RI; HPLC-RT correlation, Swann et al. 1983)
40	(20–25°C, selected, Wauchope et al. 1992; Hornsby et al. 1996)

Vapor Pressure (Pa at 25°C or as indicated):

0.37	(23°C, Spencer 1982; Worthing & Walker 1983, 1987)
0.373	(20°C, Montgomery 1993)
0.373	(20–25°C, Wauchope et al. 1992; Hornsby et al. 1996)

Henry's Law Constant (Pa·m^3/mol at 25°C):

216	(calculated-P/C, Montgomery 1993)

Octanol/Water Partition Coefficient, log K_{OW}:

3.02	(shake flask-UV, Briggs 1981)
3.02–3.41	(Montgomery 1993)
3.325	(Tomlin 1994)
3.41	(recommended, Hansch et al. 1995)
3.41	(LOGPSTAR or CLOGP data, Sabljic et al. 1995)

Octanol/Air Partition Coefficient, log K_{OA}:

Bioconcentration Factor, log BCF or log K_B:

1.87, 1.36	(calcd-solubility, K_{OW}, Kenaga 1980b)

Sorption Partition Coefficient, log K_{OC}:

1.93–2.42; 2.19	(quoted: 10 soils range; mean, Briggs 1981)
2.0	(Cottenham soil, shake flask-GC, 20°C, Briggs 1981)

2.76	(calculated, Kenaga 1980b)
2.66	(average of 3 soils, HPLC-RT correlation, McCall et al. 1980)
2.64, 2.68, 2.66; 2.66	(Commeree soil, Tracy soil, Catlin soil; mean, HPLC-RT, Swann et al. 1981; quoted, McCall et al. 1981)
2.24–2.76	(quoted literature range, Wauchope et al. 1992)
2.76	(soil, Wauchope et al. 1992; Hornsby et al. 1996)
2.62–2.68	(soil, Montgomery 1993)
2.40–3.96	(soil, Tomlin 1994)
2.62	(soil, calculated-MCI $^1\chi$, Sabljic et al. 1995)

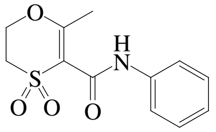
Environmental Fate Rate Constants, k, or Half-Lives, $t_{½}$:

Volatilization:
Photolysis: water photolysis $t_{½}$ = 2 h (Tomlin 1994).
Oxidation:
Hydrolysis: hydrolysis $t_{½}$ = 2 d at pH 7 (Tomlin 1994).
Biodegradation:
Biotransformation:
Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants:

Half-Lives in the Environment:

Air:
Surface water: hydrolysis $t_{½}$ = 2 d at pH 7, water photolysis $t_{½}$ = 2 h (Tomlin 1994).
Groundwater:
Sediment:
Soil: field $t_{½}$ = 10 d (Wauchope et al. 1992; Hornsby et al. 1992);
aerobic soil metabolism $t_{½}$ = 6.42 d, anaerobic metabolism $t_{½}$ ~ 2.5 h (Tomlin 1994).
Biota:

19.1.28 OXYCARBOXIN



Common Name: Oxycarboxin
Synonym: DCMOD, Oxycarboxine
Chemical Name: 5,6-dihydro-2-methyl-1,4-oxathi-ine-3-carboxanilide 4,4-dioxide; 5,6-dihydro-2-methyl-*N*-phenyl-1,4-oxathin-3-carboxamide 4,4-dioxide
CAS Registry No: 5259-88-1
Uses: as fungicide for control of rust diseases on ornamentals, cereals, and nursery trees, etc.
Molecular Formula: $C_{12}H_{13}NO_4S$
Molecular Weight: 267.301
Melting Point (°C):
129 (Lide 2003)
Boiling Point (°C):
Density (g/cm^3 at 20°C): 1.14 (Tomlin 1994)
Molar Volume (cm^3/mol):
261.4 (calculated-Le Bas method at normal boiling point)
234.5 (calculated-density)
Dissociation Constant pK_a:
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
Entropy of Fusion, ΔS_{fus} (J/mol K):
Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F: 0.054 (mp at 129°C)

Water Solubility (g/m^3 or mg/L at 25°C or as indicated):
1000 (Martin & Worthing 1977; quoted, Kenaga 1980)
1000 (Hartley & Kidd 1987; Worthing & Hance 1991; Tomlin 1994)
1000 (20–25°C, selected, Wauchope et al. 1992; Hornsby et al. 1996)
1000 (selected, Lohninger 1994)

Vapor Pressure (Pa at 25°C or as indicated):
0.0010 (20°C, Hartley & Kidd 1987)
< 133 (20°C, Worthing & Hance 1991)
5.60×10^{-6} (Tomlin 1994)
1.33×10^{-3} (20–25°C, selected, Wauchope et al. 1992; Hornsby et al. 1996)

Henry's Law Constant (Pa·m^3/mol at 25°C or as indicated):
3.56×10^{-4} (20–25°C, calculated-P/C, this work)

Octanol/Water Partition Coefficient, log K_{OW}:
0.74 (shake flask-UV, Mathre 1971)
0.74 (recommended, Sangster 1993)
0.772 (Tomlin 1994)
0.740 (selected, Hansch et al. 1995)
1.13 (RP-HPLC-RT correlation using short ODP column, Donovan & Pescatore 2002)

Bioconcentration Factor, log BCF:
1.11 (calculated-S, Kenaga 1980)

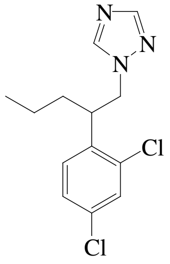
Sorption Partition Coefficient, log K_{OC}:
1.99 (calculated-S, Kenaga 1980)

1.98 (soil, estimated, Wauchope et al. 1992; Hornsby et al. 1996)
1.98 (selected, Lohninger 1994)

Environmental Fate Rate Constants, k, or Half-Lives, $t_{½}$:
Hydrolysis: $t_{½}$ = 44 d at pH 6, 25°C (Tomlin 1994).

Half-Lives in the Environment:
Soil: $t_{½}$ = 2.5–8 wk in sandy loam by aerobic soil metabolism (Tomlin 1994);
field $t_{½}$ = 20 d (Wauchope et al. 1992; Hornsby et al. 1996).

19.1.29 PENCONAZOLE



Common Name: Penconazole
Synonym: Award, CGA 71818, Topas, Topaz, Topaze
Chemical Name: 1-(2,4-dichloro-β-propylphenylethyl)-1*H*-1,2,4-triazole;1-[2-(2,4-dichlorophenyl)pentyl]-1*H*-1,2,4-triazole
CAS Registry No: 66246-88-6
Uses: as fungicide for control of pathogenic *Ascomycetes, Basidiomycetes* and *Deuteromycetes* (especially powdery mildews) on vines, cucurbits, pome fruit, ornamentals and vegetables.
Molecular Formula: $C_{13}H_{15}Cl_2N_3$
Molecular Weight: 284.184
Melting Point (°C):
60.0 (Hartley & Kidd 1987; Worthing & Hance 1991)
62.1 (Rordorf 1989)
57.6–60.3 (Tomlin 1994)
Boiling Point (°C):
Density (g/cm^3 at 20°C): 1.30 (Tomlin 1994)
Molar Volume (cm^3/mol):
312.3 (calculated-Le Bas method at normal boiling point)
218.6 (calculated-density)
Dissociation Constant pK_a:
1.51 (Tomlin 1994)
Enthalpy of Vaporization, ΔH_V (kJ/mol):
91.45 (Rordorf 1989)
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
27.1 (Rordorf 1989)
Entropy of Fusion, ΔS_{fus} (J/mol K):
81 (Rordorf 1989)
Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F: 0.454 (mp at 60°C)

Water Solubility (g/m^3 or mg/L at 25°C or as indicated):
70 (20°C, Hartley & Kidd 1987; Worthing & Hance 1991)
73 (20°C, Tomlin 1994)

Vapor Pressure (Pa at 25°C or as indicated and reported temperature dependence equations):
0.00021 (20°C, Hartley & Kidd 1987; Worthing & Hance 1991; Tomlin 1994)
3.70×10^{-4}, 1.30×10^{-2}, 0.28, 4.0, 41.0 (25, 50, 70, 100, 125°C, gas saturation-GC, Rordorf 1989)
$\log (P_S/Pa) = 16.671 - 5995.1/(T/K)$; measured range 36.6–58.3°C (solid, gas saturation-GC, Rordorf 1989)
$\log (P_L/Pa) = 13.088 - 4777.0/(T/K)$; measured range 60.9–129°C (liquid, gas saturation-GC, Rordorf 1989)

Henry's Law Constant (Pa·m^3/mol at 25°C or as indicated):
0.00082 (20°C, calculated-P/C, this work)

Octanol/Water Partition Coefficient, log K_{OW}:
3.40 (shake flask-HPLC, Bateman et al. 1990)
3.20 (shake flask-HPLC, Chamberlain et al. 1991)

3.72	(pH 5.7, Tomlin 1994)
3.40, 3.20	(Sangster 1993)
3.40, 3.50	(Hansch et al. 1995)

Bioconcentration Factor, log BCF:

1.75	(20°C, calculated-S as per Kenaga 1980, this work)

Sorption Partition Coefficient, log K_{OC}:

2.62	(20°C, calculated-S as per Kenaga 1980, this work)

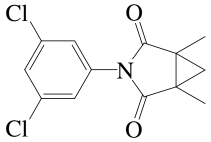
Environmental Fate Rate Constants, k, or Half-Lives, $t_{½}$:

Hydrolysis: stable to hydrolysis pH 1–13, and to temperature up to 350°C (Tomlin 1994).

Half-Lives in the Environment:

Soil: half-life is several months (Tomlin 1994).

19.1.30 PROCYMIDONE



Common Name: Procymidone
Synonym: S-7131, Sialex, Sumiboto, Sumilex, Sumisclex
Chemical Name: *N*-(3,5-dichlorophenyl)-1,2-dimethylcyclopropane-1,2-dicarboximide; 3-(3,5-dichlorophenyl)-1,5-dimethyl-3-azabicyclo[3,1,0]hexane-2,4-dione
CAS Registry No: 32809-16-8
Uses: as fungicide for control of *Botrytis, Sclerotinia, Monilia,* and *Helminthosporium* spp. on fruit, vines, vegetables, cereals and ornamentals, etc.
Molecular Formula: $C_{13}H_{11}Cl_2NO_2$
Molecular Weight: 284.138
Melting Point (°C):
166 (Lide 2003)
Boiling Point (°C):
Density (g/cm^3 at 20°C):
1.452 (25°C, Hartley & Kidd 1987; Tomlin 1994; Milne 1995)
Molar Volume (cm^3/mol):
225.9 (calculated-Le Bas method at normal boiling point)
195.7 (calculated-density)
Dissociation Constant pK_a:
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
Entropy of Fusion, ΔS_{fus} (J/mol K):
Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F: 0.0414 (mp at 166°C)

Water Solubility (g/m^3 or mg/L at 25°C or as indicated):
4.50 (Hartley & Kidd 1987; Worthing & Hance 1991; Tomlin 1994; Milne 1995)
4.50 (20–25°C, selected, Augustijn-Beckers et al. 1994; Hornsby et al. 1996)

Vapor Pressure (Pa at 25°C or as indicated):
0.018 (Hartley & Kidd 1987)
0.011 (20°C, Worthing & Hance 1991)
0.018, 0.0105 (20, 25°C, Tomlin 1994)
0.0187 (20–25°C, selected, Augustijn-Beckers et al. 1994; Hornsby et al. 1996)

Henry's Law Constant (Pa·m^3/mol at 25°C or as indicated):
1.181 (20–25°C, calculated-P/C, this work)

Octanol/Water Partition Coefficient, log K_{OW}:
3.14 (26°C, Worthing & Hance 1991; Tomlin 1994; Milne 1995)
3.0 (selected, Hansch et al. 1995)

Bioconcentration Factor, log BCF:
2.42 (calculated-S as per Kenaga 1980, this work)

Sorption Partition Coefficient, log K_{OC}:
3.18 (soil, estimated, Augustijn-Beckers et al. 1994; Hornsby et al. 1996)
3.28 (soil, calculated-S as per Kenaga 1980, this work)

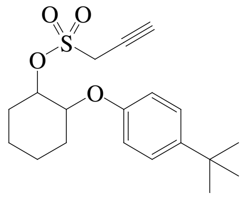
Environmental Fate Rate Constants, k, or Half-Lives, $t_{½}$:

Photolysis: when irradiation with UV light, $\lambda \geq 290$ nm, for procymidone solution (2 ppm): 9% and 11% photodegraded in 1 h, in the presence of 1 ppm humic acid and 1 ppm fulvic acid, respectively; rapid degradation with $t_{½} = 3$ min in the presence of TiO_2 (20 ppm), but degraded slowly as 9% transformation in 2 h with Fe_2O_3 (100 ppm). (Hustert & Moza 1997)

Half-Lives in the Environment:

Air:
Surface water: photodegradation of procymidone solution (2 ppm), $t_{½} = 3$ min in the presence of TiO_2 (20 ppm) when irradiated with UV light (Hustert & Moza 1997)
Groundwater:
Sediment:
Soil: persists for ca. 4–12 weeks (Hartley & Kidd 1987; Tomlin 1994);
field $t_{½} = 7$ d (Augustijn-Beckers et al. 1994; Hornsby et al. 1996).
Biota:

19.1.31 PROPARGITE



Common Name: Propargite
Synonym: Comite, Omite
Chemical Name: 2-[4-(1,1-dimethylethyl)phenoxy]cyclohexyl 2-propynyl sulfite
CAS Registry No: 2312-35-8
Uses: acaricide
Molecular Formula: $C_{16}H_{26}O_4S$
Molecular Weight: 360.472
Melting Point (°C):
dark brown liquid (Hartley & Kidd 1987)
Boiling Point (°C):
Density (g/cm^3 at 25°C):
1.085–1.115 (Hartley & Kidd 1987; Worthing & Walker 1983, 1987)
Molar Volume (cm^3/mol):
Dissociation Constant pK_a:
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
Entropy of Fusion, ΔS_{fus} (J/mol K):
Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F: 1.0

Water Solubility (g/m^3 or mg/L at 25°C or as indicated):
practically insoluble in water (Worthing & Walker 1983, 1987)

0.5	(20°C, Hartley & Kidd 1987)
0.50	(20–25°C, selected, Wauchope et al. 1992; Hornsby et al. 1996)
0.5	(20–25°C, Majewski & Capel 1995)

Vapor Pressure (Pa at 25°C or as indicated):

400	(20°C, Worthing & Walker 1983, 1987; Hartley & Kidd 1987)
0.4	(20–25°C, selected, Wauchope et al. 1992; Hornsby et al. 1996)
0.4	(20–25°C, quoted, Majewski & Capel 1995)

Henry's Law Constant (Pa·m^3/mol at 25°C or as indicated)

280	(20–25°C, Majewski & Capel 1995)

Octanol/Water Partition Coefficient, log K_{OW}:

Octanol/Air Partition Coefficient, log K_{OA}:

Bioconcentration Factor, log BCF or log K_B:

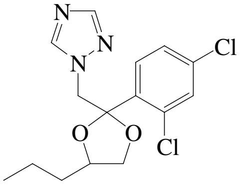
Sorption Partition Coefficient, log K_{OC}:

3.60	(soil, estimated, Wauchope et al. 1992; Hornsby et al. 1996)

Environmental Fate Rate Constants, k, or Half-Lives, $t_{1/2}$:

Half-Lives in the Environment:
Soil: field $t_{1/2}$ = 40 and 56 d, the recommended $t_{1/2}$ = 56 d (Wauchope et al. 1992; Hornsby et al. 1996).

19.1.32 PROPICONAZOLE



Common Name: Propiconazole
Synonym: Alamo, Banner, CGA 64250, Desmel, Orbit, Practis, Radar, Spire, Tilt
Chemical Name: (±)-1-[2-(2,4-dichlorophenyl)-4-propyl-1,3-dioxalan-2-ylmethyl]-1H-1,2,4-triazole; 1-[2-(2,4-dichlorophenyl)-4-propyl-1,3-dioxalan-2-ylmethyl]-1H-1,2,4-triazole
CAS Registry No: 60207-90-1
Uses: as fungicide for control of mildews, rusts on cereals, ornamentals, fruits and other crops; and also used for other diseases of turf and grass seed crops, etc.
Molecular Formula: $C_{15}H_{17}Cl_2N_3O_2$
Molecular Weight: 342.221
Melting Point (°C): liquid
Boiling Point (°C):
180 (at 0.1 mmHg, Hartley & Kidd 1987; Worthing & Hance 1991; Tomlin 1994; Milne 1995)
Density (g/cm^3 at 20°C):
1.27 (Hartley & Kidd 1987; Worthing & Hance 1991; Milne 1995)
1.29 (20°C, Tomlin 1994)
Molar Volume (cm^3/mol):
358.6 (calculated-Le Bas method at normal boiling point)
267.3 (calculated-density)
Dissociation Constant pK_a:
1.09 (Tomlin 1994)
Enthalpy of Vaporization, ΔH_V (kJ/mol):
106.8 (Rordorf 1989)
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
Entropy of Fusion, ΔS_{fus} (J/mol K):
Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F: 1.0

Water Solubility (g/m^3 or mg/L at 25°C or as indicated):
110 (20°C, Hartley & Kidd; Worthing & Hance 1991; Milne 1995)
100 (20°C, Tomlin 1994)
110 (20–25°C, selected, Wauchope et al. 1992; Hornsby et al. 1996)
110 (selected, Lohninger 1994)
110 (20°C, quoted, Siebers et al. 1994)

Vapor Pressure (Pa at 25°C or as indicated and reported temperature dependence equations):
0.00013 (20°C, Hartley & Kidd 1987)
5.60×10^{-5}, 1.60×10^{-3}, 0.027, 0.32, 28.0 (25, 50, 70, 100, 125°C, gas saturation-GC, Rordorf 1989)
$\log (P_L/\text{Pa}) = 14.468 - 5581.2/(T/\text{K})$; measured range 32.5–124°C (liquid, gas saturation-GC, Rordorf 1989)
0.000133 (20°C, Worthing & Hance 1991)
5.6×10^{-5} (20–25°C, Wauchope et al. 1992; Hornsby et al. 1996)
5.6×10^{-5} (Tomlin 1994)

Henry's Law Constant (Pa·m^3/mol at 25°C or as indicated):
4.0×10^{-4} (20°C, calculated-P/C, Siebers et al. 1994)
0.00017 (20–25°C, calculated-P/C, this work)

Octanol/Water Partition Coefficient, log K_{OW}:

3.50	(Bateman et al. 1990; quoted, Sangster 1993)
3.72	(Siebers et al. 1994)
3.72	(pH 6.6, Tomlin 1994)
3.50	(selected, Hansch et al. 1995)
3.50	(LOGPSTAR or CLOGP data, Sabljic et al. 1995)
3.33	(RP-HPLC-RT correlation using short ODP column, Donovan & Pescatore 2002)

Bioconcentration Factor, log BCF:

Sorption Partition Coefficient, log K_{OC}:

2.81	(soil, selected, Wauchope et al. 1992; Hornsby et al. 1996)
2.52	(soil, calculated-S as per Kenaga 1980, this work)
2.81	(selected, Lohninger 1994)
3.39	(soil, calculated-MCI $^1\chi$, Sabljic et al. 1995)
3.39; 3.62	(soil, quoted obs.; estimated-general model using molecular descriptors, Gramatica et al. 2000)

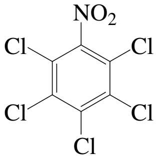
Environmental Fate Rate Constants, k, or Half-Lives, $t_{½}$:

Hydrolysis: no significant hydrolysis (Tomlin 1994).

