
18 Insecticides

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18.1. List of Chemicals and Data Compilations (by Functional Group):

Organophosphorus compounds:

a) Phosphates:

Chlorfenvinphos	3758
Crotoxyphos	3767
Dichlorvos	3811
Dicrotophos	3816
Mevinphos	3925
Monocrotophos	3930
Naled	3932

b) Phosphorothioates:

Acephate	3715
Bromophos	3734
Bromophos-ethyl	3736
Chlorpyrifos	3760
Chlorpyrifos-methyl	3765
Demeton	3800
Diazinon	3804
Fenitrothion	3851
Fensulfothion	3857
Fenthion	3859
Leptophos	3896
Parathion	3936
Parathion-methyl	3942
Ronnel	3969
Trichlorfon	3980

c) Phosphorodithioates (Phosphorothiolothionates):

Azinphos-methyl	3729
Carbophenothion	3746
Dialifor	3802
Dimethoate	3829
Disulfoton	3832
Ethion	3847
Ethoprop	3849
Fonofos	3867
Malathion	3912
Phenthoate	3957
Phorate	3959
Phosmet	3962
Terbufos	3971

Carbamates:

Aldicarb	3717
Aminocarb	3728
Bendiocarb	3732
Carbaryl	3738
Carbofuran	3742
Carbosulfan	3748
Ethiofencarb	3845
Fenoxycarb	3854
Methiocarb	3916
Methomyl	3918
Oxamyl	3934
Pirimicarb	3964
Propoxur	3966
Thiodicarb	3973

Organochlorines:

Aldrin	3721
Chlordane	3750
DDD	3774
DDE	3779
DDT	3785
Dieldrin	3819
Endrin	3840
α -HCH	3869
β -HCH	3876
δ -HCH	3881
Heptachlor	3885
Heptachlor epoxide	3890
Kepone	3893
Lindane (γ -HCH)	3898
Methoxychlor	3920
Mirex	3927
Toxaphene	3975

Phenols:

Pentachlorophenol (PCP)	3947
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Synthetic pyrethroids:

Cypermethrin	3772
Cyhalothrin	3769
Lambda-cyhalothrin	3770
Deltamethrin	3798
Fenpropathrin	3855
Fenvalerate	3862
Permethrin	3953

Miscellaneous:

Diflubenzuron	3827
Endosulfan	3835
Flucythrinate	3865

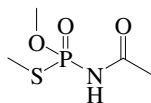
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18.1 LIST OF CHEMICALS AND DATA COMPILATIONS

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 ($^{\circ}C$):

88 (Lide 2003)

Boiling Point ($^{\circ}C$):

Density (g/cm^3 at $20^{\circ}C$):

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 $25^{\circ}C$ (assuming $\Delta S_{fus} = 56$ J/mol K), F: 0.241 (mp at $88^{\circ}C$)

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$ or as indicated):

650000 (Spencer 1973, 1982; Martin & Worthing 1977; Worthing & Walker 1987, Worthing & Hance 1991)
 > 5000 ($20^{\circ}C$, shake flask-GC, Bowman & Sans 1983a)
 790000 ($20^{\circ}C$, Hartley & Kidd 1987)
 818000 (Wauchope 1989)
 818000 (20 – $25^{\circ}C$, selected, Wauchope et al. 1992; Hornsby et al. 1996)
 790000 ($20^{\circ}C$, Montgomery 1993; Tomlin 1994; Milne 1995)

Vapor Pressure (Pa at $25^{\circ}C$ or as indicated):

2.26×10^{-4} ($20^{\circ}C$, Hartley & Kidd 1987)
 2.26×10^{-4} ($24^{\circ}C$, Worthing & Walker 1987, Worthing & Hance 1991; Tomlin 1994)
 2.27×10^{-4} (20 – $25^{\circ}C$, selected, Wauchope et al. 1992; Hornsby et al. 1996)
 2.27×10^{-4} ($20^{\circ}C$, 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 ($Pa \cdot m^3/mol$ at $25^{\circ}C$ or as indicated):

5.27×10^{-8} (20 – $25^{\circ}C$, calculated-P/C, Montgomery 1993)
 6.37×10^{-8} (20 – $25^{\circ}C$, 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, $t_{1/2}$:

Volatilization:

Photolysis:

Oxidation: calculated rate constant $k \sim 51 \times 10^{-12} \text{ cm}^3/\text{molecules}$ 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)

$t_{1/2} = 60 \text{ h}$ at pH 9 and $t_{1/2} = 710 \text{ h}$ 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:

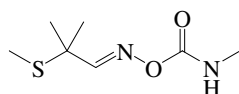
Sediment: degradation increased greatly when treated samples were incubated in the presence of sediments, ~ 20% recovered after 42 d and ~ 28% recovered after 58 d after incubating acephate-treated pond and creek water with their respective sediments (Szeto et al. 1979)