Half-Lives in the Environment:

Air:
Surface water: $t_{½}$ = 25–85 d in aerobic aquatic systems at 25°C (Tomlin 1994).
Groundwater:
Sediment:
Soil: field $t_{½}$ = 110 d (Wauchope et al. 1992; Hornsby et al. 1996);
$t_{½}$ = 40–70 d in aerobic soils at 25°C (Tomlin 1994).
Biota:

19.1.33 QUINTOZENE



Common Name: Quintozene
Synonym: Avicol, Batrilex, Brassicol, Chinozan, earthcide, Fartox, Folosan, Fomac 2, Fungiclor, Kobutol, KOBU, KP 2, Marisan forte, Olpisan, PCNB, Pentagen, Phomasan, PKhNB, Quinosan, Quinocene, saniclor 30, Terraclor, Terrafun
Chemical Name: pentachloronitrobenzene
CAS Registry No: 82-68-8
Uses: as fungicide for seed and soil treatment, for control of *Botrytis, Rhizoctonia*, and *Sclerotinia* spp. on brassicas, vegetables, ornamentals and other crops, and *Telletia caries* of wheat.
Molecular Formula: $C_6Cl_5NO_2$
Molecular Weight: 295.335
Melting Point (°C):
144 (Lide 2003)
Boiling Point (°C):
328 (dec, Lide 2003)
Density (g/cm^3 at 20°C):
1.718 (25°C, Spencer 1982; Hartley & Kidd 1987; Worthing & Hance 1991; Milne 1995)
1.907 (21°C, Tomlin 1994)
Molar Volume (cm^3/mol):
207.3 (calculated-Le Bas method at normal boiling point)
154.9 (calculated-density)
Dissociation Constant pK_a:
Enthalpy of Vaporization, ΔH_V (kJ/mol):
77.3 (Rordorf 1989)
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
18 (Rordorf 1989)
Entropy of Fusion, ΔS_{fus} (J/mol K):
43 (Rordorf 1989)
Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F: 0.0680 (mp at 144°C)

Water Solubility (g/m^3 or mg/L at 25°C or as indicated):
practically insoluble (Spencer 1982; Worthing & Hance 1991; Milne 1995)
0.55 (20–25°C, shake flask-GC, Kanazawa 1981)
0.44 (20°C, Hartley & Kidd 1987; Pait et al. 1992; Milne 1995)
0.40 (Davies & Lee 1987)
0.44 (20–25°C, selected, Wauchope et al. 1992; Hornsby et al. 1996)
0.10 (selected, Lohninger 1994)
0.10 (20°C, Tomlin 1994)

Vapor Pressure (Pa at 25°C or as indicated and reported temperature dependence equations):
0.0151 (Spencer 1982)
6.60×10^{-3} (20°C, Hartley & Kidd 1987)
8.40×10^{-3}, 0.16, 1.90, 17.0, 110 (25, 50, 70, 100, 125°C, gas saturation-GC, Rordorf 1989)
$\log (P_S/Pa) = 14.34 - 4893.9/(T/K)$; measured range 49.9–140°C (solid, gas saturation-GC, Rordorf 1989)
$\log (P_L/Pa) = 12.234 - 4037.9/(T/K)$; measured range 150–196°C (liquid, gas saturation-GC, Rordorf 1989)
1.80 (Worthing & Hance 1991)
0.0147 (20–25°C, selected, Wauchope et al. 1992; Hornsby et al. 1996)
0.0127 (Tomlin 1994)

Henry's Law Constant ($Pa \cdot m^3/mol$ at 25°C):

0.3718	(known LWAPC of Kawamoto & Urano 1989, Meylan & Howard 1991)
0.4812	(calculated-bond contribution method LWAPC, Meylan & Howard 1991)

Octanol/Water Partition Coefficient, log K_{OW}:

4.22	(20°C, shake flask-GC, Kanazawa 1981)
5.21	(HPLC-RT correlation, McDuffie 1981)
5.00	(HPLC-RT correlation, Ohori & Ihashi 1987)
5.18	(HPLC-RT correlation, Kawamoto & Urano 1989)
4.77; 5.40	(shake flask-GC; calculated-fragment const., Niimi et al. 1989)
5.02	(RP-HPLC-RT correlation, Saito et al. 1993)
4.64	(recommended, Sangster 1993)
5.0–6.0	(Tomlin 1994)
4.22	(selected, Hansch et al. 1995)
4.89	(Pomona-database, Müller & Kördel 1996)
5.01	(RP-HPLC-RT correlation, Nakamura et al. 2001)
5.30	(RP-HPLC-RT correlation using short ODP column, Donovan & Pescatore 2002)

Bioconcentration Factor, log BCF:

2.38	(topmouth gudgeon, Kanazawa 1981)
3.49, 3.65, 3.06	(algae, activated sludge, fish, Freitag et al. 1985)
2.23	(rainbow trout, Niimi et al. 1989)
2.91	(quoted, Pait et al. 1992)

Sorption Partition Coefficient, log K_{OC}:

4.30	(correlated-Freundlich Isotherm, Kawamoto & Urano 1989)
4.30, 3.38	(soil, quoted exptl., calculated-MCI χ and fragments contribution, Meylan et al. 1992)
3.70	(soil, estimated, Wauchope et al. 1992; Hornsby et al. 1996)
4.34	(soil, HPLC-screening method, mean value of different stationary and mobile phases, Kördel et al. 1993, 1995)
3.78, 3.47	(for adsorption: silt loam, sand, Tomlin 1994)
3.98, 3.52	(for desorption: silt loam, sand, Tomlin 1994)
4.30	(estimated-chemical structure, Lohninger 1994)
4.34; 3.38	(HPLC-screening method; calculated-PCKOC fragment method, Müller & Kördel 1996)

Environmental Fate Rate Constants, k, or Half-Lives, $t_{1/2}$:

Biodegradation: rate constant k(aerobic) = 0.16 d^{-1} with $t_{1/2}$ = 4.3 d at 20°C by aerobic activated sludge and k(anaerobic) = 0.16 d^{-1} with $t_{1/2}$ = 4.3 d at 20°C by anaerobic microorganisms cultivated an artificial sewage (Kawamoto & Urano 1990)

rate constant k = 6.5 d^{-1} with $t_{1/2}$ = 0.11 d (Corrigendum, Kawamoto & Urano 1991).

Half-Lives in the Environment:

Air:

Surface water: biodegradation $t_{1/2}$ = 4.3 d at 20°C by aerobic activated sludge or anaerobic microorganisms cultivated by an artificial sewage (Kawamoto & Urano 1990)

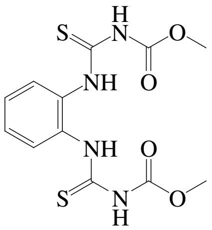
Groundwater:

Sediment:

Soil: $t_{1/2}$ ~ 4–10 months (Hartley & Kidd 1987; Tomlin 1994),
$t_{1/2}$ = 4 d (Pait et al. 1992);
field $t_{1/2}$ = 21 d (Wauchope et al. 1992; Hornsby et al. 1996).

Biota:

19.1.34 THIOPHANATE-METHYL



Common Name: Thiophanate-methyl

Synonym: Cerobin, Enovit, Fumidor, Fungitox, Fungo, Fungus Fighter, Labilite, Mildothane, Neotosin, NF-44, Pelt 44, Seal 7 Heal, Sigma, Sipcaplant, Sipcasan, Topsin M, Trevin

Chemical Name: dimethyl 4,4′-(*o*-phenylene)bis(3-thioallophanate; dimethyl [1,2-phenylene-bis(monocarbonothioyl)]-biscarbamate

Uses: fungicide/wound protectant

CAS Registry No: 23564-05-8

Molecular Formula: $C_{12}H_{14}N_4O_4S_2$

Molecular Weight: 342.394

Melting Point (C):

172	(dec., Worthing & Hance 1991; Tomlin 1994; Milne 1995; Lide 2003)

Boiling Point (°C):

Density (g/cm^3 at 20°C):

Molar Volume (cm^3/mol):

344.0	(calculated-Le Bas method at normal boiling point)

Dissociation Constant pK_a:

7.28	(Worthing & Hance 1991; Tomlin 1994)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

Entropy of Fusion, ΔS_{fus} (J/mol K):

Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F: 0.0361 (mp at 172°C)

Water Solubility (g/m^3 or mg/L at 25°C or as indicated):

3.50	(20°C, Hartley & Kidd 1987)
26.6	(Worthing & Hance 1991)
3.50	(20–25°C, selected, Wauchope et al. 1992; Hornsby et al. 1996)
3.50	(selected, Lohninger 1994)
26.6	(20°C, Milne 1995)

Vapor Pressure (Pa at 25°C or as indicated):

$< 1.0 \times 10^{-5}$	(20°C, Hartley & Kidd 1987)
$< 1.33 \times 10^{-5}$	(20–25°C, selected, Wauchope et al. 1992; Hornsby et al. 1996)
9.50×10^{-6}	(Tomlin 1994)

Henry's Law Constant (Pa·m^3/mol at 25°C):

0.0013	(calculated-P/C, this work)

Octanol/Water Partition Coefficient, log K_{OW}:

1.40	(Worthing & Hance 1991; Milne 1995)
1.50	(Tomlin 1994)
1.40	(selected, Hansch et al. 1995)
1.86	(RP-HPLC-RT correlation, pH 3.5, Hu et al. 1997)

Bioconcentration Factor, log BCF:

Sorption Partition Coefficient, log K_{OC}:

0.079	(Worthing & Hance 1991)
3.26	(20–25°C, estimated, Wauchope et al. 1992; Hornsby et al. 1996)
3.26	(selected, Lohninger 1994)

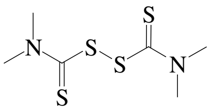
Environmental Fate Rate Constants, k, or Half-Lives, $t_{1/2}$:

Hydrolysis: stable neutral, aqueous solution, $t_{1/2}$ = 24.5 h at pH 9, 22°C (Tomlin 1994).

Half-Lives in the Environment:

Soil: field $t_{1/2}$ = 10 d (Wauchope et al. 1992; Hornsby et al. 1996);
persistence ca. 3–4 weeks (Tomlin 1994).

19.1.35 Thiram



Common Name: Thiram
Synonym: Aapirol, Aatiram, Accel TMT, Accelerator T, Aceto TETD, Arasan, Atiram, Cyuram, Delsan, Ekagom TB, ENT-987, Falitiram, Fermide, Fernacol, Fernasan, Fernide, Thiuram, TMTD
Chemical Name: tetramethylthiuram disulphide; bis(dimethylthiocarbomoyl) disulfide
CAS Registry No: 137-26-8
Uses: fungicide and also as seed disinfectant.
Molecular Formula: $C_6H_{12}N_2S_4$
Molecular Weight: 240.432
Melting Point (°C):

155.6	(Lide 2003)

Boiling Point (°C):

129	(20 mmHg, Howard 1991)
310–315	(15 mmHg, Montgomery 1993)

Density (g/cm^3 at 20°C):

1.29	(Spencer 1982; Worthing & Hance 1991; Montgomery 1993; Tomlin 1994; Milne 1995)

Molar Volume (cm^3/mol):

256.6	(calculated-Le Bas method at normal boiling point)
186.4	(calculated-density,)

Dissociation Constant pK_a:
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
Entropy of Fusion, ΔS_{fus} (J/mol K):
Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F: 0.0523 (mp at 155.6°C)

Water Solubility (g/m^3 or mg/L at 25°C or as indicated):

17.4	(22°C, Spencer 1973, 1982)
30	(Martin & Worthing 1977; Worthing & Walker 1987, Worthing & Hance 1991)
30	(Hartley & Kidd 1987; Montgomery 1993; Milne 1995)
30	(20–25°C, selected, Wauchope et al. 1992; Hornsby et al. 1996)
18	(room temp., Tomlin 1994)

Vapor Pressure (Pa at 25°C or as indicated):

negligible	(Hartley & Kidd 1987; Worthing & Hance 1991)
0.00133	(Halfon et al. 1996)
< 0.00133	(20–25°C, selected, Wauchope et al. 1992; Hornsby et al. 1996)
0.307	(Tomlin 1994)

Henry's Law Constant (Pa·m^3/mol at 25°C):

< 0.008	(calculated-P/C, Lyman et al. 1982)
0.0107	(calculated-P/C, this work)

Octanol/Water Partition Coefficient, log K_{OW}:

1.73	(Tomlin 1994)

Bioconcentration Factor, log BCF:

1.96	(calculated-S, Kenaga 1980)
1.96	(calculated-S, Lyman et al. 1982; quoted, Howard 1991)

Sorption Partition Coefficient, log K_{OC}:

2.83	(calculated-S, Kenaga 1980)
2.83	(calculated-S, Lyman et al. 1982; quoted, Howard 1991)
2.83	(20–25°C, selected, Wauchope et al. 1992; Hornsby et al. 1996)
2.82–3.39	(soil, Montgomery 1993)
2.83	(estimated-chemical structure, Lohninger 1994)

Environmental Fate Rate Constants, k, or Half-Lives, $t_{½}$:

Volatilization:

Photolysis:

Oxidation: assuming an ambient hydroxyl radical concn. of 8.0×10^5 mol/cm^3, the photooxidation reaction $t_{½}$ ~ 26.6 d at 25°C (estimated, GEMS 1986; quoted, Howard 1991).

Hydrolysis: $t_{½}$ = 5.3 d was estimated based on exptl. rate k = 5.0×10^{-3} h^{-1} (Ellington et al. 1988; quoted, Howard 1991; Montgomery 1993);

$t_{½}$ = 128 d at pH 4, $t_{½}$ = 18 d at pH 7 and $t_{½}$ = 9 h at pH 9 (Tomlin 1994).

Biodegradation:

Biotransformation:

Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants:

Half-Lives in the Environment:

Air: assuming an ambient hydroxyl radical concn. of 8.0×10^5 mol/cm^3, the photooxidation reaction $t_{½}$ ~ 26.6 d at 25°C (estimated, GEMS 1986; quoted, Howard 1991).

Surface water: calculated hydrolysis $t_{½}$ = 5.3 d at pH 7 (Ellington et al. 1988);

hydrolysis $t_{½}$ = 128 d, $t_{½}$ = 18 d and $t_{½}$ = 9 h at pH 4,7 and 9 (Tomlin 1994).

Groundwater:

Sediment:

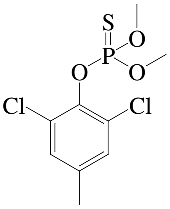
Soil: $t_{½}$ = 15 d in soil (Halfon et al. 1996);

field $t_{½}$ = 15 d (20–25°C, selected, Wauchope et al. 1992; Hornsby et al. 1996);

degradation $t_{½}$ = 0.5 d in sandy soil at pH 6.7 (Tomlin 1994).

Biota:

19.1.36 TOLCLOFOS-METHYL



Common Name: Tolclofos-methyl
Synonym: Risolex, Rizolex, S-3349
Chemical Name: *O*-2,6-dichloro-*p*-tolyl *O,O*-dimethyl phosphorothioate; *O*-(2,6-dichloro-4-methylphenyl) *O,O*-dimethyl phosphorothioate
CAS Registry No: 57018-04-9
Uses: as fungicide for control of soil-borne diseases caused by *Rhizoctonia, Sclerotium* and *Typhula* spp.; also used as a seed, bulb or tuber treatment, soil drench, foliar spray, or by soil incorporation.
Molecular Formula: $C_9H_{11}Cl_2O_3PS$
Molecular Weight: 301.127
Melting Point (°C):
78–80 (Hartley & Kidd 1987; Worthing & Hance 1991; Tomlin 1994; Milne 1995)
Boiling Point (°C):
Density (g/cm^3 at 20°C):
Molar Volume (cm^3/mol):
Dissociation Constant pK_a:
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
Entropy of Fusion, ΔS_{fus} (J/mol K):
Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F:

Water Solubility (g/m^3 or mg/L at 25°C or as indicated):
0.3–0.4 (23°C, Hartley & Kidd 1987)
0.3–0.4 (23°C, Worthing & Hance 1991)
1.10 (Tomlin 1994)
0.30 (20–25°C, selected, Augustiijn-Beckers et al. 1994; Hornsby et al. 1996)

Vapor Pressure (Pa at 25°C or as indicated):
0.057 (20°C, Hartley & Kidd 1987)
0.057 (20°C, Worthing & Hance 1991; Tomlin 1995)
0.0573 (20–25°C, selected, Augustijn-Beckers et al. 1994; Hornsby et al. 1996)
5.25×10^{-3}; 6.61×10^{-3}, 0.0234 (gradient GC method; estimation using modified Watson method: Sugden's parachor, McGowan's parachor, Tsuzuki 2000)

Henry's Law Constant (Pa·m^3/mol at 25°C):
57.5 (calculated-P/C, this work)

Octanol/Water Partition Coefficient, log K_{OW}:
4.56 (Worthing & Hance 1991; Tomlin 1994)

Bioconcentration Factor, log BCF:

Sorption Partition Coefficient, log K_{OC}:
3.30 (soil, estimated, Augustijn-Beckers et al. 1994; Hornsby et al. 1996)

Environmental Fate Rate Constants, k, or Half-Lives, $t_{½}$:

Photolysis: photodegradable with 8 h of sunlight: $t_{½}$ = 44 d in water, $t_{½}$ = 15–28 d in lake and river water, and $t_{½}$ < 2 d on soil surface (Hartley & Kidd 1987; Tomlin 1994).

Half-Lives in the Environment:

Air:

Surface water: photodegradable with 8 hours of sunlight in water with $t_{½}$ = 44 d, $t_{½}$ = 15–28 d in lake and river water, and $t_{½}$ < 2 d on soil surface (Hartley & Kidd 1987);

Photodegration $t_{½}$ = 44 d in water, $t_{½}$ = 15–28 d in lake (Tomlin 1994).

Groundwater:

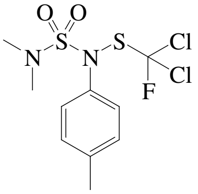
Sediment:

Soil: $t_{½}$ < 2 d from soil surface by photodegradation (Tomlin 1994);

field $t_{½}$ = 30 d (20–25°C, Augustijn-Beckers et al. 1994; Hornsby et al. 1996)

Biota:

19.1.37 TOLYLFLUANID



Common Name: Tolylfluanid

Synonym: Tolylfluanide

Chemical Name: *N*-dichlorofluoromethylthio-*N′N′*-dimethyl-*N*-*p*-tolylsulphamide; 1,1-dichloro-*N*-[(dimethylamino)-sulfonyl]-1-fluoro-*N*-(4-methylphenyl)methane-sulfenamide

Uses: fungicide/acaricide; to control scab on apples and pears; *Botrytis* on strawberries, raspberries, blackberries, currants, grapes, ornamentals, etc.

CAS Registry No: 731-27-1

Molecular Formula: $C_{10}H_{13}Cl_2FN_2O_2S_2$

Molecular Weight: 347.257

Melting Point (°C):

95–97	(Hartley & Kidd 1987; Worthing & Hance 1991; Milne 1995)
96	(Tomlin 1994)

Boiling Point (°C): dec. on distillation (Tomlin 1994)

Density (g/cm^3 at 20°C): 1.52 (Tomlin 1994)

Molar Volume (cm^3/mol):

326.0	(calculated-Le Bas method at normal boiling point)

Dissociation Constant pK_a:

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

Entropy of Fusion, ΔS_{fus} (J/mol K):

Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F: 0.201 (mp at 96°C)

Water Solubility (g/m^3 or mg/L at 25°C or as indicated):

4000	(Martin & Worthing 1977; quoted, Kenaga 1980)
4000	(room temp., Hartley & Kidd 1987; Worthing & Hance 1991)
0.90	(room temp., Tomlin 1994)

Vapor Pressure (Pa at 25°C or as indicated):

< 0.001	(20°C, Hartley & Kidd 1987)
1.3×10^{-5}	(45°C, Worthing & Hance 1991)
1.6×10^{-5}	(20°C, Tomlin 1994)

Henry's Law Constant (Pa·m^3/mol):

Octanol/Water Partition Coefficient, log K_{OW}:

3.95	(20°C, Worthing & Hance 1991)
3.90	(Tomlin 1994)
3.95	(selected, Hansch et al. 1995)
4.36	(RP-HPLC-RT correlation, Nakamura et al. 2001)

Bioconcentration Factor, log BCF:

0.778	(calculated, Kenaga 1980)

Sorption Partition Coefficient, log K_{OC}:

1.66	(soil, calculated-S, Kenaga 1980)

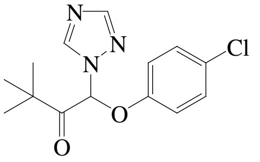
Environmental Fate Rate Constants, k, or Half-Lives, $t_{½}$:

Hydrolysis: $t_{½}$ = 12 d at 22°C and pH 4, $t_{½}$ = 29 h at pH 7 and $t_{½}$ < 10 min at pH 9 (Worthing & Hance 1991; Tomlin 1994).

Half-Lives in the Environment:

Soil: half-life of a few days (Tomlin 1994).

19.1.38 TRIADIMEFON



Common Name: Triadimefon
Synonym: Amiral, Bayleton, MEB 6447, Triadimefone
Chemical Name: 1-(4-chlorophenoxy)-3,3-dimethyl-1-(1*H*-1,2,4-triazol-1-yl)butanone; 1-(4-chlorophenoxy)-3,3-dimethyl-1-(1*H*-1,2,4-triazol-1-yl)-2-butanone
CAS Registry No: 43121-43-3
Uses: as fungicide for control of powdery mildews, rusts in cereals and *Rhynchosporium* in cereals and control of bunt, smuts, *Typhula* spp., seedling blight, leaf stripe, net blotch, and other cereal diseases when used for seed treatment, etc.
Molecular Formula: $C_{14}H_{16}ClN_3O_2$
Molecular Weight: 293.749
Melting Point (°C):
82 (Lide 2003)
Boiling Point (°C):
Density (g/cm^3 at 20°C):
1.22 (Hartley & Kidd 1987; Tomlin 1994; Milne 1995)
Molar Volume (cm^3/mol):
321 (calculated-Le Bas method at normal boiling point)
240.8 (calculated-density)
Dissociation Constant pK_a:
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
Entropy of Fusion, ΔS_{fus} (J/mol K):
Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F: 0.276 (mp at 82°C)

Water Solubility (g/m^3 or mg/L at 25°C or as indicated):
260 (Martin & Worthing 1977)
260 (20°C, Hartley & Kidd 1987; Worthing & Hance 1991; Milne 1995)
71.5 (20–25°C, selected, Wauchope et al. 1992; Hornsby et al. 1996)
71.5 (selected, Lohninger 1994)
64 (20°C, Tomlin 1994)
69; 72 (calculated-group contribution fragmentation method; quoted exptl., Kühne et al. 1995)

Vapor Pressure (Pa at 25°C or as indicated):
$< 1.0 \times 10^{-4}$ (20°C, Hartley & Kidd 1987; Worthing & Hance 1991)
2.00×10^{-6} (20–25°C, selected, Wauchope et al. 1992; Hornsby et al. 1996)
2.00×10^{-5}, 6.0×10^{-5} (20, 25°C, Tomlin 1994)

Henry's Law Constant (Pa·m^3/mol):

Octanol/Water Partition Coefficient, log K_{OW}:
1.80 (shake flask-UV at pH 5, Barak et al. 1983)
3.26 (shake flask, Hansch & Leo 1987)
2.77 (shake flask-LC, Patil et al. 1988)
3.18 (Worthing & Hance 1991; Milne 1995)
2.90 (shake flask at pH 7, Baker et al. 1992)
3.26 (recommended, Sangster 1993)
2.77 (recommended, Hansch et al. 1995)

3.03 (Pomona-database, Müller & Kördel 1996)
3.12 (RP-HPLC-RT correlation using short ODP column, Donovan & Pescatore 2002)

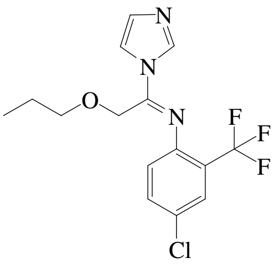
Bioconcentration Factor, log BCF:
1.43 (calculated, Kenaga 1980)

Sorption Partition Coefficient, log K_{OC}:
2.41 (soil, calculated-S, Kenaga 1980)
2.48 (20–25°C, selected, Wauchope et al. 1992; Hornsby et al. 1996)
2.57 (HPLC-screening method, Kördel et al. 1993)
2.48 (estimated-chemical structure, Lohninger 1994)
2.48 (soil, Tomlin 1994)
2.71 (soil, calculated-MCI $^1\chi$, Sabljic et al. 1995)
2.57; 3.72 (HPLC-screening method; calculated-PCKOC fragment method, Müller & Kördel 1996)
3.19, 2.277, 2.536, 2.39, 2.96 (first generation Eurosoils ES-1, ES-2, ES-3, ES-4, ES-5, shake flask/batch equilibrium-HPLC/UV, Gawlik et al. 1998, 1999)
2.826, 2.56, 2.512, 2.381, 3.046 (second generation Eurosoils ES-1, ES-2, ES-3, ES-4, ES-5, shake flask/batch equilibrium-HPLC/UV Gawlik et al. 1999)
2.826, 2.560, 2.512, 2.381, 3.046 (second generation Eurosoils ES-1, ES-2, ES-3, ES-4, ES-5, shake flask/batch equilibrium-HPLC/UV and HPLC-k′ correlation, Gawlik et al. 2000)
2.71; 2.43 (soil, quoted obs.; estimated-general model using molecular descriptors, Gramatica et al. 2000)

Environmental Fate Rate Constants, k, or Half-Lives, $t_{½}$:
Hydrolysis: $t_{½}$ > 1 yr at 22°C and pH 3, 6, and 9 (Worthing & Hance 1991; Tomlin 1994).

Half-Lives in the Environment:
Soil: field $t_{½}$ = 26 d (20–25°C, selected, Wauchope et al. 1992; Hornsby et al. 1996).

19.1.39 TRIFLUMIZOLE



Common Name: Triflumizole
Synonym: NF-114, Triflumizol, Trifmine
Chemical Name: (*E*)-4-chloro-α,α,α,-trifluoro-*N*-(1-imidazol-1-yl-2-propoxyethylidene)-*o*-tolui-dine; 1-[1-[[4-chloro-2-(trifluoromethyl)phenyl]imino]-2-propoxyethyl]-1*H*-imidazole
CAS Registry No: 68694-11-1
Uses: as fungicide for control of powdery mildews in fruit, vines, and vegetables; scab and rust in apples and pears; also used as seed treatment for barley, etc.
Molecular Formula: $C_{15}H_{15}ClF_3N_3O$
Molecular Weight: 345.574
Melting Point (°C):
63.5 (Hartley & Kidd 1987; Worthing & Hance 1991; Tomlin 1994; Milne 1995; Lide 2003)
Boiling Point (°C):
Density (g/cm^3 at 20°C):
Molar Volume (cm^3/mol):
359.5 (calculated-Le Bas method at normal boiling point)
Dissociation Constant pK_a:
3.70 (Augustijn-Beckers et al. 1994; Tomlin 1994; Hornsby et al. 1996)
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
Entropy of Fusion, ΔS_{fus} (J/mol K):
Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F: 0.419 (mp at 63.5°C)

Water Solubility (g/m^3 or mg/L at 25°C or as indicated):
12500 (20°C, Hartley & Kidd 1987; Worthing & Hance 1991; Tomlin 1994; Milne 1995)
12500 (20–25°C, selected, Augustijn-Beckers et al. 1994; Hornsby et al. 1996)

Vapor Pressure (Pa at 25°C or as indicated):
1.40×10^{-6} (Worthing & Hance 1991)
1.47×10^{-6} (20–25°C, selected, Augustijn-Beckers et al. 1992; Hornsby et al. 1996)
1.86×10^{-4} (Tomlin 1994)

Henry's Law Constant (Pa·m^3/mol at 25°C or as indicated):
4.07×10^{-8} (20–25°C, calculated-P/C, this work)

Octanol/Water Partition Coefficient, log K_{OW}:
1.40 (Worthing & Hance 1991; Milne 1995; Tomlin 1994)
1.40 (selected, Hansch et al. 1995)

Bioconcentration Factor, log BCF:

Sorption Partition Coefficient, log K_{OC}:
3.03–3.22 (Tomlin 1994)
1.60 (20–25°C, estimated, Augustijn-Beckers et al. 1994; Hornsby et al. 1996)

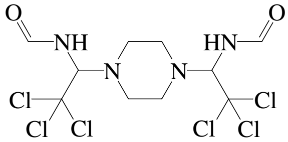
Environmental Fate Rate Constants, k, or Half-Lives, $t_{1/2}$:

Photolysis: aqueous solutions degraded by sunlight with $t_{1/2}$ = 29 h (Worthing & Hance 1991; Tomlin 1994).

Half-Lives in the Environment:

Soil: $t_{1/2}$ = 14 d on clay (Worthing & Hance 1991);
field $t_{1/2}$ = 14 d (20–25°C, selected, Augustijn-Beckers et al. 1994; Hornsby et al. 1996).

19.1.40 TRIFORINE



Common Name: Triforine

Synonym: Biformychloazin, Cela W524, Compound W, Denarin, FMC, Funginex, Saprol, W 524

Chemical Name: 1.1′-piperazine-1,4-diyldi-[*N*-(2,2,2-trichloroethyl)formamide]; 1,4-bis(2,2,2-trichloro-1-formamidoethyl) piperazine; *N,N′*-[1,4-piperazinediylbis(2,2,2-trichloro-ethylidene)]bisformamide

Uses: systemic fungicide to control powdery mildews on cereals, fruit, vines, hops, cucurbits, vegetables, and ornamentals, etc.; also used to suppress spider mite activity.

CAS Registry No: 26644-46-2

Molecular Formula: $C_{10}H_{14}Cl_6N_4O_2$

Molecular Weight: 434.962

Melting Point (°C):

155	(dec., Hartley & Kidd 1987; Worthing & Hance 1991; Tomlin 1994; Milne 1995; Lide 2003)

Boiling Point (°C):

Density (g/cm^3 at 20°C): 1.554 (Tomlin 1994)

Molar Volume (cm^3/mol):

389.2	(calculated-Le Bas method at normal boiling point)
279.9	(calculated-density)

Dissociation Constant pK_a:

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

Entropy of Fusion, ΔS_{fus} (J/mol K):

Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F: 0.053 (mp at 155°C)

Water Solubility (g/m^3 or mg/L at 25°C or as indicated):

30	(rm. temp., Hartley & Kidd 1987; Worthing & Hance 1991)
6.0	(rm. temp., Worthing & Hance 1991; Milne 1995)
30	(20–25°C, selected, Wauchope et al. 1992; Hornsby et al. 1996)
30	(selected, Lohninger 1994)
9.0	(20°C, Tomlin 1994)

Vapor Pressure (Pa at 25°C or as indicated):

2.6×10^{-5}	(Hartley & Kidd 1987)
2.7×10^{-5}	(Worthing & Hance 1991; Tomlin 1994)
2.7×10^{-5}	(20–25°C, selected, Wauchope et al. 1992; Hornsby et al. 1996)

Henry's Law Constant (Pa·m^3/mol):

Octanol/Water Partition Coefficient, log K_{OW}:

2.20	(Worthing & Hance 1991; Tomlin 1994; Milne 1995)

Bioconcentration Factor, log BCF:

Sorption Partition Coefficient, log K_{OC}:

2.73	(20–25°C, estimated, Wauchope et al. 1992; Hornsby et al. 1996)
2.30	(estimated-chemical structure, Lohninger 1994)

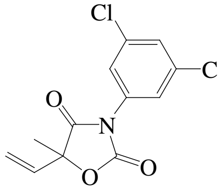
Environmental Fate Rate Constants, k, or Half-Lives, $t_{½}$:

Hydrolysis: $t_{½}$ = 3.5 d at pH 5, 25°C in aqueous solutions (Tomlin 1994).

Half-Lives in the Environment:

Soil: $t_{½}$ ~ 3 wk in soil (Hartley & Kidd 1987; Tomlin 1994);
field $t_{½}$ = 21 d (20–25°C, estimated, Wauchope et al. 1992; Hornsby et al. 1996).

19.1.41 VINCLOZOLIN



Common Name: Vinclozolin
Synonym: BAS 352F, Ronilan, Vorlan
Chemical Name: (*RS*)-3-(3,5-dichlorophenyl)-5-vinyl-1,3-oxazolidine-2,4-dione; 3-(3,5-dichlorophenyl)-5-ethenyl-5-methyl-2,4-oxazolidinedione
CAS Registry No: 50471-44-8
Uses: fungicide to control *Botrytis/Sclerotinie* spp. in vines, oilseed rape, vegetables, fruit, and ornamentals, etc.
Molecular Formula: $C_{12}H_9Cl_2NO_3$
Molecular Weight: 286.110
Melting Point (°C):
108 (Hartley & Kidd 1987; Worthing & Hance 1991; Tomlin 1994; Milne 1995: Lide 2003)
Boiling Point (°C):
131 (at 0.05 mmHg, Hartley & Kidd 1987; Tomlin 1994; Milne 1995)
Density (g/cm^3 at 20°C):
1.51 (Worthing & Hance 1991; Tomlin 1994; Milne 1995)
Molar Volume (cm^3/mol):
266.3 (calculated-Le Bas method at normal boiling point, this work)
189.5 (calculated-density, this work)
Dissociation Constant pK_a:
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
Entropy of Fusion, ΔS_{fus} (J/mol K):
Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F: 0.153 (mp at 108°C)

Water Solubility (g/m^3 or mg/L at 25°C or as indicated):
1000 (Martin & Worthing 1977)
1000 (20°C, Hartley & Kidd 1987)
3.40 (20°C, Worthing & Hance 1991; Tomlin 1994; Milne 1995)
1000 (20–25°C, estimated, Augustijn-Beckers et al. 1994; Hornsby et al. 1996)

Vapor Pressure (Pa at 25°C or as indicated):
< 0.010 (20°C, Hartley & Kidd 1987)
1.6×10^{-5} (20°C, Worthing & Hance 1991; Tomlin 1994)
1.6×10^{-5} (20–25°C, selected, Augustijn-Beckers et al. 1994; Hornsby et al. 1996)
1.3×10^{-4} (20°C, Siebers et al. 1994)

Henry's Law Constant (Pa·^{3}/mol at 25°C or as indicated):
0.011 (20°C, quoted, Siebers et al. 1994)

Octanol/Water Partition Coefficient, log K_{OW}:
3.00 (Stevens et al. 1988)
3.00 (pH 7, Worthing & Hance 1991; Tomlin 1994; Milne 1995)
2.47 (shake flask-HPLC at pH 6, Nielsen et al. 1992)
3.00, 2.47 (Sangster 1993)
3.10 (recommended, Hansch et al. 1995)

Bioconcentration Factor, log BCF:
1.26 (calculated, Kenaga 1980)

Sorption Partition Coefficient, log K_{OC}:

1.99	(soil, calculated-S, Kenaga 1980)
2.0–2.87	(soil, Tomlin 1994)
2.0	(soil, 20–25°C, estimated, Augustijn-Beckers et al. 1994; Hornsby et al. 1996)

Environmental Fate Rate Constants, k, or Half-Lives, $t_{½}$:

Volatilization:

Photolysis: when irradiation with UV light, $\lambda \geq 290$ nm, for vinclozolin aqueous solution (1 ppm): 10% and 11% photodegraded in 1 h, in the presence of 1 ppm humic acid and 1 ppm fulvic acid, respectively; irradiation of vinclozolin (2 ppm) in water with $t_{½}$ = 7 min and 92 min in the presence of TiO_2 (20 ppm), and Fe_2O_3 (100 ppm), respectively. (Hustert & Moza 1997)

Oxidation:

Hydrolysis: stable in neutral and weakly acidic media, in 0.1 N NaOH, 50% hydrolysis occurs in 3.8 h (Hartley & Kidd 1987; Tomlin 1994).

Biodegradation:

Biotransformation:

Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants:

Half-Lives in the Environment:

Air:

Surface water: photodegradation of vinclozolin aqueous solution (2 ppm), $t_{½}$ = 7 min and 92 min in the presence of TiO_2 (20 ppm), and Fe_2O_3 (100 ppm), respectively, when irradiated with UV light (Hustert & Moza 1997)

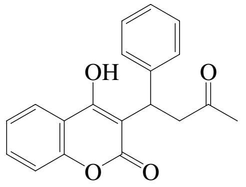
Groundwater:

Sediment:

Soil: field $t_{½}$ = 20 d (20–25°C, selected, Augustijn-Beckers et al. 1994; Hornsby et al. 1996).

Biota:

19.1.42 WARFARIN



Common Name: Warfarin
Synonym: Coumafen, Zoocoumarin
Chemical Name: 3-(α-acetonylbenzyl)-4-hydroxycoumarin
CAS Registry No: 81-81-2
Use: rodenticide
Molecular Formula: $C_{19}H_{16}O_4$
Molecular Weight: 308.328
Melting Point (°C):

161	(Lide 2003)

Boiling Point (°C): dec. (Montgomery 1993)
Density (g/cm^3 at 20°C):
Molar Volume (cm^3/mol):
Dissociation Constant pK_a:
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
Entropy of Fusion, ΔS_{fus} (J/mol K):
Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F: 0.0463 (mp at 161°C)

Water Solubility (g/m^3 or mg/L at 25°C or as indicated):

40	(shake flask, Coon et al. 1954)
17	(20°C, Hartley & Kidd 1987; Worthing & Walker 1987)
17	(20°C, Montgomery 1993; Tomlin 1994)

Vapor Pressure (Pa at 25°C or as indicated):

1.55×10^{-4}	(21.5°C, Hartley & Kidd 1987)
9.0	(21.5°C, Worthing & Walker 1987; Tomlin 1994)

Henry's Law Constant (Pa·m^3/mol at 25°C):

2.86×10^{-4}	(calculated-P/C, Howard 1991)

Octanol/Water Partition Coefficient, log K_{OW}:

2.52	(at pH 3, Howard 1991)
3.20	(calculated, Montgomery 1993)
3.12	(RP-HPLC-RT correlation using short ODP column, Donovan & Pescatore 2002)

Octanol/Air Partition Coefficient, log K_{OA}:

Bioconcentration Factor, log BCF:

1.68	(calculated, Howard 1991)

Sorption Partition Coefficient, log K_{OC}:

2.75	(estimated, Howard 1991)
2.96	(calculated, Montgomery 1993)

Environmental Fate Rate Constants, k, or Half-Lives, $t_{1/2}$:
Volatilization:
Photolysis:

Oxidation: Photooxidation $t_{½}$ = 0.254–1.87 h was estimated based on rate constants for reaction with hydroxyl radicals and ozone in air (Howard et al. 1991).

Hydrolysis: very slow with a $t_{½}$ = 16 yr at pH 7; the chemical hydrolysis rate constants, k = 1.4×10^{-4} M^{-1} h^{-1} for acid, neutral-k = 4.9×10^{-6} M^{-1} h^{-1} and k = 0.026 M^{-1} h^{-1} for base (Ellington et al. 1988; quoted, Howard 1991).

Biodegradation: aqueous aerobic $t_{½}$ = 168–672 h, anaerobic $t_{½}$ = 672–2688 h were estimated based on aqueous aerobic biodegradation (Howard et al. 1991).