Soil: selected field $t_{1/2} = 3.0 \text{ d}$ (Wauchope et al. 1992; Dowd et al. 1993; Hornsby et al. 1996);

$t_{1/2} = 7\text{--}10 \text{ d}$ 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)propional *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: C₇H₁₄N₂O₂S

Molecular Weight: 190.263

Melting Point (°C):

99 (Lide 2003)

Boiling Point (°C):

100 (decomposes above this temp., Howard 1991)

Density (g/cm³ at 20°C):

1.195 (25°C, Hartley & Kidd 1987; Montgomery 1993; Tomlin 1994; Milne 1995)

Molar Volume (cm³/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/m³ 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·m³/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 $\geq 0.5\%$, average, Delle Site 2001)

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_{NO_3} with NO_3 radical and k_{O_3} with O_3 or as indicated, *data at other temperatures see reference:

photooxidation $t_{1/2} = 1\text{--}9.5$ h, based on an estimated rate constant for vapor-phase reaction with hydroxyl radical in air (Atkinson 1987; quoted, Howard et al. 1991)

$t_{1/2} = 1.7\text{--}12$ d in soil for pH 1–10 with little change in rate between pH 4.4–10 (Lemley et al. 1988; quoted, Howard 1991)

$k(aq.) = 5.9 \times 10^9 \text{ M}^{-1} \text{ s}^{-1}$ for the reaction (Fenton with reference to acetophenone) with hydroxyl radical in aqueous solutions at pH 3.5 and at $24 \pm 1^\circ\text{C}$ (Buxton et al. 1988; quoted, Faust & Hoigné 1990; Haag & Yao 1992)

$k(aq.) = (4.4 \pm 0.1) \times 10^4 \text{ M}^{-1} \text{ s}^{-1}$ for direct reaction with ozone in water at pH 2.1; $k = (4.3 \pm 0.2) \times 10^5 \text{ M}^{-1} \text{ s}^{-1}$ at pH 7.0 and $24 \pm 1^\circ\text{C}$, with $t_{1/2} = 0.08$ s at pH 7 (Yao & Haag 1991).

$k(aq.) = (8.1 \pm 1.1) \times 10^9 \text{ M}^{-1} \text{ s}^{-1}$ for the reaction (Fenton with reference to acetophenone) with hydroxyl radical in aqueous solutions at pH 3.5 and at $24 \pm 1^\circ\text{C}$ (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 $k = 1.51 \times 10^{-4} \text{ d}^{-1}$ 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 $k = 5.3 \times 10^{-3} \text{ d}^{-1}$ with $t_{1/2} = 131$ d at pH 3.95, $k = 1.3 \times 10^{-3} \text{ d}^{-1}$ with $t_{1/2} = 559$ d at pH 6.02, $k = 2.1 \times 10^{-3} \text{ d}^{-1}$ with $t_{1/2} = 324$ d at pH 7.96, $k = 1.3 \times 10^{-2} \text{ d}^{-1}$ with $t_{1/2} = 55$ d at pH 8.85 in period of 89 d; and $k = 1.2 \times 10^{-1} \text{ d}^{-1}$ 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:

$k = 0.000222 \text{ h}^{-1}$ for discharge rate of 30 cm/year and $k = 0.000233 \text{ h}^{-1}$ for discharge rate of 61 cm/year with $t_{1/2} = 30$ d (Jones & Back 1984)

Aerobic mineralization $k = (1.93\text{--}34.2) \times 10^{-3} \text{ d}^{-1}$ with $t_{1/2} = 20\text{--}361$ d in surface soils and $k = 2.97\text{--}5.28) \times 10^{-3} \text{ d}^{-1}$ with $t_{1/2} = 131\text{--}233$ d in subsurface soils; anaerobic mineralization $k = (8.09\text{--}31.1) \times 10^{-4} \text{ d}^{-1}$ with $t_{1/2} = 223\text{--}1130$ 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).

$t_{1/2}(\text{aq. aerobic}) = 480\text{--}8664$ h, based on unacclimated aerobic soil grab sample data; $t_{1/2}(\text{aq. anaerobic}) = 1488\text{--}15240$ 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: $t_{1/2} = 1\text{--}9.5$ 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)

$t_{1/2} = 480\text{--}8664$ 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 $24 \pm 1^\circ\text{C}$ (Yao & Haag 1991)

Ground water: $t_{1/2} = 960\text{--}15240$ 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);