Biotransformation:

Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants:

Half-Lives in the Environment:

Air: estimated $t_{½}$ = 11.6 min due to reaction with photochemically produced hydroxyl radicals and ozone in the vapor phase (Howard 1991);

$t_{½}$ = 0.254–1.87 h based on estimated photooxidation in air (Howard et al. 1991).

Surface water: $t_{½}$ = 168–672 h based on estimated unacclimated aqueous aerobic biodegradation (Howard et al. 1991);

slow hydrolysis $t_{½}$ = 15 yr at pH 7 (Howard 1991).

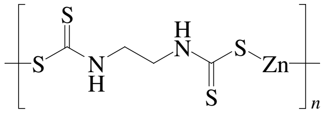
Groundwater: $t_{½}$ = 336–1344 h based on estimated aqueous aerobic biodegradation (Howard et al. 1991).

Sediment:

Soil: $t_{½}$ = 168–672 h based on estimated unacclimated aqueous aerobic biodegradation (Howard et al. 1991).

Biota:

19.1.43 ZINEB



Common Name: Zineb
Synonym: Dithane Z-78, Parzate Zineb, Lonaol, Aspor
Chemical Name: zinc ethylene-1,2-bisdithiocarbamate
CAS Registry No: 12122-67-7
Uses: fungicide
Molecular Formula: $(C_4H_6N_2S_4Zn)_x$
Molecular Weight: $(275.773)_x$
Melting Point (°C):
decomposes without melting (Worthing & Walker 1983)

157	(dec., Tomlin 1994; Lide 2003)

Boiling Point (°C):
Density (g/cm^3 at 20°C):
Molar Volume (cm^3/mol):
Dissociation Constant pK_a:
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
Entropy of Fusion, ΔS_{fus} (J/mol K):
Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F: 0.0507 (mp at 157°C)

Water Solubility (g/m^3 or mg/L at 25°C or as indicated):

1	(Melnikov 1971)
10	(Spencer 1982)
≈10	(Worthing & Walker 1983, 1987; quoted, Howard 1991)
10	(room temp., Tomlin 1994)
10	(20–25°C, selected, Augustijn-Beckers et al. 1994; Hornsby et al. 1996)

Vapor Pressure (Pa at 25°C or as indicated):

negligible at rm. temp. (Worthing & Walker 1983)

1.07×10^{-5}	(20°C, quoted, Howard 1991)
$< 1 \times 10^{-5}$	(20°C, Hartley & Kidd 1987; Tomlin 1994)
1.0×10^{-5}	(10–25°C, estimated, Augustijn-Beckers et al. 1994; Hornsby et al. 1996)

Henry's Law Constant (Pa·m^3/mol at 25°C):

Octanol/Water Partition Coefficient, log K_{OW}:

≤ 1.30	(Tomlin 1994)

Octanol/Air Partition Coefficient, log K_{OA}:

Bioconcentration Factor, log BCF:

2.11, 2.23, < 1.0,	(activated sludge, algae, Golden ide, Freitag et al. 1985)
2.28	(calculated-S, Kenaga 1980b; quoted, Howard 1991)

Sorption Partition Coefficient, log K_{OC}:

3.08	(soil, calculated-S, Kenaga 1980b; quoted, Howard 1991)
3.0	(soil, selected, Augustijn-Beckers et al. 1994; Hornsby et al. 1996)

Environmental Fate Rate Constants, k, or Half-Lives, $t_{1/2}$:

Photolysis: unstable to light, moisture and heat on prolonged storage (Tomlin 1994).

Half-Lives in the Environment:

Air: $t_{1/2}$ = 11–14 d in greenhouse experiment, microagroecosystem chambers (Nash & Beall 1980);
$t_{1/2}$ = 11–14 d by gravitational settling and degradation (Howard 1991).

Surface water:

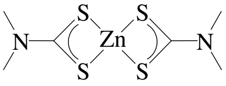
Groundwater:

Sediment:

Soil: $t_{1/2}$ = 23 d in 1-cm surface soil (sandy loam with pH 6.7), greenhouse experiment in microagroecosystem chambers (Nash & Beall 1980);
$t_{1/2}$ = 16–23 d upper layer of soil (Howard 1991);
field $t_{1/2}$ ~ 30 d (estimated, Augustijn-Beckers et al. 1994; Hornsby et al. 1996).

Biota: $t_{1/2}$ = 14 d on tomato leaves, green house experiment, microagroecosystem chambers (Nash & Beall 1980);
$t_{1/2}$ = 7 d for tomato fruit in the field, $t_{1/2}$ = 3.4 d for soybean leaves and $t_{1/2}$ = 9 d for tomatoes (Nash 1983);
$t_{1/2}$ = 14 d for tomato leaves, $t_{1/2}$ = 7 d for tomatoes, $t_{1/2}$ = 11 d for lettuce and $t_{1/2}$ = 35 d for grapes (Howard 1991).

19.1.44 ZIRAM



Common Name: Ziram
Synonym: Aaprotect, Fuklasin, Zerlate, zirmane
Chemical Name: zinc bis(dimethyldithiocarbamate)
CAS Registry No: 137-30-4
Uses: fungicide, bird and rodent repellent
Molecular Formula: $C_6H_{12}N_2S_4Zn$
Molecular Weight: 305.841
Melting Point (°C):
  250 (Howard 1991; Lide 2003)
Boiling Point (°C):
Density (g/cm^3 at 20°C):
  2.00 (Spencer 1982)
  1.66 (25°C, Hartley & Kidd 1987; Tomlin 1994; Milne 1995)
Molar Volume (cm^3/mol):
Dissociation Constant pK$_a$:
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
Entropy of Fusion, ΔS_{fus} (J/mol K):
Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F: 0.0062 (mp at 250°C)

Water Solubility (g/m^3 or mg/L at 25°C or as indicated):
  65 (Melnikov 1971)
  65 (Martin & Worthing 1977; Worthing & Walker 1983, 1987)
  4.0 (20°C, Spencer 1982)
  65 (Hartley & Kidd 1987)
  0.03 (20°C, Tomlin 1994)
  65 (20–25°C, selected, Augustijn-Beckers et al. 1994; Hornsby et al. 1996)
  65 (Milne 1995)

Vapor Pressure (Pa at 25°C or as indicated):
  negligible (Worthing & Walker 1983, 1987; quoted, Howard 1991)
  1.33×10^{-5} (20–25°C, Augustijn-Beckers et al. 1994; Hornsby et al. 1996)
  $< 1 \times 10^{-6}$ (extrapolated, Tomlin 1994)

Henry's Law Constant (Pa·m^3/mol at 25°C):

Octanol/Water Partition Coefficient, log K_{OW}:
  1.086 (Tomlin 1994)

Octanol/Air Partition Coefficient, log K_{OA}:

Bioconcentration Factor, log BCF:
  1.77 (calculated-S, Kenaga 1980b; quoted, Howard 1991)

Sorption Partition Coefficient, log K_{OC}:
  2.64 (soil, calculated-solubility, Kenaga 1980b; quoted, Howard 1991)
  2.60 (soil, estimated, Augustijn-Beckers et al. 1994; Hornsby et al. 1996)

Environmental Fate Rate Constants, k, or Half-Lives, $t_{1/2}$:
  Hydrolysis: decomposed in acidic media (Tomlin 1994).

Half-Lives in the Environment:

Air:
Surface water: decomposed in acidic media, and by UV irradiation (Tomlin 1994).
Groundwater:
Sediment:
Soil: field $t_{1/2}$ ~ 30 d (estimated, Augustijn-Beckers et al. 1992; Hornsby et al. 1996).
Biota: for orally administered to rate was mostly eliminated within 1–2 d (Tomlin 1994).

19.2 SUMMARY TABLES

TABLE 19.2.1
Common names, chemical names and physical properties of fungicides

Name	Synonym	Chemical name	Molecular formula	Molecular weight, MW g/mol	m.p. °C	Fugacity ratio, F at 25°C*	pK_a
Anilazine [101-05-3]	Botrysan, Direz, Dyren	2-chloro-*N*-(4,6-dichloro-1,3,5-triazin-2-yl)aniline	$C_9H_5Cl_3N_4$	275.522	160	0.0474	
Benalaxyl [71626-11-4]	Galben	methyl *N*-phenylacetyl-*N*-2,6-xylyl-*DL*-alaninate	$C_{20}H_{23}NO_3$	325.402	79	0.295	
Benodanil [15310-01-8]	Calirux	2-iodo-*N*-phenylbenzamide	$C_{13}H_{10}INO$	323.129	137	0.0796	
Benomyl [17804-35-2]	Benlate	methyl 1-(butylcarbamoyl)benz-imidazol-2-ylcarbamate	$C_{14}H_{18}N_4O_3$	290.318	140	0.0744	
Bitertanol [70585-36-3]	Baycor, Baymat, Biloxa, Siibutol	1-(biphenyl-4-yloxy)-3,3-dimethyl-1-1*H*-1,2,4-triazol-1-yl)butan-2-ol	$C_{20}H_{23}N_3O_2$	337.415	118 eutectic	0.122	
diastereoisomer A [70585–38–5]			337.415	136.7	0.0802		
diastereoisomer B [55179–31–2]			337.415	145.2	0.0662		
Buprirmate [41483-43-6]	Nimrod, Nimrod T	5-butyl-2-ethylamino-6-methyl-pyrimidinyl dimethylsulfamate	$C_{13}H_{24}N_4O_3S$	316.419	50–51	0.562	
Captan [133-06-2]	Aacaptan, Amercide, Captab, orthocide	*N*-trichloromethylthio-4-cyclohexene-1,2-dicarboximide	$C_9H_8Cl_3NO_2S$	300.590	172.5	0.0357	
Carbendazim [10605-21-7]	Bavistin, BCM, Carbendazol	carbamic acid, methyl-1*H*-benzimidazol-2-yl	$C_9H_9N_3O_2$	191.186	300 dec	0.0020	4.48 4.2
Carboxin [5234-68-4]	Vitavax, carbathiin	5,6-dihydro-2-methy-1,4-oxathi-ine-3-carboxanilide	$C_{12}H_{13}NO_2S$	235.302	94	0.210	
Chloroneb [2675-77-6]	Tersan SP	1,4-dichloro-2,5-dimethoxybenzene	$C_8H_8Cl_2O_2$	207.055	134	0.0852	
Chloropicrin [76-06-2]	Nitrochloroform	trichloronitromethane	CCl_3NO_2	164.376	–64	1	
Chlorothalonil [1897-45-6]	Bravo, Daconil	2,4,6-tetrachloro-1,3-benzene-dicarbonitrile	$C_8Cl_4N_2$	265.911	250	0.0062	
Dazomet (Fum.) [533-74-4]	Salvo, Mylone, Basamid	3,5-dimethyl-1,3,5-thiadiazinane-2-thione	$C_5H_{10}N_2S_2$	162.276	106	0.16	
Dichlofluanid [1085-98-9]	Euaren, Elvaron	*N*-dichlorofluoromethylthio-*N,N'*-dimethyl-*N*-phenylsuphamide	$C_9H_{11}Cl_2FN_2O_2S_2$	333.229	105.3	0.163	
Dichlone [117–80–6]	Phygon	2,3-dichloro-1,4-naphthoquinone	$C_{10}H_4Cl_2O_2$	227.044	195	0.0215	
Dicofol [115–32–2]	Kelthan	2,2,2-trichloro-1,1-bis(4-chlorophenyl) ethenol	$C_{14}H_9Cl_5O$	370.485	77.5	0.305	
Dithianon [3347-22-6]	Delan	5,10-dihydro-5,10-dioxonaphtho[2,3-*b*-]-1,4-dithi-in-2,3-dicarbonitrile	$C_{13}H_4N_2O_2S_2$	296.324	220	0.0122	

Edifenphos [17109-49-8]	EDDP, Hinosan	*O*-ethyl *S,S*-diphenyl-phosphoradithioate	$C_{14}H_{15}O_2PS_2$	310.371	–25	1	
Ethirimol [23947-60-6]		5-butyl-2-ethylamino-6-methyl-pyrimidim-4-ol	$C_{11}H_{19}N_3O$	209.288	160	0.0474	
Etridiazole [2593-15-9]	ethazol, ethazole, Terazole	ethyl 3-trichloromethyl-1,2,4-thiadiazolyl ether	$C_5H_5Cl_3N_2OS$	247.530	19.9	1	2.27
Fenarimol [60168-88-9]	Bloc, Rimidin, Rubigan	(±)-2,4-dichloro-α-(pyrimidin-5-yl) benzhydryl alcohol	$C_{17}H_{12}Cl_2N_2O$	331.195	118	0.122	
Fenfuram [24691-80-3]	fenfurame	2-methyl-3-fruanilide	$C_{12}H_{11}NO_2$	201.221	109–110	0.148	
Fenpropimorph [67564-91-4]	Corbel, Mistral	(±)-*cis*-4-[3-(4-*tert*-butylphenyl)-2-methylpropyl]-2,6-dimethylmorpholine	$C_{20}H_{33}NO$	303.482	oil	1	6.98
Folpet [133-07-3]	Foltan, Folpan, Folpel, Spolacid	*N*-(trichloromethylthio)phthalimide	$C_9H_4Cl_3NO_2S$	296.558	177	0.0323	
Formaldehyde [50–00–0]	Formalin, methanal	formaldehyde	HCHO	30.026	–92	1	
Furalaxyl [57646-30-7]	Fongarid	methyl-*N*-(2-furoyl)-*N*-(2,6-xylyl)-*DL*-alaninate	$C_{17}H_{19}NO_4$	301.337	70	0.362	
Hexachlorobenzene [118–74-1]	HCB	hexachlorobenzene	C_6Cl_6	284.782	228.83	0.010	
Imazalil [35554-44-0]	Bromazil, Deccozil	(±)-1-(β-allyloxy-2,4-dichlorophenyl-ethyl)imidazole	$C_{14}H_{14}Cl_2N_2O$	297.179	50	0.568	
Iprobenfos [26087-47-8]	Kitazin	*S*-benzy *O,O*-di-isopropyl phosphoro-thioate	$C_{13}H_{21}O_3PS$	288.342	oil	1	
Mancozeb [8018–01–7]	Dithane ultra, Dithane M45				192–194 dec		
Maneb [12427–38–2]	MEB, Dithane, Bravo	manganese ethylenebis(dithiocarbamate)	$(C_4H_6MnN_2S_4)_x$	$(265.302)_x$	dec 200		
Metalaxyl [57837-19-1]	Ridomil, Apron Fubol	methyl *N*-(2-methoxyacetyl)-2,6-xylyl)-*DL*-alaninate	$C_{15}H_{21}NO_4$	279.333	71	0.354	<< 0
Metiram [9006-42-4]	Carbatene, Polyram	zinc ammoniate ethylenebisdithio-carbamate-poly(ethylenethiurmdisulfide)					
Nitrapyrin [1929–82–4]	N-Serve	2-chloro-6-(trichloromethyl)pyridine	$C_6H_3C_{14}N$	230.907	63	0.424	
Oxycarboxin [5259-88-1]	Plantvax	5,6-dihydro-2-methyl-1,4-oxathi-ine-3- carboxanilide 4,4-dioxide	$C_{12}H_{13}NO_4S$	267.301	129	0.0954	
Penconazole [66246-88-6]	Topas, Topaz, Topaze	1-(2,4-dichloro-β-propylphenyl-ethyl)-1*H*-1,2,4-trizaole	$C_{13}H_{15}Cl_2N_3$	284.184	60	0.454	1.51
Procymidone [32809-16-8]	Sumisclex, Sumilex	*N*-(3,5-dichlorophenyl)-1,2-dimethyl-cyclopropane-1,2-dicarboximide	$C_{13}H_{11}Cl_2NO_2$	284.138	166	0.0414	
Propargite [2312–35–8]	Comite, Omite	2-[4-(1,1-dimethylethyl)phenoxy] cyclohexyl 2-propynyl sulfite	$C_{16}H_{26}O_4S$	360.472	liquid	1	
Propiconazole [60207-90-1]		(±)-1-[2,4-(dichlorophenyl)-4-propyl-1,3-dioxolan-2-methyl]-	$C_{15}H_{17}Cl_2N_3O_2$	342.221	liquid	1	1.09

(*Continued*)

TABLE 19.2.1 (*Continued*)

Name	Synonym	Chemical name	Molecular formula	Molecular weight, MW g/mol	m.p. °C	Fugacity ratio, F at 25°C*	pK_a
Quintozene [82-68-8]	Tritisan, Botrilex, Terrachlor	pentachloronitrobenzene	$C_6Cl_5NO_2$	295.335	144	0.0680	
Tecnazene [117-18-0]	Folosan, Fusarex	1,2,4,5-tetrachloro-3-nitrobenzene	$C_6HCl_4NO_2$	260.890	99.5	0.186	
Thiabendazole [148-79-8]	Mertect, Storite	2-(thiazol-4-yl)benzimidazole	$C_{10}H_7N_3S$	201.248	304–305	0.00181	
Thiophanate-methyl [23564-05-8]	Topsin M, Mildothane	dimethyl 4,4'-(*o*-phenylene)bis(3-thioallphanate)	$C_{12}H_{14}N_4O_4S_2$	342.394	172 dec	0.0361	7.28
Thiram [137-26-8]	Arasan, Tersan, Fernasan	tetramethylthiuram disulphide	$C_6H_{12}N_2S_4$	240.432	155.6	0.0523	
Tolclofos-methyl [57018-04-9]	Rizolex	*O*-2,6-dichloro-*p*-tolyl *O*,*O*-dimethyl phosphorothioate	$C_9H_{11}Cl_2O_3PS$	301.127	78-80	0.295	
Tolylfluanid [731-27-1]	Euparen M	*N*-dichlorofluoromethylthio-*N*,*N*'-dimethyl-*N*-*p*-tolysulphamide	$C_{10}H_{13}Cl_2FN_2O_2S_2$	347.257	96	0.201	
Triadimefon [43121-43-3]	Amiral, Bayeton	1-(-chlorophenoxy)-3,3-dimethyl-1-1*H*-1,2,4-triazol-1-yl)butanone	$C_{14}H_{16}ClN_3O_2$	293.749	82	0.276	
Triadimenol [55219-65-3]	Baytan	1-(4-chlorophenoxy)-3,3-dimethyl-1-(1*H*-1,2,4-triazol-1-yl)butan-2-ol	$C_{14}H_{18}ClN_3O_2$	295.764	121–127		
Tricyclazole [41814-78-2]	Beam, Bim, Blascide	5-methyl-1,2,4-triazolo[3,4-*b*]-benzothiazole	$C_9H_7N_3S$	189.237	187	0.0257	
Triflumizole [99387–89–0]	Trifmine	(*E*)-4-chloro-α,α,α-trifluoro-*N*-(1-imidazol-1-yl-propoxyethylidene)-*o*-toluidine	$C_{15}H_{15}ClF_3N_3O$	345.747	63.5	0.419	3.70
Triforine [26644-46-2]		1,4-bis(2,2,2-trichloro-1-formamido-ethyl) piperazine	$C_{10}H_{14}Cl_6N_4O_2$	434.962	155 dec	0.0530	
Vinclozolin [50471-44-8]	Ronilan	(*RS*)-3-(3,5-dichlorophenyl)-5-methyl-5-vinyl-1,3-oxazolidine-2,4-dione	$C_{12}H_9Cl_2NO_3$	286.110	108	0.153	
Warfarin (R.) [81-81-2]	Coumarin Dethmor	4-hydroxy-3-(3-*oxo*-1-phenylbutyl)-2*H*-1-benzopyran-2-one	$C_{19}H_{16}O_4$	308.328	161	0.0463	
Zineb [12122-67-7]	Zinebe	zine ethylenebis(dithiocarbamate)	$C_4H_6N_2S_4Zn$	275.773	157 dec	0.0507	
Ziram [137-30-4]	Zirame	zinc bis(dimethyldithiocarbamate)	$C_6H_{12}N_2S_4Zn$	305.841	250	0.0062	

Note: Fum.—fumigant, I—insecticide, R.—rodenticide

* Assuming ΔS_{fus} = 56 J/mol K

TABLE 19.2.2
Summary of selected physical-chemical properties of fungicides at 25°C

	Selected properties							
	Vapor pressure		Solubility				Henry's law constant H/(Pa·m^3/mol) calcd P/C	log K_{OC} reported
Compound	P^S/Pa	P_L/Pa	S/(g/m^3)	C^S/(mol/m^3)	C_L/(mol/m^3)	log K_{OW}		
Anilazine	8.20×10^{-7}	1.77×10^{-5}	8	0.0290	0.628	3.80	2.82×10^{-5}	3.0
Benalaxyl	0.00133	4.65×10^{-3}	37	0.1137	0.398	3.40	0.012	3.44–3.86
Benodanil	1.00×10^{-8}	1.28×10^{-7}	2	0.0062	0.0793		1.62×10^{-6}	2.85
Benomyl	1.33×10^{-8}*	1.82×10^{-7}	2.0*	0.0069	0.0945	2.30	1.93×10^{-6}	3.28
Bitertanol	1.00×10^{-6}	8.31×10^{-6}	5	0.0118	0.0984		8.45×10^{-5}	
diastereoisomer A	2.20×10^{-9}	2.80×10^{-8}	2.9	0.0069	0.0874	4.10	3.20×10^{-7}	
diastereoisomer B	2.50×10^{-9}	3.86×10^{-8}	1.6	0.0038	0.0585	4.40	6.60×10^{-7}	
Buprirmate	0.00067	1.21×10^{-3}	22	0.0695	0.126	3.90	9.64×10^{-3}	2.9
Captan	1.10×10^{-5}	4.23×10^{-4}	5.1	0.0170	0.653	2.30	6.48×10^{-4}	2.29
Carbendazim	6.50×10^{-8}	3.82×10^{-5}	8	0.0418	24.60	1.52	1.55×10^{-6}	2.35
Carboxin	1.30×10^{-5}	5.98×10^{-5}	195	0.829	3.811	2.17	1.57×10^{-5}	2.41
Chloroneb	0.40	4.788	8	0.0386	0.462		173.8	3.06
Chloropicrin (I,Fum.)	2400	2400	2270	13.81	13.81	2.07	197.3	1.79
Chlorothalonil	0.133*	22.86	0.6	0.0023	0.388	2.64	58.94	3.2
Dazomet (Fum.)	4.0×10^{-4}	2.47×10^{-3}	3000	18.48	114.3	0.15	2.16×10^{-5}	0.48
Dichlofluanid	2.10×10^{-5}	1.32×10^{-4}	1.3	0.0039	0.0245	3.70	5.38×10^{-3}	
Dithianon	6.60×10^{-5}	6.28×10^{-4}	0.5	0.0017	0.1605	3.20	0.0391	
Edifenphos	0.013	0.013	56	0.180	0.180	3.48	0.072	
Ethirimol	2.67×10^{-4}	5.78×10^{-3}	200	0.956	20.68	2.3	2.79×10^{-4}	
Etridiazole	0.013	0.013	50	0.202	0.202	3.37	0.0644	
Fenarimol	2.93×10^{-5}	2.44×10^{-4}	14	0.0423	0.351	3.69	6.93×10^{-4}	2.78
Fenfuram	2.0×10^{-5}	1.39×10^{-4}	100	0.497	3.444		4.02×10^{-5}	2.48
Fenpropimorph	0.0023	2.30×10^{-3}	4.3	0.0142	0.014		0.162	2.94–3.65
Folpet	0.0013	0.0414	1	0.0034	0.107	3.63	0.386	3.27
Formaldehyde	> 1 atm		miscible			0.35		
Furalaxyl			230	0.763	2.127	2.61		
Imazalil	9.30×10^{-6}	1.75×10^{-5}	1400	4.71	8.853	3.82	1.97×10^{-6}	3.60
Metalaxyl	7.47×10^{-4}	2.18×10^{-3}	8400	30.08	87.71	1.75	2.48×10^{-5}	1.7
Metiram	< 0.00001		0.1			0.30		5.7
Oxycarboxin	0.00133	0.0139	1000	3.741	39.06	0.74	3.56×10^{-4}	1.98
Penconazole	0.00021	4.66×10^{-4}	73	0.257	0.570	3.72	8.18×10^{-4}	2.62

(Continued)

TABLE 19.2.2 (*Continued*)

	Selected properties							
	Vapor pressure		Solubility				Henry's law constant H/(Pa·m³/mol)	log K_{OC}
Compound	P^S/Pa	P_L/Pa	S/(g/m³)	C^S/(mol/m³)	C_L/(mol/m³)	log K_{OW}	calcd P/C	reported
Procymidone	0.0187	0.4534	4.5	0.0158	0.384	3.14	1.181	3.18
Propiconazole	5.60×10^{-5}	5.60×10^{-5}	110	0.321	0.321	3.72	1.74×10^{-4}	2.82
Quintozene	0.0066	0.104	0.44	0.0015	0.023	4.64	4.430	4.3, 3.38
Tecnazene			0.44	0.0017	0.0091			
Thiabendazole	5.33×10^{-7}	3.13×10^{-4}	50	0.249	146.1	2.69	2.14×10^{-6}	3.4
Thiophanate-methyl	1.30×10^{-5}	3.70×10^{-4}	3.5	0.0102	0.291	1.50	1.27×10^{-3}	3.26
Thiram	0.00133	0.0209	30	0.125	1.963	1.73	0.0107	2.83
Tolclofos-methyl	0.0573	0.196	0.3	0.001	0.0034	4.56	57.51	3.3
Tolylfluanid	1.6×10^{-5}	8.06×10^{-5}	0.9	0.0026	0.0131	3.90	6.17×10^{-3}	1.66
Triadimefon	2.0×10^{-6}	7.37×10^{-6}	71.5	0.243	0.897	3.26	8.22×10^{-6}	
Triadimenol	4.13×10^{-8}	4.03×10^{-7}	47	0.159	1.549	3.08	2.60×10^{-7}	3.00
diastereoisomer A	< 0.001		62	0.210	2.761	3.08		
diastereoisomer B	4.10×10^{-8}	4.85×10^{-7}	32	0.108	1.280	3.28		
Tricyclazole	2.67×10^{-5}	1.09×10^{-3}	1600	8.46	346.2	1.40	3.16×10^{-6}	3.00
Triflumizole	1.47×10^{-6}	3.53×10^{-6}	12500	36.16	86.90		4.07×10^{-8}	
Triforine	2.67×10^{-5}	5.16×10^{-4}	30	0.069	1.332	2.20	3.87×10^{-4}	2.3
Vinclozolin	1.33×10^{-5}	8.81×10^{-5}	1000	3.495	23.14	3.00	3.81×10^{-6}	2.6
Warfarin (R.)	1.55×10^{-4}	3.43×10^{-3}	17	0.0551	1.221	3.20	2.81×10^{-3}	2.96
Zineb	1.33×10^{-5}		10	0.0363		1.30	3.67×10^{-4}	3.00
Ziram	1.0×10^{-6}	1.53×10^{-4}	65	0.213	32.61	1.086	4.70×10^{-6}	2.60

Note: * The reported values for this quantity vary considerably, whereas this selected value represents the best judgment of the authors. The reader is cautioned that it may be subject to a large error.

TABLE 19.2.3
Suggested half-life classes of fungicides in various environmental compartments at 25°C

Compound	Air class	Water class	Soil class	Sediment class
Benomyl	1	4	6	7
Captan	2	2	5	5
Chloropicrin	4	3	3	4
Chlorothalonil	4	4	5	6
Thiram	4	4	5	6

Class	Mean half-life (hours)	Range (hours)
1	5	< 10
2	17 (~ 1 day)	10–30
3	55 (~ 2 days)	30–100
4	170 (~ 1 week)	100–300
5	550 (~ 3 weeks)	300–1,000
6	1700 (~ 2 months)	1,000–3,000
7	5500 (~ 8 months)	3,000–10,000
8	17000 (~ 2 years)	10,000–30,000
9	55000 (~ 6 years)	> 30,000

19.3 REFERENCES

Agnihotri, V P. (1970) Persistent of captan and its effects on microflora, respiration, and nitrification of a forest nursery soil. *Can. J. Microbiol.* 17, 377–383.

Anliker, R., Moser, P. (1987) The limits of bioaccumulation of organic pigments in fish: their relation to the partition coefficient and the solubility in water and octanol. *Ecotoxicol. Environ. Saf.* 13, 43–52.

Atlas, E., Foster, R., Giam, C.S. (1982) Air-sea exchange of high molecular weight organic pollutants: laboratory studies. *Environ. Sci. Technol.* 16, 283–286.

Atkinson, R. (1985) Kinetics and mechanisms of the gas-phase reactions of OH radicals with organic compounds under atmospheric conditions. *Chem. Rev.* 85, 69–201.

Atkinson, R. (1987) Structure-activity relationship for the estimation of rate constants for the gas-phase reactions of OH radicals with organic compounds. *Int. J. Chem. Kinetics* 19, 799–828.

Atkinson, R., Carter, W.P.L. (1984) Kinetics and mechanisms of the gas-phase reactions of ozone with organic compounds under atmospheric conditions. *Chem. Rev.* 84, 437–470.

Atkinson, R., Lloyd, A.C. (1984) Evaluation of kinetic and mechanistic data for modeling of photochemical smog. *J. Phys. Chem. Ref. Data* 13, 315–444.

Augustijn-Beckers, P.W.M., Hornsby, A.G., Wauchope, R.D. (1994) The SCS/ARS/CES pesticide-properties database for environmental decision making. II. Additional compounds. *Rev. Environ. Contam. Toxicol.* 137, 1–82.

Austin, D.J., Briggs, G.G. (1976) A new extraction method for benomyl residues in soil and its application in movement and persistence studies. *Pestic. Sci.* 7, 201–210.

Austin, D.J., Lord, K.A., Williams, I.H. (1976) *Pestic. Sci.* 7, 211.

Baker, E.A., Hayes, A.L., Butler, R.C. (1992) Physicochemical properties of agrochemicals: Their effects on foliar penetration. *Pest. Sci.* 34(2), 167–182.

Ballschmiter, K., Wittlinger, R. (1991) Interhemisphere exchange of hexachlorohexanes, hexachlorobenzene, polychlorobiphenyl and 1,1,1-trichloro-2,2-bis(*p*-chloro-phenyl)-ethane in the lower atmosphere. *Environ. Sci. Technol.* 25, 1103–1111.

Banerjee, S. (1985) Calculation of water solubility of organic compounds with UNIFAC-derived parameters. *Environ. Sci. Technol.* 19, 369–370.

Banerjee, S., Howard, P. H. (1988) Improved estimation of solubility and partitioning through correction of UNIFAC-derived activity coefficients. *Environ. Sci. Technol.* 22, 839–841.

Banerjee, S., Howard, P.H., Lande, S.S. (1990) General structure vapor pressure relationship for organics. *Chemosphere* 21, 1173–1180.

Barak, E., Dinoor, A., Jacoby, B. (1983) Adsorption of systemic fungicides and a herbicide by some components of plant tissues, in relation to some physicochemical properties of the pesticides. *Pest. Sci.* 14(3), 213–219.

Barber, M.C., Suárez, L.A., Lassiter, R.R. (1988) Modeling bioconcentration of nonpolar organic pollutants by fish. *Environ. Toxicol. Chem.* 7, 545–558.

Bateman, G.L., Nicholls, P.H., Chamberlain, K. (1990) The effectiveness of eleven sterol biosynthesis-inhibiting fungicides against the take-all fungus (*Gaeumannomyces gramminis, var. tritici*) in relation to their physical properties. *Pest. Sci.* 29, 109–122.

Baulch, D.L., Cox, R.A., Hampson, R.F., Jr., Kerr, J.A., Troe, J., Watson, R.T. (1984) Evaluated kinetic and photochemical data for atmospheric chemistry (Supplement II). *J. Phys. Chem. Ref. Data* 13, 1255–1380.

Baxter, G.P., Bezzenberger, F.K., Wilson, C.H. (1920) The vapor pressures of certain substances: Chloropicrin, cyanogen bromide, methyl-dichloro-arsine, phenyl-dichloro-arsine, diphenyl-chloro-arsine and arsenic trichloride. *J. Am. Chem. Soc*. 42, 1386–1393.

Beck, J., Hansen, K.E. (1974) The degradation of quintozene, pentachlorobenzene, hexachloro-benzene and pentachloroaniline in soil. *Pest. Sci.* 5, 41–48.

Biagi, G.L., Guerra, M.C., Barbaro, A.M., Recanatini, M., Borea, P.A. (1991) Lipophilicity indices of triazine herbicides. *Sci. Total Environ.* 109/110, 33–40.

Bidleman, T.F. (1984) Estimation of vapor pressures for nonpolar organic compounds by capillary gas chromatography. *Anal. Chem.* 56, 2490–2496.

Bidleman, T.F., Foreman, W.T. (1987) Vapor-particle partitioning of semivolatile organic compounds. In: *Sources and Fate of Aquatic Pollutants*. Hite, R.A., Eisenreich, S.J., Editors, pp. 127–56, Advances in Chemistry Series 216, American Chemical Society, Washington, DC.

Bintein, S., Devillers, J. (1994) QSAR for organic chemical sorption in soils and sediments. *Chemosphere* 28(6), 1171–1188.

Bobra, A.M., Shiu, W.Y., Mackay, D. (1985) Quantitative structure-activity relationships for the acute toxicity of chlorobenzenes to *Daphnia magna*. *Environ. Toxicol. Chem.* 4, 297–305.

Briggs, G.G. (1981) Theoretical and experimental relationships between soil adsorption, octanol-water partition coefficients, water solubilities, bioconcentration factors, and the Parachor. *J. Agric. Food Chem.* 29, 1050–1059.

Brooke, D.N., Dobbs, A.J., Williams, N. (1986) Octanol/water partition coefficients (P): Measurement, estimation, and interpretation, particularly for chemicals with $P > 10^5$. *Ecotoxicol. Environ. Saf.* 11, 251–260.

Brouwer, D.H., Ravensberg, J.C., De Kort, W.L A.M., Van Hemmen, J.J. (1994) A personal sampler for inhalable mixed-phase aerosols: Modification to an existing sampler and validation test with three pesticides. *Chemosphere* 28(6), 1135–1146.

Brown, S., Chan, F., Jones, J., Liu, D., MaCalab, K., Mill, T., Supios, K., Schendel, D. (1975) Research program on hazard priority ranking of manufactured chemicals: Phase II. Final report, Stanford Research Institute, Menlo Park, California.

Brusseau, M.L., Rao, P.S.C. (1989) The influence of sorbate-organic matter interactions on sorption nonequilibrium. *Chemosphere* 18, 1691–1706.

Burchfield, H.P. (1959) Comparative stabilities of dyrene, 1-fluoro-2,4-dinitrobenzene, dichlone and captan in a silt loam soil. *Contrib. D. Boyce Thompson Inst.* 20, 205–215.

Burkhard, L.P., Kuehl, D.W., Veith, G.D. (1985) Evaluation of reversed phase LC/MS for estimation of *n*-octanol/water partition coefficients of organic chemicals. *Chemosphere* 14, 1551–1560.

Burkhard, N., Guth, J.A. (1981) Rate of volatilisation of pesticides from soil surfaces; Comparison of calculated results with those determined in a laboratory model system. *Pest. Sci.* 12(1), 37–44.

Buser, H.-R., Müller, M.D., Poiger, T., Balmer, M.E. (2002) Environmental behavior of the chiral acetamide pesticide metalaxyl: enantioselective degradation and chiral stability in soil. *Environ. Sci. Technol.* 36, 221–226.

Bysshe, S.E. (1982) Chapter 5, Bioconcentration factor in aquatic organisms. In: *Handbook on Chemical Property Estimation Methods, Environmental Behavior of Organic Compounds*. Lyman, W. J., Reehl, W. F., Rosenblatt, D. H., Editors, McGraw-Hill, Inc., New York.

Calamari, D., Galassi, S., Sette, F., Vighi, M. (1983) Toxicity of selected chlorobenzenes to aquatic organisms. *Chemosphere* 12, 253–262.

Callahan, M.A., Slimak, M.W., Gabel, N.W., May, I.P., Fowler, C.F., Freed, J.R., Jennings, P., Durfee, R.L., Whitmore, F.C., Maestri, B., Mabey, W.R., Holt, B.R., Gould, C. (1979) *Water-Related Environmental Fate of 129 Priority Pollutants.* Vol. 1, EPA Report No. 440/4–79–029a, Versar, Inc., Springfield, Virginia.

Calvert, J.G., Demeyan, K.L., Kerr, J.A., McQuigg, R.D. (1972) Photolysis of formaldehyde as a hydrogen atom source in the lower atmosphere. *Science* 175, 751–752.

Carlier, P., Hannachi, H., Mouvier, G. (1986) The chemistry of carbonyl compounds in the atmosphere-A review. *Atmos. Environ.* 20(11), 2079–2099.

Carlson, A.R., Kosian, P.A. (1987) Toxicity of chlorinated benzenes to fathead minnows (*Pimephales promelas*). *Arch. Environ. Contam. Toxicol.* 16, 129–135.

Carris, L.M. (1983) Movement of the systemic fungicide metalaxyl in soils and its translocation in plants. M.S. Thesis, Washington State University, Pullman, Washington.

Chamberlain, K., Bateman, G.L., Nicholls, P.H. (1991) Volatile analogoues of penconazole and their activity against the take-all fungus (*Gaeumannomyces gramminis, var. tritici*). *Pest. Sci.* 31(2), 185–196.

Chin, Y.P., Weber, Jr., W.J., Voice, T.C. (1986) Determination of partition coefficients and aqueous solubilities by reverse phase chromatography-II. *Water Res.* 20, 1443–1450.

Chiou, C.T. (1981) Partition coefficient and water solubility in environmental chemistry. In: *Hazard Assessment of Chemicals. Current Development*. Vol. 1, Saxena, J., Fisher, S, Editors, pp. 117–153, Academic Press, Inc., New York.

Chiou, C.T. (1985) Partition coefficients of organic compounds in lipid-water systems and correlations with fish concentration factors. *Environ. Sci. Technol.* 19, 57–62.

Chiou, C.T., Schmedding, D.W., Manes, M. (1982) Partitioning of organic compounds in octanol-water system. *Environ. Sci. Technol.* 16, 4–10.

Connell, D.W., Hawker, D.W. (1988) Use of polynomial expressions to describe the bio-concentration of hydrophobic chemicals by fish. *Ecotoxicol. Environ. Saf.* 16, 242–257.

Connell, D.W., Markwell, R D. (1990) Bioaccumulation in the soil to earthworm system. *Chemosphere* 20, 91–100.

Coon, F.B., Richter, E.F., Hein, L.W., Krieger, C.H. (1954) Problems encountered in physicochemical determination of warfarin. *J. Agric. Food Chem.* 2, 739–741.

Davies, J.E., Lee, J.A. (1987) Changing profiles in human health effects of pesticides. *Pest. Sci. Biotechnol. Proc. 6th Int'l Congr. Pesticide Chem.* 533–538.

Dean, J., Editor (1985) *Lange's Handbook of Chemistry.* 13th Edition, McGraw-Hill, New York.

De Bruijn, J., Busser, F., Seinen, W., Hermens, J. (1989) Determination of octanol/water partition coefficients for hydrophobic organic chemicals with the "slow-stirring" method. *Environ. Toxicol. Chem.* 8, 499–512.

De Bruijn, J., Hermens, J. (1990) Relationships between octanol/water partition coefficients and total molecular surface area and total molecular volume of hydrophobic organic chemicals. *Quant. Struct.-Act. Relat.* 9, 11–21.

De Kock, A.C., Lord, D.A. (1987) A simple procedure for determining octanol-water partition coefficients using reversed phase high performance liquid chromatography (RPHPLC). *Chemosphere* 16(1), 133–142.

Deneer, J.W., Seinen, W., Hermens, J.L.M. (1988) The acute toxicity of aldehydes to the guppy. *Aqua. Toxicol.* 12, 185–192.

Deutsche Forschungsgemeinschaft (1983) *Hexachlorcyclohexan als Schadstoff in Lebensmitteln.* Verlag Chemie, Weinheim, Germany. pp.11–17.

DiToro, D.M., O'Conner, D.J., Thomann, R.V., St. John, J.P. (1981) Analysis of fate of chemicals in receiving waters. Phase I, Hydroqual, Inc., Prepared for the Chemical Manufacturing Association, Washington, DC., May, 1981.

Dobbs, A.J., Cull, M.R. (1982) Volatilization of chemicals-relative loss rates and the estimation of vapor pressures. *Environ. Pollut.* B3, 289–298.

Dong, S., Dasgupta, P. K. (1986) Solubility of gaseous formaldehyde in liquid water and generation of trace standard gaseous formaldehyde. *Environ. Sci. Technol.* 6(20), 637–640.

Donovan, S.F. (1996) New method for estimating vapor pressure by the use of gas chromatography. *J. Chromatogr.* A, 749, 123–129.

Donovan, S.F., Pescatore, M.C. (2002) Method for measuring the logarithm of the octanol-water partition coefficient by using short octadecyl-poly-(vinyl alcohol) high-performance liquid chromatography columns. *J. Chromatog.* A, 952, 47–61.

Dorfman, L M., Adams, G.E. (1973) Reactivity of the Hydroxyl Radicals in Aqueous Solution. NSRD-NDB-46. NTIS COM-73–50623. National Bureau of Standards, Washington, DC., 51 pp.

Doucette, W.J., Andren, A.W. (1988) Estimation of octanol/water partition coefficients: Evaluation of six methods for highly hydrophobic aromatic hydrocarbons. *Chemosphere* 17, 345–359.

Dreisbach, R.R. (1961) *Physical Properties of Chemical Compounds—III.* Advances in Chemistry Series, American Chemical Society Applied Publications. American Chemical Society.

Eadsforth, C.V., Moser, P. (1983) Assessment of reverse phase chromatographic methods for determining partition coefficients. *Chemosphere* 12, 1459–1475.

Ellgehausen, H., D'Hondt, C., Fuerer, R. (1981) Reversed-phase chromatography as a general method for determining octanol/water partition coefficients. *Pest. Sci.* 12, 219–227.

Ellgehausen, H., Guth, J.A., Esser, H.O. (1980) Factors determining bioaccumulation potential of pesticides in the individual compartments of aquatic food chains. *Ecotoxicol. Environ. Saf.* 4, 134–157.

Ellington, J.J., Stancil, F.E., Payne, W.D. (1987) *Measurement of Hydrolysis Rate Constants for Evaluation of Hazardous Waste Land Disposal.* Vol. 1, Data on 32 chemicals. EPA-600/3–86/043, U.S. EPA, Washington, DC.

Ellington, J.J., Stancil, F.E., Payne, W.D. (1987) *Measurement of Hydrolysis Rate Constants for Evaluation of Hazardous Waste Land Disposal.* Vol. 2, Data on 54 chemicals. EPA-600/53–87/019, U.S. EPA, Washington, DC.

Ellington, J.J., Stancil, F.E., Payne, W.D. (1988) *Measurement of Hydrolysis Rate Constants for Evaluation of Hazardous Waste Land Disposal.* Vol. 3, EPA 600/3–88/028, U.S. EPA, Washington, DC.

Farmer, W.J., Yang, M.S., Spencer, W.F. (1980) Hexachlorobenzene: Its vapor pressure and vapor phase diffusion in soil. *Soil Sci. Soc. Am. J.* 44, 676–680.

Figueroa, I. del C., Simmons, M.S. (1991) Structure-activity relationships of chlorobenzenes using DNA measurement as a toxicity parameter in algae. *Environ. Toxicol. Chem.* 10, 323–329.

Finizio, A., Vighi, M., Sandroni, D. (1997) Determination of N-octanolwater partition coefficient (Kow) of pesticide critical review and comparison of methods. *Chemosphere* 34, 131–161.

Fischer, R.C., Krämer, W., Ballschmiter, K. (1991) Hexachlorocyclohexane isomers as markers in the water flow of the Atlantic Ocean. *Chemosphere* 23, 889–900.

Foschi, S., Cesari, A., Ponti, I., Bentivogli, P.G., Bencivelli, A. (1970) Degradation and vertical movement of pesticides in the soil. *Notiz. Mal. Piante*. 82–83, 37–49.

Freed, V.H. (1976) Solubility, hydrolysis, dissolution constants and other constants of benchmark pesticides. In: *Literature Survey of Benchmark Pesticides.* George Washington University Medical Center, Washington, DC.

Freitag, D., Balhorn, L., Geyer, H., Körte, F. (1985) Environmental hazard profile of organic chemicals. An experimental method for the assessment of the behaviour of chemicals in the ecosphere by simple laboratory tests with C-14 labelled chemicals. *Chemosphere* 14, 1589–1616.

Freitag, D., Lay, J.P., Körte, F. (1984) Environmental hazard profile - Test results as related to structure and translation into the environment. In: *QSAR in Environmental Toxicology.* Kaiser, K. L. E., Ed., D. Reidel Publishing Co., Dordrecht, The Netherlands.

Gaffney, J.S., Streit, G.E., Spall, W.D., Hall, J.H. (1987) Beyond acid rain. Do soluble oxidants and organic toxins interact with SO_2 and NO_2 to increase ecosystem effects? *Environ. Sci. Technol.* 21(6), 519–524.

Garst, J.E. (1984) Accurate wide-range, automated, high-performance liquid chromatographic method for the estimation of octanol/water partition coefficients. II. Equilibrium in partition coefficient measurements, additivity of subsequent constants, and correlation of biological data. *J. Pharm. Sci.* 73, 1623–1629.

Garst, J.E., Wilson, W.C. (1984) Accurate wide-range, automated, high-performance liquid chromatographic method for the estimation of octanol/water partition coefficients. I. Effects of chromatographic conditions and procedure variables on accuracy and reproducibility of the method. *J. Pharm. Sci.* 73, 1616–1622.

Garten, C.T., Jr., Trabalka, J.R. (1983) Evaluation of models for predicting terrestrial food chain behavior of xenobiotics. *Environ. Sci. Technol.* 17, 590–595.

Gawlik, B.M., Feicht, E.A., Karcher, W., Kettrup, A., Muntau, H. (1998) Application of the European soil set (Eurosoils) to a HPLC-screening method for the estimation of soil adsorption coefficients of organic compounds. *Chemosphere* 36, 2903–2919.

Gawlik, B.M., Kettrup, A., Muntau, H. (1999) Characterisation of a second generation of European reference soils for sorption studies in the framework of chemical testing - Part II: soil adsorption behaviour of organic chemicals. *Sci. Total Environ*. 229, 109–120.

Gawlik, B.M., Kettrup, A., Muntau, H. (2000) Estimation of soil adsorption coefficients of organic compounds by HPLC screening using the second generation of the European reference soil set. *Chemosphere* 41, 1337–1347.

Gellman, I., Heukelekian, H. (1950) Biological oxidation of formaldehyde. *Sew. Indus. Waste* 22, 13–21.

GEMS (1986) *Graphical Exposure Modeling Systems.* Fate of Atmosphere Pollutants (FAP). Office of Toxic Substances, U.S. EPA, Washington, DC.

Geyer, H., Kraus, A.G., Klein, W., Richter, E., Körte, F. (1980) Relationship between water solubility and bioaccumulation potential of organic chemicals in rats. *Chemosphere* 9, 277–291.

Geyer, H., Politzki, G.R., Freitag, D. (1984) Prediction of ecotoxicological behaviour of chemicals: relationships between *n*-octanol/water partition coefficient and bioaccumulation of organic chemicals by alga *Chlorella. Chemosphere* 13, 269–284.

Geyer, H., Scheunert, I., Korte, F. (1987) Correlation between the bioconcentration potential of organic environmental chemicals in humans and their n-octanol/water partition coefficients. *Chemosphere* 16(1), 239–252.

Geyer, H., Visvanathan, R., Freitag, D., Körte, F. (1981) Relationship between water solubility of organic chemicals and their bioaccumulation by the alga *Chlorella*. *Chemosphere* 10, 1307–1313.

Giam, C.S., Atlas, E., Chan, H.S., Neff, G.S. (1980) Phthalate esters, PCB and DDT residues in the Gulf of Mexico atmosphere. *Atmos. Environ.* 14, 65–69.

Gobas, F.A.P.C., Bedard, D.C., Ciborowski, J.J.H. (1989b) Bioconcentration of chlorinated hydrocarbons by the mayfly (*Hexgenia limbata*) in Lake St. Clair. *J. Great Lakes Res.* 15(4), 581–588.

Gobas, F.A.P.C., Clark, K., Shiu, W.Y., Mackay, D. (1989a) Bioconcentration of polybrominated benzenes and biphenyls and related superhydrophobic chemicals in fish: Role of bioavailability and elimination into feces. *Environ. Toxicol Chem.* 8, 231–245.

Gobas, F.A.P.C., Shiu, W.Y., Mackay, D. (1987) Factors determining partitioning of hydrophobic organic chemicals in aquatic organisms. In: *QSAR in Environmental Toxicology II.,* Kaiser, K.L.E., Ed., pp. 107–124, D. Reidel Publishing Company, Dordrecht, The Netherlands.

Gramatica, P., Corradi, M., Consonni, V. (2000) Modelling and prediction of soil sorption coefficients of non-ionic organic pesticides by molecular descriptors. *Chemosphere* 41, 763–777.

Grayson, B.T., Fosbracey, L.A. (1982) Determination of the vapour pressure of pesticides. *Pest. Sci.* 13(3), 269–278.

Gückel, W., Kistel, R., Lewerenz, J., Synnatschke, G. (1982) A method for determining the volatility of active ingredients used in plant protection. Part III: the temperature relationship between vapor pressure and evaporation rate. *Pest. Sci.* 13, 161–168.

Gustafson, D.I. (1989) Groundwater ubiquity score: A simple method for assessing pesticide leachability. *Environ. Toxicol. Chem.* 8, 339–357.

Halfon, E., Galassi, S., Brüggemann, R., Provini, A. (1996) Selection of priority properties to assess environmental hazard of pesticides. *Chemosphere* 33(8), 1543–1562.

Halfon, E., Reggiani, M.G. (1986) On ranking chemicals for environmental hazard. *Environ. Sci. Technol.* 20, 1173–1179.

Hamaker, J.W., Thompson, J.M. (1972) Adsorption. In: *Organic Chemistry in Soil Environment.* Goring, C. A. I., Hamaker, J.W., Eds., pp. 49–143, Vol. 1, Marcel Dekker, New York.

Hammers, W.E., Meurs, G.J., De Ligny, C.L. (1982) Correlations between liquid chromatographic capacity ratio data on lichrosorb RP-18 and partition coefficients in the octanol-water system. *J. Chromatogr.* 247, 1–13.

Hansch, C., Leo, A. (1979) *Substituent Constants for Correlation Analysis in Chemistry and Biology.* John Wiley & Sons, Inc., New York.

Hansch, C., Leo, A. (1985) *Medchem. Project Issue No. 26,* Pomona College, Claremont, California.

Hansch, C., Leo, A. (1987) *Medchem. Project Issue No. 28,* Pomona College, Claremont, California.

Hansch, C., Leo, A., Hoekman, D. (1995) *Exploring QSAR. Hydrophobic, Electronic, and Steric Constants.* ACS Professional Reference Book, Am. Chem. Soc., Washington, DC.

Harnish, M., Möckel, H. J., Schulze, G. (1983) Relationship between log P_{OW} shake-flask values and capacity factors derived from reversed-phase HPLC for *n*-alkylbenzenes and some OECD reference substances. *J. Chromatogr.* 282, 315–332.

Hartley, D., Kidd, H., Eds. (1987) *The Agrochemicals Handbook.* 2nd Edition, The Royal Society of Chemistry, London, England.

Hartley, G.S., Graham-Bryce, I.J. (1980) *Physical Principles and Pesticide Behavior.* Volume 2, Academic Press, New York.

Hashimoto, Y., Tokura, K., Ozaki, K., Strachan, W. M. J. (1982) A comparison of water solubility by the flask and micro-column methods. *Chemosphere* 11, 991–1001.

Hawker, D.W. (1990) Description of fish bioconcentration factors in terms of solvatochromic parameters. *Chemosphere* 20, 467–477.

Hawker, D.W., Connell, D.W. (1985) Relationships between partition coefficient and uptake rate constant, clearance rate constant, and time to equilibration for bioaccumulation. *Chemosphere* 14, 1205–1219.

Hawker, D.W., Connell, D.W. (1986) Bioconcentration of lipophilic compounds by some aquatic organisms. *Ecotoxicol. Environ. Saf.* 11, 184–197.

Heukelekian, H., Rand, M.C. (1955) Biochemical oxygen demand for pure organic compounds. *J. Water Pollut. Control Assoc.* 29, 1040–1053.

Hinckley, D.A., Bidleman, T.F., Foreman, W.T. (1990) Determination of vapor pressures for nonpolar and semipolar organic compounds from gas chromatographic retention data. *J. Chem. Eng. Data* 35, 232–237.

Hine, J., Mookerjee, P.K. (1975) The intrinsic hydrophilic character of organic compounds. Correlations in terms of structural contributions. *J. Org. Chem.* 40, 292–298.

Hine, R.B., Johnson, D.L., Wenger, C.J. (1969) Persistence of two benzimidazole fungicides in soil and their fungistatic activity against *Phymatotrichum omnivorum*. *Phytopathology* 59, 798–801.

Hodnett, E. M., Wongwiechintana, C., Dunn, III, W. J., Marrs, P. (1983) Substituted 1,4-naphthoquinones vs. the ascitic Sarcoma 180 of mice. *J. Med. Chem.* 26, 570–574.

Hodson, J., Williams, N. A. (1988) The estimation of the adsorption coefficient (K_{OC}) for soils by high performance liquid chromatography. *Chemosphere* 17, 67–77.

Hollifield, H.C. (1979) Rapid nephelometric estimate of water solubility of highly insoluble organic chemicals of environmental interests. *Bull. Environ. Contam. Toxicol.* 23, 579–586.

Hornsby, A.G., Wauchope, R.D., Herner, A.E. (1996) *Pesticide Properties in The Environment.* Springer-Verlag, Inc., New York.

Horvath, A.L., Editor (1982) *Halogenated Hydrocarbons, Solubility-Miscibility with Water.* Marcel Dekker, Inc., New York.

Howard, P.H., Editor (1989) *Handbook of Fate Exposure Data for Organic Chemicals. Vol. I. Large Production and Priority Pollutants.* Lewis Publishers, Inc., Chelsea, Michigan.

Howard, P.H., Editor (1991) *Handbook of Fate Exposure Data for Organic Chemicals. Vol. III. Pesticides.* Lewis Publishers, Inc., Chelsea, Michigan.

Howard, P.H., Boethling, R.S., Jarvis, W.F., Meylan, W.M., Michalenko, E.M., Eds. (1991) *Handbook of Environmental Degradation Rates.* Lewis Publishers, Inc., Chelsea, Michigan.

Hu. J.-Y., Aizawa, T., Magara, Y. (1997) Evaluation of adsorbability of pesticides in water on powdered activated carbon using octanol-water partition coefficient. *Wat. Sci. Tech*. 35, 219–226.

Hustert, K., Moza, P.N. (1997) Photochemical degradation of dicarboximide fungicides in the presence of soil constituents. *Chemosphere* 35, 33–37.

Isnard, P., Lambert, S. (1988) Estimating bioconcentration factors from octanol-water partition coefficient and aqueous solubility. *Chemosphere* 17, 21–34.

Isnard, P., Lambert, S. (1989) Aqueous solubility and octanol-water partition coefficient correlations. *Chemosphere* 18, 1837–1853.

IUPAC Solubility Data series (1985) Volume 20: *Halogenated Benzenes, Toluenes and Phenols with Water.* Horvath, A. L, Getzen, F.W., Eds., Pergamon Press, Oxford, England.

Jalali, L., Anderson, J.P.E. (1976) Uptake of benomyl by the cultivated mushroom, *Agricus bisporus. J. Agric. Food Chem*. 24, 431–432.

Jury, W.A., Focht, D.D., Farmer, W.J. (1987b) Evaluation of pesticide groundwater pollution potential from standard indices of soil-chemical adsorption and biodegradation. *J. Environ. Qual.* 16(4), 422–428.

Jury, W.A., Winer, A.M., Spencer, W.F., Focht, D.D. (1987a) Transport and transformations of organic chemicals in the soil-air water ecosystem. *Rev. Environ. Contam. Toxicol.* 99, 120–164.

Kaiser, K.L.E., Valdmanis, I. (1982) Apparent octanol/water partition coefficients of pentachlorophenol as a function of pH. *Can J. Chem.,* 60, 2104–2106.

Kaiser, K.L.E. (1983) COMPUTOX databank, National Water Research Institute Burlington, Ontario, Canada.

Kaiser, K.L.E., Dixon, D.G., Hodson, P.V. (1984) QSAR studies on chlorophenols, chlorobenzenes and para-substituted phenols. In: *QSAR in Environmental Toxicology.* Kaiser, K. L. E., Ed., pp. 189–206, D. Reidel Publishing Co., Dordrecht, The Netherlands.

Kamlet, M.J., Doherty, R.M., Carr, P.W., Mackay, D., Abraham, M.H., Taft, R.W. (1988) Linear solvation energy relationship. 44. Parameter estimation rules that allow accurate prediction of octanol/water partition coefficients and other solubility and toxicity properties of polychlorinated biphenyls and polycyclic aromatic hydrocarbons. *Environ. Sci. Technol.* 22, 503–509.

Kanazawa, J. (1981) Measurement of the bioconcentration factors of pesticides by fresh-water fish and their correlation with physicochemical properties of acute toxicities. *Pest. Sci.* 12, 417–424.

Karickhoff, S.W., Morris, K.R. (1985a) Impact of tubificid oligochaetes on pollutant transport in bottom sediments. *Environ. Sci. Technol.* 19(1), 51–56.

Karickhoff, S. W., Morris, K. R. (1985b) Sorption dynamics of hydrophobic pollutants in sediment suspensions. *Environ. Toxicol. Chem.* 4, 469–479.

Kawamoto, K., Urano, K. (1989) Parameters for predicting fate of organochlorine pesticides in the environment. (I) Octanol-water and air-water partition coefficients. *Chemosphere* 18, 1987–1996.

Kawamoto, K., Urano, K. (1989) Parameters for predicting fate of organochlorine pesticides in the environment. (II) Adsorption constant to soil. *Chemosphere* 18, 1987–1996.

Kawamoto, K., Urano, K. (1990) Parameters for predicting fate of organochlorine pesticides in the environment. (III) Biodegradation rate constants. *Chemosphere* 21, 1141–1152.

Kawanoto, K., Urano, K. (1991) Corrigendum. *Chemosphere* 23, 813.

Kelly, T.J., Mukund, R., Spicer, C.W., Pollack, A.J. (1994) Concentrations and trans-formations of hazardous air pollutants. *Environ. Sci. Technol.* 28, 378A-387A.

Kenaga, E.E. (1980a) Predicted bioconcentration factors and soil sorption coefficients of pesticides and other chemicals. *Ecotoxicol. Environ. Saf.* 4, 26–38.

Kenaga, E.E. (1980b) Correlation of bioconcentration factors of chemicals in aquatic and terrestrial organisms with their physical and chemical properties. *Environ. Sci. Technol.* 14, 553–556.

Kenaga E.E., Goring, C.A. (1980) Relationship between water solubility, soil sorption, octanol-water partitioning, and bioconcentration of chemicals in biota. In: *Aquatic Toxicology.* ASTM STP 707, Eaton, J.G., Parrish, P.R., Hendricks, A.C., Eds., pp. 78–115, American Society for Testing and Materials, Philadelphia, Pennsylvania.

Kerler, F., Schönherr, J. (1988) Accumulation of lipophilic chemicals in plant cuticles: Prediction from octanol/water partition coefficients. *Arch. Environ. Contam. Toxicol.* 17, 1–6.

Khan, U. K. (1980) *Pesticides in the Soil Environment, Fundamental Aspects of Pollution Control and Environmental Series 5.* Elsevier, Amsterdam, The Netherlands.

Kilzer, L., Scheunert, I., Geyer, H., Klein, W., Korte, F. (1979) Laboratory screening of the volatilization rates of organic chemicals from water and soil. *Chemosphere* 10, 751–761.

Klein, A.W., Harnish, M., Porenski, H.J., Schmidt-Bleek, F. (1981) OECD chemicals testing program physico-chemical tests. *Chemosphere* 10, 153–207.

Klein, W., Geyer, H., Freitag, D., Rohleder, H. (1984) Sensitivity of schemes of ecotoxicological hazard ranking of chemicals. *Chemosphere* 13, 203–211.

Koch, R. (1983) Molecular connectivity index for assessing ecotoxicological behaviour of organic compounds. *Toxicol. Environ. Chem.* 6, 87–96.

Könemann, H. (1981) Quantitative structure-activity relationships in fish toxicity studies. Part 1: Relationship for 50 industrial pollutants. *Toxicology* 19, 209–221.

Könemann, H., van Leeuwen, K. (1980) Toxicokinetics in fish: Accumulation and elimination of six chlorobenzenes by guppies. *Chemosphere* 9, 3–19.

Könemann, H., Zelle, R., Busser, F. (1979) Determination of log P_{oct} values of chloro-substituted benzenes, toluenes and anilines by high-performance liquid chromatography on ODS-silica. *J. Chromatogr.* 178, 559–565.

Kördel, W., Stutte, J., Kotthoff, G. (1993) HPLC-screening method for the determination of the adsorption coefficient on soil-Comparison of different stationary phases. *Chemosphere* 27(12), 2341–2352.

Kördel, W., Stutte, J., Kotthoff, G. (1995) HPLC-screening method to determine the adsorption coefficient in soil-Comparison of immobilized humic acid and clay mineral phases for cyanopropyl columns. *Sci. Total Environ.* 162, 119–125.

Körte, F., Freitag, D., Geyer, H., Klein, W., Kraus, A. G., Lahaniatus, E. (1978) Ecotoxicologic profile analysis-A concept for establishing ecotoxicologic priority lists for chemicals. *Chemosphere* No.1, 79–102.

Kühne, R., Ebert, R.-U., Kleint, F., Schmidt, G., Schüürmann, G. (1995) Group contribution methods to estimate water solubility of organic chemicals. *Chemosphere* 30, 2061–2077.

Leo, A., Hansch, C., Elkins, D. (1971) Partition coefficients and their uses. *Chem. Rev.* 71, 525–616.

Lide, D.R., Editor (2003) *Handbook of Chemistry and Physics*. 84th Edition, CRC Press, LLC. Boca Raton, Florida

Lohninger, H. (1994) Estimation of soil partition coefficients of pesticides from their chemical structure. *Chemosphere* 29(8), 1611–1626.

Lord, K.A., Briggs, G.C., Nearle, M.C., Manlove, R. (1980) Uptake of pesticides from water and soil by earthworms. *Pest. Sci.* 11, 401–408.

Lu, P.Y., Metcalf, R.L. (1975) Environmental fate and biodegradability of benzene derivatives as studied in a model aquatic ecosystem. *Environ. Health Perspect.* 10, 269–284.

Lyman, W.J. (1982) Chapter 2, Solubility in water and Chapter 4, Adsorption coefficient for soils and sediments. In: *Handbook on Chemical Property Estimation Methods, Environmental Behavior of Organic Compounds.* Lyman, W. J., Reehl, W. F., Rosenblatt, D. H., Eds., McGraw-Hill, New York.

Lyman, W.J., Reehl, W.F., Rosenblatt, D.H., Eds. (1982) *Handbook on Chemical Property Estimation Methods, Environmental Behavior of Organic Compounds.* McGraw-Hill, Inc., New York.

Mabey, W., Mill, T. (1978) Critical review of hydrolysis of organic compounds in water under environmental conditions. *J. Phys. Chem. Ref. Data* 7, 383–415.

Mabey, W.R., Smith, J.H., Podoll, R.T., Johnson, H.L., Mill, T., Chou, T.W., Gates, J., Waight-Partridge, I., Jaber, H., Vanderberg, D. (1982) Aquatic Fate Process for Organic Priority Pollutants. EPA Report No. 440/4–81–014, U.S. EPA, Washington, DC.

Mackay, D. (1982) Correlation of bioconcentration factors. *Environ. Sci. Technol.* 16, 274–278.

Mackay, D. (1985) Chapter 5, Air/water exchange coefficients. In: *Environmental Exposure from Chemicals.* Neely, W.B., Blau, G.E., Eds., pp. 91–108, CRC Press, Inc., Boca Raton, Florida.

Mackay, D., Paterson, S. (1991) Evaluating the multimedia fate of organic chemicals. A level III fugacity model. *Environ. Sci. Technol.* 25, 427–436.

Mackay, D., Paterson, S., Chung, B., Neely, W. B. (1985) Evaluation of the environmental behaviour of chemicals with level III fugacity model. *Chemosphere* 13, 335–374.

Mackay, D., Shiu, W.Y. (1981) A critical review of Henry's law constants for chemicals of environmental interest. *J. Phys. Chem. Ref. Data* 10, 1175–1199.

Mackay, D., Shiu, W.Y., Ma, K C. (1992) *Illustrated Handbook of Physical-Chemical Properties and Environmental Fate for Organic Chemicals, Vol. I. Monoaromatic-Hydrocarbons, Chlorobenzenes, and PCBs*. Lewis Publishers, Inc., Chelsea, Michigan.

Mailhot, H. (1987) Prediction of algae bioaccumulation and uptake rate of nine organic compounds by ten physico-chemical properties. *Environ. Sci. Technol.* 21, 1009–1013.

Majewski, M S., Capel, P.D. (1995) *Pesticides in the Atmosphere. Distribution, Trends, and Governing Factors.* Vol. 1 in the series Pesticides in the Hydrologic System. Gilliom, R. J., Series Editor., Ann Arbor Press, Inc., Chelsea, Michigan.

Martin, H., Worthing, C.R., Eds. (1977) *Pesticide Manual.* 5th Edition, British Crop Protection Council, Thornton, United Kingdom.

Martin, R.A., Edgington, L.V. (1981) Comparative systemic translocation of several xenobiotics and sucrose. *Pest. Biochem. Physiol.* 16(2), 87–96.

Mathre, D.E. (1971) Mode of action of oxathiin systemic fungicides. Structure-activity relations. *J. Agric. Food Chem.* 19(5), 872–874.

McCall, P.J., Swann, R.L., Laskowski, D.A., Unger, S.M., Vrona, S.A., Dishburger, H.J. (1980) Estimation of chemical mobility in soil from liquid chromatographic retention times. *Bull. Environ. Contam. Toxicol.* 24, 190–195.

McDuffie, B. (1981) Estimation of octanol/water partition coefficients for organic pollutants using reverse-phase HPLC. *Chemosphere* 10(1), 73–83.

McKim, J., Schnieder, P., Veith, G. (1985) Absorption dynamics of organic chemical transport across trout gills as related to octanol-water partition coefficients. *Toxicol. Appl. Pharmacol.* 77, 1–10.

Melnikov, N.N. (1971) Chemistry of pesticides. *Res. Rev.* 36, 1–447.

Meylan, W., Howard, P.H. (1991) Bond contribution method for estimating Henry's law constants. *Environ. Toxicol. Chem.* 10, 1283–1293.

Meylan, W., Howard, P.H., Boethling, R.S. (1992) Molecular topology/fragment contribution method for predicting soil sorption coefficients. *Environ. Sci. Technol.* 26, 1560–1567.

Miller, M.M., Ghodbane, S., Wasik, S.P., Tewari, Y.B., Martire, D.E. (1984) Aqueous solubilities, octanol/water partition coefficients and entropies of melting of chlorinated benzenes and biphenyls. *J. Chem. Eng. Data* 29, 184–190.

Miller, M.M., Wasik, S.P., Huang, G.L., Shiu, W.Y., Mackay, D. (1985) Relationship between octanol-water partition coefficient and aqueous solubility. *Environ. Sci. Technol.* 19, 522–529.

Mills, W.B., Dean, J.D., Porcella, D.B., Gherini, S.A., Huson, R.J.M., Frick, W.E., Rupp, G.L. (1982) *Water Quality Assessment: A Screening Procedure for Toxic and Conventional Pollutants.* Part 1. U.S. EPA Report EPA-600/6-82-004a.

Milne, G.W.A., Editor (1995) *CRC Handbook of Pesticides.* CRC Press, Inc., Boca Raton, Florida.

Monkiedje, A., Spiteller, M., Bester, K. (2003) Degradation of racemic and enantiopure metalaxyl in tropical and temperate soils. *Environ. Sci. Technol.* 37, 707–712.

Montgomery, J.H., Editor (1993) *Agrochemicals Desk Reference. Environmental Data.* Lewis Publishers, Inc., Chelsea, Michigan.

Mortimer, M.R., Connell, D.W. (1995) A model of the environmental fate of chloro-hydrocarbon contaminants associated with Sydney sewage discharge. *Chemosphere* 30, 2021–2038.

Moza, P.N., Sukul, P., Hustert, K., Kettrup, A. (1994) Photooxidation of metalaxyl in aqueous solution in the presence of hydrogen peroxide and titanium dioxide. *Chemosphere* 28, 341–347.

Müller, M., Kördel, W. (1996) Comparison of screening methods for the estimation of adsorption coefficients on soil. *Chemosphere* 32, 2493–2504.

Müller, M.D., Buser, H.-R. (1995) Environmental behavior of acetamide pesticide stereoisomers. 2. Stereo- and enantioselective degradation in sewage sludge and soil. *Environ. Sci. Technol.* 29, 2031–2037.

Nakamura, M., Suzuki, T., Amano, K., Yamada, S. (2001) Relation of sorption behavior of agricultural chemicals in solid-phase extraction with their *n*-octanol/water partition coefficients evaluated by high-performance liquid chromatography (HPLC). *Anal. Chim. Acta* 428, 219–226.

Nash, R.G. (1983) Determining environmental fate of pesticides with microagroecosystems. *Res. Rev.* 85, 199–215.

Nash, R.G. (1989) Models for estimating pesticide dissipation from soil and vapor decline in air. *Chemosphere* 18(11/12), 2375–2381.

Nash, R.G., Beall, M.L. (1980) Distribution of silvex, 2,4-D, and TCDD applied to turf in chambers and field plots. *J. Agric. Food Chem.* 28, 614.

Neely, W.B. (1980) A method for selecting the most appropriate environmental experiments on a new chemical. In: *Dynamic, Exposure and Hazard Assessment of Toxic Chemicals.* Haque, R., Ed., pp. 287–298, Ann Arbor Science Publishers, Ann Arbor, Michigan.

Neely, W.B., Branson, D.R., Blau, G.E. (1974) Partition coefficient to measure bio-concentration potential of organic chemicals in fish. *Environ. Sci. Technol.* 8, 1113–1115.

Neuhauser, E.F., Loehr, R.C., Malecki, M.R., Milligan, D.l., Durin, P.R. (1985) The toxicity of selected organic chemicals to earthworm *Eisenia fetida. J. Environ. Qual.* 14(3), 383–388.

Nielsen, L.S., Bundgaard, H., Falch, E. (1992) Prodrugs of thiabendazole with increased water-solubility. *Acta Pharm. Nord.* 4(1), 43–49.

Nigg, H.N., Stamper, J.H., Queen, R.M. (1986) Dicofol exposure to Florida citrus applicators: Effect of protective clothing. *Arch. Environ. Contam. Toxicol.* 15, 121–134.

Niimi, A.J., Lee, H.B., Kisson, G.P. (1989) Octanol/water partition coefficients and bioconcentration factors of chloronitrobenzenes in rainbow trout (*Salmo gairdneri*). *Environ. Toxicol. Chem.* 8, 817–823.

Niimi, A.J., Palazzo, V. (1985) Temperature effect on the elimination of pentachlorophenol, hexachlorobenzene and mirex by rainbow trout (*Salmo gairdneri*). *Water Res.* 19, 205–207.

Nirmalakhandan, N.N., Speece, R.E. (1988) QSAR model for predicting Henry's law constant. *Environ. Sci. Technol.* 22, 1349–1357.

OECD (1979) OECD Environmental Committee Chemicals Group, OECD Chemical Testing Programme Expert Group, Physical Chemical Final Report Vol. 1, Part 1 and Part 2, Summary of the OECD Laboratory Intercomparison Testing Programme Part 1-On the Physico-Chemical Properties. p. 33, Dec., 1979, Berlin, Germany.

Ohori, Y., Ihashi, Y. (1987) Foliar absorption of pesticides using an isolated cucumber membrane. *Res. Dev. Rev.-Mitsubishi Chem.* 1(2), 22–26.

Oliver, B.G. (1985) Desorption of chlorinated hydrocarbons from spiked and anthropogenically contaminated sediments. *Chemosphere* 14, 1087–1106.

Oliver, B.G. (1987a) Biouptake of chlorinated hydrocarbons from laboratory-spiked and field sediments by oligochaete worms. *Environ. Sci. Technol.* 21, 785–790.

Oliver, B.G. (1987b) Fate of some chlorobenzenes from the Niagara River in Lake Ontario. In: *Sources and Fates of Aquatic Pollutants.* Hite, R.A., Eisenreich, S.J., Eds., pp. 471–489, Advances in Chemistry Series 216, American Chemical Society, Washington, DC.

Oliver, B.G. (1987c) Partitioning relationships for chlorinated organics between water and particulates in the St. Clair, Detroit and Niagara Rivers. In: *QSAR in Environmental Toxicology II.* Kaiser, K.L.E., Ed., pp. 251–260, D. Reidel Publishing Co., Dordrecht, The Netherlands.

Oliver, B.G., Charlton, M.N. (1984) Chlorinated organic contaminants on settling particulates in the Niagara River vicinity of Lake Ontario. *Environ. Sci. Technol*. 18, 903–908.

Oliver, B.G., Niimi, A.J. (1983) Bioconcentration of chlorobenzenes from water by rainbow trout: correlations with partition coefficients and environmental residues. *Environ. Sci. Technol.* 17, 287–291.

Oliver, B.G., Niimi, A.J. (1985) Bioconcentration factors of some halogenated organics for rainbow trout: Limitations in their use for prediction of environmental residues. *Environ. Sci. Technol.* 19, 842–849.

Opperhuizen, A. (1986) Bioconcentration of hydrophobic chemicals in fish. In: *Aquatic Toxicology and Environmental Fate.* 9th Vol. ASTM STP 921, Poston, T.M., Purdy, R., Eds., pp. 304–315, American Society for Testing and Materials, Philadelphia, Pennsylvania.

Pait, A.S., De Souza, A.E., Farrow, D.R.D. (1992) *Agriculture Pesticide Use in Coastal Areas: A National Summary.* National Oceanic and Atmospheric Administration (NOAA) Rockville, Maryland.

Pankow, J.F., Isabelle, L.M., Asher, W.E. (1984) Trace organic compounds in rain. 1. Sample design and analysis by adsorption/thermal desorption (ATD). *Environ. Sci. Technol.* 18, 310–318.

Patil, G.S. (1994) Prediction of aqueous solubility and octanol-water coefficient for pesticides based on their molecular structure. *J. Hazard. Materials* 36, 35–43.

Patil, G.S., Nicholls, P.H., Chamberlain, K., Briggs, G.G., Bromilow, R.H. (1988) Degradation rates in soil of 1-benzyltriazoles and two triazole fungicides. *Pest. Sci.* 22(4), 333–342.

Pereira, W.E., Rostad, C.E., Chiou, C.T., Brinton, T.I., Barber, I.,L.B., Demcheck, D.K., Demas, C.R. (1988) Contamination of estuarine water, biota and sediment by halogenated organic compounds: A field study. *Environ. Sci. Technol.* 22, 772–778.

Pinsuwan, S., Li, A., Yalkowsky, S.H. (1995) Correlation of octanol/water solubility and partition coefficients. *J. Chem. Eng. Data* 40, 623–626.

Plato, C. (1972) Differential scanning calorimetry as a general method for determining the purity and heat of fusion of high-purity organic chemicals. Application to 64 compounds. *Anal. Chem.* 44(8), 1531–1534.

Plato, C., Glasgow, A.R., Jr. (1969) Differential scanning calorimetry as a general method for determining the purity and heat of fusion of high purity organic chemicals. Application to 95 compounds. *Anal. Chem*. 41, 330–336.

Popov, V.I., Sboeva, J.N. (1974) Determination of benomyl in cotton leaves. *J. Environ. Qual. Saf.* 3.

Rao, P.S.C., Davidson, J.M. (1980) Estimation of pesticide retention and transformation parameters required in nonpoint source pollutant models. In: *Environmental Impact of Nonpoint Pollution.* Overcash, M.R., Davidson, J.M., Eds., Ann Arbor Science Publishers Inc., Ann Arbor, Michigan.

Rao, P.S.C., Davidson, J.M. (1982) Retention and Transformation of Selected Pesticides and Phosphorus in Soil Water System: A Critical Review. U.S. EPA-600/3–82–060.

Reischl, A., Reissinger, M., Thoma, H., Hutzinger, O. (1989) Uptake and accumulation of PCDD/F in terrestrial plants: Basic considerations. *Chemosphere* 19, 467–474.

Rekker, R.F. (1977) *The Hydrophobic Fragmental Constants. Its Derivation and Application, A Means of Characterizing Membrane Systems*. Elsevier Science Publishing Co., Oxford, England.

Rippen, G., Ilgenstein, M., Klöpffer, W., Poreniski, H.J. (1982) Screening of the adsorption behavior of new chemicals: natural soils and model adsorbents. *Ecotoxicol. Environ. Saf.* 6, 236–245.

Rordorf, B.F. (1989) Unpublished data, private communication.

Ryan, J.A., Bell, R.M., Davidson, J.M., O'Connor, G.A. (1988) Plant uptake of non-ionic organic chemicals from soils. *Chemosphere* 17, 2299–2323.

Sabljic, A., Güsten, H., Verhaar, H., Hermens, J. (1995) QSAR modelling of soil sorption. Improvements and systematics of log K_{OC} vs. log K_{OW} correlations. *Chemosphere* 31, 4489–4514.

Saito, S., Tanoue, A., Matsuo, M. (1992) Applicability of the i/o-characters to a quantitative description of bioconcentration of organic chemicals in fish. *Chemosphere* 24, 81–87.

Saito, S., Koyasu, J., Yoshida, K., Shigeoka, T., Koike, S. (1993) Cytotoxicity of 109 chemicals to goldfish GFS cells and relationships with 1-octanol/water partition coefficients. *Chemosphere* 26(5), 1015–1028.

Sangster, J. (1989) Octanol-water partition coefficients of simple organic compounds. *J. Phy. Chem. Ref. Data* 18, 1111–1230.

Sangster, J. (1993) LOGKOW Databank, Sangster Research Labs., Montreal, Canada.

Sarna, I.P., Hodge, P.E., Webster, G.R.B. (1984) Octanol-water partition coefficients of chlorinated dioxins and dibenzofurans by reversed-phase HPLC using several C_{18} columns. *Chemosphere* 13, 975–983.

Schreiber, L., Schönherr, J. (1992) Uptake of organic chemicals in conifer needles: Surface adsorption and permeability of cuticles. *Environ. Sci. Technol.* 26, 153–159.

Schwack, W., Flößer-Müller, H. (1990) Fungicides and photochemistry. Photodehalogenation of captan. *Chemosphere* 21(7), 905–912.

Sears, G.W., Hopke, E.R. (1949) Vapor pressures of naphthalene, anthracene, and hexachlorobenzene in a low pressure region. *J. Am. Chem. Soc.* 71, 1632–1634.

Sharom, M.S., Edgington, L.V. (1982) The adsorption, mobility, and persistence of metalaxyl in soil and aqueous systems. *Can. J. Plant Pathol.* 4, 334–340.

Sicbaldi, F., Finizio, A. (1993) K_{OW} estimation by combination of RP-HPLC and molecular indexes for a heterogeneous set of pesticide. In: *Proceedings IX Symposium Pesticide Chemistry, Mobility and Degradation of Xenobiotics*. 11–13, Oct. 1993, Picenza, Italy.

Siebers, J., Gottschild, D., Nolting, H.-G. (1994) Pesticides in precipitation in Northern Germany. *Chemosphere* 28(8), 1559–1570.

Sijm, D.T.H.M., Middlekoop, J., Vrisekoop, K. (1995) Algal density dependent bio-concentration factors of hydrophobic chemicals. *Chemosphere* 31(9), 4001–4012.

Singh, R.P., Chiba, M. (1985) Solubility of benomyl in water at different pHs and its conversion to methyl 2-benzimidazolecarbamate, 3-butyl-2,4-dioxo[1,2-α]-*s*-triazino-benzimidazole, and 1-(2-benzimidazolyl)-3-*n*-butylurea. *J. Agric. Food Chem.* 33(1), 63–67.

Spencer, E.Y., Editor (1973) *Guide to the Chemicals Used in Crop Protection.* 6th Edition, Research Branch Agriculture Canada, Ontario, Canada.

Spencer, E.Y., Editor (1982) *Guide to the Chemicals Used in Crop Protection.* 7th Edition, Research Branch Agriculture Canada, Ontario, Canada.

Stevens, P.J.G., Baker, E.A., Anderson, N.H. (1988) Factors affecting the foliar absorption and redistribution of pesticides. 2. Physicochemical properties of the active ingredient and the role of surfactant. *Pest. Sci.* 24(1), 31–53.

Stull, D.R. (1947) Vapor pressure of pure substances. Organic compounds. *Ind. Eng. Chem.* 39, 517–560.

Su, F., Calvert, J.G., Shaw, J.H. (1979) Mechanism of the photooxidation of gaseous formaldehyde. *J. Phys. Chem.* 83, 3185–3191.

Sukop, M., Cogger, C.G. (1992) Adsorption of carbofuran, metalaxyl, and simazine: KOC evaluation and relation to soil transport. *J. Environ. Sci. Health* B27, 565–590.

Suntio, L.R., Shiu, W.Y., Mackay, D., Seiber, J.N., Glotfelty, D. (1988) Critical review of Henry's law constants. *Rev. Environ. Contam. Toxicol.* 103, 1–59.

Swann, R.L., Laskowski, D.A., McCall, P.J., Vander, Kuy K., Dishburger, H. J. (1983) A rapid method for estimation of the environmental parameters octanol/water partition coefficient, soil sorption constant, water to air ratio, and water solubility. *Res. Rev.* 85, 17–28.

Swann, R.L., McCall, P.J., Laskowski, D.A., Dishburger, H.J. (1981) Estimation of soil sorption constants of organic chemicals by high-performance liquid chromatography. In: *Aquatic Toxicology and Hazard Assessment. Forth Conference ASTM STP 737*. Branson, B.R., Dickson, K.L., Eds. Pp. 43–48, American Society for Testing and Materials, Philadelphia, PA.

Tabak, H.H., Quave, S.A., Mahni, C.I., Barth, E.F. (1981) Biodegradability studies with organic priority pollutant compound. *J. Water Pollut. Control Fed.* 53, 1503–1518.

Tadokoro, H., Tomita, Y. (1987) The relationship between bioaccumulation and lipid content of fish. In: *QSAR in Environmental Toxicology II*. Kaiser, K.L.E., Editor, pp. 363–373, D. Reidel Publishing Co., Dordrecht, The Netherlands.

Thomann, R. V. (1989) Bioconcentration model of organic chemical distribution in aquatic food chains. *Environ. Sci. Technol.* 23, 699–707.

Tomlin, C. (1994) *The Pesticide Manual (A World Compendium)*. 10th Ed., Incorporating the Agrochemicals Handbook. The British Crop Protection Council, Surrey, UK and The Royal Society of Chemistry, Cambridge, UK.

Travis, C.C., Arms, A.D. (1988) Bioconcentration of organics in beef, milk, and vegetation. *Environ. Sci. Technol.* 22, 271–273.

Tsonopoulos, C., Prausnitz, J.M. (1971) Activity coefficients of aromatic solutes in dilute aqueous solutions. *Ind. Eng. Chem. Fundam.* 10, 593–600.

Tsuzuki, M. (2000) Thermodynamic estimation of vapor pressure for organophosphorus pesticides. *Environ. Toxicol. Chem.* 19, 1717–1736.

Valvani, S.C., Yalkowsky, S H. (1980) Solubility and partitioning in drug design. In: *Physical Chemical Properties of Drug*. Medical Research Series, Vol. 10, Yalkowsky, S H., Sinkinla, A.A., Valvani, S., Eds., pp. 201–229, Marcel Dekker, Inc., New York, New York.

Veith, G.D., Austin, N.M., Morris, R T. (1979a) A rapid method for estimation log P for organic chemicals. *Water Res.* 13, 43–47.

Veith, G.D., Defoe, D.L., Bergstedt, B.V. (1979b) Measuring and estimating the bio-concentration factor of chemicals in fish. *J. Fish Res. Board Can.* 26, 1040–1048.

Veith, G.D., Kosian, P. (1983) Estimating bioconcentration potential from octanol/water partition coefficients. In: *Physical Behaviour of PCBs in the Great Lakes*. D. Mackay, S. Patterson, S.J. Eisenreich, M.S. Simmons Eds., pp. 269–282, Ann Arbor Science Publishers, Ann Arbor, Michigan.

Verschueren, K. (1977) *Handbook of Environmental Data on Organic Chemicals*. Van Nostrand Reinhold, New York.

Verschueren, K. (1983) *Handbook of Environmental Data on Organic Chemicals*. 2nd Edition, Van Nostrand Reinhold, New York.

Walker, W.W., Cripe, C R., Pritchard, P.H., Bourquin, A.W. (1988) Biological and abiotic degradation of xenobiotic compounds in vitro estuarine water and sediment/water systems. *Chemosphere* 17(12), 2255–2270.

Wang, X., Harada, S., Wantanabe, M., Koshikawa, H., Geyer, H.J. (1996) Modelling the bioconcentration of hydrophobic organic chemicals in aquatic organisms. *Chemosphere* 32(9), 1783–1793.

Watarai, H., Tanaka, M., Suzuki, N. (1982) Determination of water partition coefficients of halobenzenes in heptane/water and 1-octanol/water systems and comparison with the scaled particle calculation. *Anal. Chem.* 54, 702–705.

Wauchope, R.D., Buttler, T.M., Hornsby, A. G., Augustijn-Beckers, P.W.M., Burt, J.P. (1992) The SCS/ARS/SCS Pesticide Properties Database for Environmental Decision Making. *Rev. Environ. Contam. Toxicol.* 123, 1–164.

Weast, R.C., Ed. (1972–73) *Handbook of Chemistry and Physics*. 53rd edition, CRC Press, Inc., Cleveland, Ohio.

Weast, R.C., Ed. (1982–83) *Handbook of Chemistry and Physics*. 62th edition, CRC Press, Inc., Boca Raton, Florida.

Weil, V.G., Dure, G., Quentin, K.E. (1974) Solubility in water of insecticide chlorinated hydrocarbons and polychlorinated biphenyls in view of water pollution. *Z. Wasser Abwasser Forsch* 7(6), 169–175.

Wolfe, N.L., Zepp, R.G., Baughman, G.L., Fincher, R.C., Gordon, T.A. (1976) *Chemical and Photochemical Transformation of Selected Pesticides in Aquatic Environments.* U.S. EPA-600/3–76–067, U.S. EPA, Athens, Georgia.

Worthing, C.R., Walker, S., Eds. (1983) *The Pesticide Manual* (*A World Compendium*). 7th edition, The British Crop Protection Council, Croydon, England.

Worthing, C.R., Walker, S., Eds. (1987) *The Pesticide Manual* (*A World Compendium*). 8th edition, The British Crop Protection Council, Croydon, England.

Worthing, C.R., Hance, R.J., Eds. (1991) *The Pesticide Manual* (*A World Compendium*). 9th edition, The British Crop Protection Council, Croydon, England.

Yalkowsky, S.H., Dannenfelser, R.M. (1994) *AQUASOL DATABASE.* 5th edition, University of Arizona, Tucson, Arizona.

Yalkowsky, S.H., Orr, R.J., Valvani, S.C. (1979) Solubility and partitioning. 3. The solubilities of halobenzenes in water. *Ind. Eng. Chem. Fundam.* 18, 351–353.

Yalkowsky, S.H., Valvani, S.C. (1979) Solubility and partitioning. 2. Relationships between aqueous solubilities, partition coefficients, and molecular surface areas of rigid aromatic hydrocarbons. *J. Chem. Eng. Data* 24, 127–129.

Yalkowsky, S.H., Valvani, S.C. (1980) Solubility and partitioning. 1. Solubility of nonelectrolytes in water. *J. Pharm. Sci.* 69, 912–922.

Yalkowsky, S. H., Valvani, S.C., Mackay, D. (1983) Estimation of the aqueous solubility of some aromatic compounds. *Res. Rev.* 85, 43–55.

Yoshioka, Y., Mizuno, T., Ose, Y., Sato, T. (1986) Estimation of toxicity on fish by physico-chemical properties. *Chemosphere* 15(2), 195–203.

Yoshida, K., Shigeoka, T., Yamauchi, F. (1983) Non-steady state equilibrium model for the preliminary prediction of the fate of chemicals in the environment. *Ecotoxicol. Environ. Saf.* 7, 179–190.

Zhou, X., Mopper, K. (1990) Apparent partition coefficients of 15 carbonyl compounds between air and seawater and between air and freshwater; implications for air-sea exchange. *Environ. Sci. Technol.* 24, 1864–1869.

Zoeteman, B.C.J., Harmsen, K.M., Linders, J.B.H.J. (1980) Persistent organic pollutants in river water and groundwater of the Netherlands. *Chemosphere* 9, 231–249.

Appendix 1

1.1 LIST OF SYMBOLS AND ABBREVIATIONS

A_i	area of phase i, m^2
ALPM	automated log-P measurement
AS	absorption spectrophotometry
BCF	bioconcentration factor
bp	boiling point, °C
C	molar concentration, mol/L or $mmol/m^3$
C^S	saturated aqueous concentration, mol/L or $mmol/m^3$
C_L	liquid or supercooled liquid concentration, mol/L or $mmol/m^3$
C_S	solid molar concentration, mol/L or $mmol/m^3$
C_A	concentration in air phase, mol/L or $mmol/m^3$
C_W	concentration in water phase, mol/L or $mmol/m^3$
^{14}C	radioactive labelled carbon-14 compound
CC	countercurrent chromatography
COD	chemical oxygen demand
CPC	centrifugal partition chromatography
D	D values, mol/Pa·h
D_A	D values for advection, mol/Pa·h
D_{Ai}	D values for advective loss in phase i, mol/Pa·h
D_R	D value for reaction, mol/Pa·h
D_{Ri}	D value for reaction loss in phase i, mol/Pa·h
D_{ij}	intermedia D values, mol/Pa·h
D_{VW}	intermedia D value for air-water diffusion (absorption), mol/Pa·h
D_{RW}	intermedia D value for air-water dissolution, mol/Pa·h
D_{QW}	D value for total particle transport (dry and wet), mol/Pa·h
D_{RS}	D value for rain dissolution (air-soil), mol/Pa·h
D_{QS}	D value for wet and dry deposition (air-soil), mol/Pa·h
D_{VS}	D value for total soil-air transport, mol/Pa·h
D_S	D value for air-soil boundary layer diffusion, mol/Pa·h
D_{SW}	D value for water transport in soil, mol/Pa·h
D_{SA}	D value for air transport in soil, mol/Pa·h
D_{Ti}	total transport D value in bulk phase i, mol/Pa·h
DOC	dissolved organic carbon
DOM	dissolved organic matter
DSC	differential scanning calorimetry
DTA	differential thermal analyzer
E	emission rate, mol/h or kg/h
EPICS	equilibrium partitioning in closed system
F	fugacity ratio
f	fugacity, Pa
f_i	fugacity in pure phase i, Pa
f-const.	fragmental constants

fluo.	fluorescence method
G	advective inflow, m^3/h
G_B	advective inflow to bottom sediment m^3/h
ΔG_v	Gibbs's free energy of vaporization kJ/mol or kcal/mol
GC	gas chromatography
GC/FID	GC analysis with flame ionization detector
GC/ECD	GC analysis with electron capture detector
GC-RT	GC retention time
gen. col.	generator-column
H, HLC	Henry's law constant, $Pa \cdot m^3/mol$, or atm m^3/mol
ΔH_{fus}	enthalpy of fusion, kJ/mol
ΔH_{subl}	enthalpy of sublimation, kJ/mol
ΔH_V	enthalpy of vaporization, kJ/mol or kcal/mol
HPLC	high pressure liquid chromatography
HPLC/MS	HPLC analysis with mass spectrometer detector
HPLC/UV	HPLC analysis with UV detector
HPLC/fluo.	HPLC analysis with fluorescence detector
HPLC-k′	HPLC-capacity factor correlation
HPLC-RI	HPLC-retention index correlation
HPLC-RT	HPLC-retention time correlation
HPLC-RV	HPLC-retention volume correlation
IP	ionization potential
IR	infrared absorption
J	intermediate quantities for fugacity calculation
K	Kjeldahl method
k	reaction rate constant
k_i	first-order rate constant in phase i, h^{-1}
k_A	air/water mass transfer coefficient, air-side, m/h
k_W	air/water mass transfer coefficient, water-side, m/h
$K_{AR/W}$	aerosol/water partition coefficient
K_{AW}	dimensionless air/water partition coefficient
k_H	Henry's law constant with units of vapor pressure
K_B	bioconcentration factor
K_h	association coefficient
K_{OC}	organic-carbon sorption partition coefficient
K_{OM}	organic-matter sorption partition coefficient
K_{OA}	octanol/air partition coefficient
K_{OW}	octanol/water partition coefficient
$K_{SD/W}$	sediment-water partition coefficient
$K_{SSD/W}$	suspended sediment/water partition coefficient
K_{SW}	soil/water partition coefficient
K_p or K_d	sorption coefficient
k_1	uptake/accumulation rate constant, d^{-1} (day^{-1})
k_2	elimination/clearance/depuration rate constant, d^{-1}
k_b	biodegradation rate constant, d^{-1}
k_h	hydrolysis rate constant, d^{-1}
k_p	photolysis rate constant, d^{-1}
k_{OH}	photooxidation rate constant for hydroxyl radical
k_{NO3}	photooxidation rate constant for NO_3 radical
k_{O3}	photooxidation rate constant for ozone
L	lipid content of fish
LSC	liquid scintillation counting
LSS	liquid scintillation spectrometry
m_i	amount of chemical in phase i, mol or kg
M	total amount of chemical, mol or kg

MCI	molecular connectivity indices
MO	molecular orbital calculation
mp.	melting point, °C
MR	molar refraction
MS	mass spectrometry
MW	molecular weight, g/mol
n_C	number of carbon atoms
n_{Cl}	number of chlorine atoms
P	vapor pressure, Pa (Pascal)
P_L	liquid or supercooled liquid vapor pressure, Pa
P_S	solid vapor pressure, Pa
Q	scavenging ratio
QSAR	quantitative structure-activity relationship
QSPR	quantitative structure-property relationship
RC	Radiochemical method
RP-HPLC	reversed phase high pressure liquid chromatography
RP-TLC	reversed phase thin layer chromatography
S	water solubility, mg/L or g/m^3
ΔS_{fus}	entropy of fusion, J/mol·K or cal/mol·K (e.u.)
$S_{octanol}$	solubility in octanol
SD	standard deviation
SPARC	a computational expert system that predicts chemical reactivity
t/°C	temperature in degree centigrade
t	residence time, h (hour)
t_o	overall residence time, h
t_A	advection persistence time, h
t_B	sediment burial residence time, h
t_R	reaction persistence time, h
$t_{1/2}$	half-life, s, h, min, d, month or yr
T_{ij}	intermedia transport rate, mol/h or kg/h
T	system temperature, K
T_B	boiling point, K
T_M	melting point, K
TLC	thin-layer chromatography
TMV	total molecular volume per molecule, $Å^3$ ($Angstrom^3$)
TN	titration method
TSA	total surface area per molecule, $Å^2$
U_1	air side, air-water MTC (same as k_A), m/h
U_2	water side, air-water MTC (same as k_W), m/h
U_3	rain rate (same as U_R), m/h
U_4	aerosol deposition rate, m/h
U_5	soil-air phase diffusion MTC, m/h
U_6	soil-water phase diffusion MTC, m/h
U_7	soil-air boundary layer MTC, m/h
U_8	sediment-water MTC, m/h
U_9	sediment deposition rate, m/h
U_{10}	sediment resuspension rate, m/h
U_{11}	soil-water run-off rate, m/h
U_{12}	soil-solids run-off rate, m/h
U_R	rain rate, m/h
U_Q	dry deposition velocity, m/h
U_B	sediment burial rate, m/h
UV	UV spectrometry
UNIFAC	UNIQUAC functional group activity coefficients
V_i	volume of pure phase i, m^3

V_S	volume of bottom sediment, m^3
V_{Bi}	volume of bulk phase i, m^3
V_I	intrinsic molar volume, cm^3/mol
V_M	molar volume, cm^3/mol
v_i	volume fraction of phase i
v_Q	volume fraction of aerosol
VOC	volatile organic chemicals
W	molecular mass, g/mol
Z_i	fugacity capacity of phase i, mol/m^3 Pa
Z_{Bi}	fugacity capacity of bulk phase i, mol/m^3 Pa

1.2 GREEK CHARACTERS

π-const.	substituent constants for K_{OW} estimation
γ	solute activity coefficient
γ_o	solute activity coefficient in octanol phase
γ_W	solute activity coefficient in water phase
ρ_i	density of pure phase i, kg/m^3
ρ_{Bi}	density of bulk phase i, kg/m^3
χ	molecular connectivity indices
ϕ_{OC} or f_{OC}	organic carbon fraction
ϕ_i	organic carbon fraction in phase i

Appendix 2

2.1 ALPHABETICAL INDEX

Appendix 3

3.1 CAS REGISTRY NUMBER INDEX