$t_{1/2} = 0.4\text{--}3.2$ d at pH 4.5–4.9 and 25°C (Rao et al. 1984; quoted, Howard 1991);

degradation rate constants $k = 0.000222 \text{ h}^{-1}$ for discharge rate of 30 cm/year and $k = 0.000233 \text{ h}^{-1}$ for discharge rate of 61 cm/yr with $t_{1/2} = 30$ d (Jones & Back 1984);

Mineralization $t_{1/2} = 20\text{--}361$ d in surface soils and $t_{1/2} = 131\text{--}233$ d in surface soils under aerobic condition, anaerobic $t_{1/2} = 223\text{--}1130$ 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 $t_{1/2} = 1.7\text{--}12$ 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 $t_{1/2} \sim 7$ 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)

$t_{1/2} \leq 2$ 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);

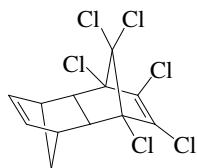
selected field $t_{1/2}$ = 30 d (Wauchope et al. 1992; Dowd et al. 1993; Hornsby et al. 1996);

$t_{1/2}$ 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, Alttox, 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 ($^{\circ}C$):

104 (Lide 2003)

Boiling Point ($^{\circ}C$):

145 (at 2 mmHg, Hartley & Kidd 1987; Montgomery 1993; Milne 1995)

Density (g/cm^3 at $20^{\circ}C$):

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 $25^{\circ}C$ (assuming $\Delta S_{fus} = 56 J/mol K$), F: 0.168 (mp at $104^{\circ}C$)

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$ 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 $25-45^{\circ}C$, Richardson & Miller 1960)

0.20 (Stephen & Stephen 1963)

0.027 ($25-29^{\circ}C$, 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 ($20-25^{\circ}C$, Wauchope 1978; Willis & McDowell 1982)

0.013 (Kenaga 1980a, b; Kenaga & Goring 1980; Garten & Trabalka 1983)

0.027 ($27^{\circ}C$, Spencer 1982; Worthing & Walker 1987)

<0.05 (rm. temp., Hartley & Kidd 1987, Milne 1995)

0.017–0.18 (Montgomery 1993)

0.027 ($20-25^{\circ}C$, 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)

$\log [C_L/(mol m^{-3})] = -1480/(T/K) + 2.42$ (supercooled liquid, linear regression of literature data, Shen & Wania 2005)

Vapor Pressure (Pa at $25^{\circ}C$ 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)

$\log (P/mmHg) 2,351 - 2035.35/(T/K)$; temp range $20-50^{\circ}C$ (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 & Fosbraey 1982)
 $\ln(P/\text{Pa}) = 32.9 - 11044/(T/\text{K})$; 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)
 $\log(P/\text{mmHg}) = 10.4514 - 4281.065/(T/\text{K})$; 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)
 $\log(P_{\text{S}}/\text{Pa}) = 15.561 - 5262.3/(T/\text{K})$; measured range 45–65.2°C (solid, gas saturation-GC, Rordorf 1989)
 $\log(P_{\text{L}}/\text{Pa}) = 12.489 - 4189.8/(T/\text{K})$; 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)
 $\log(P_{\text{L}}/\text{Pa}) = 12.04 - 3924/(T/\text{K})$ (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)
 $\log(P_{\text{L}}/\text{Pa}) = -4106/(T/\text{K}) + 12.56$ (supercooled liquid, linear regression of literature data, Shen & Wania 2005)

Henry's Law Constant ($\text{Pa}\cdot\text{m}^3/\text{mol}$ 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, $\log K_{\text{OW}}$:

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, $\log K_{\text{OA}}$ 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)
 $\log K_{\text{OA}} = -4.37 + 3709/(T/\text{K})$, 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*; *Epimeoptera*; *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*, Schaubberger & Wildman 1977)
- 2.30 (*Acacystis nidulans*, Schaubberger & Wildman 1977; quoted, Baughman & Paris 1981)
- 2.99 (*Acacystis nidulans*, Schaubberger & 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 $k = 3.8 \times 10^{-5} \text{ h}^{-1}$ 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)

$t_{1/2} = 760$ d at pH 7 in natural waters (Capel & Larson 1995).

Biodegradation: aqueous aerobic $t_{1/2} = 504\text{--}14200$ 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 $k = 0.013\text{ d}^{-1}$ by soil incubation studies from die-away tests (Rao & Davidson 1980; quoted, Scow 1982);

aqueous anaerobic $t_{1/2} = 24\text{--}168$ h, based on soil and freshwater mud grab sample data (Maule et al. 1987; quoted, Howard et al. 1991);

$t_{1/2} = 43\text{--}63$ d in a sandy loam soil incubated in the dark (McLean et al. 1988; quoted, Howard 1991)

$t_{1/2}(\text{aerobic}) = 21$ d, $t_{1/2}(\text{anaerobic}) = 1$ 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 $t_{1/2} \sim 35.5$ min for the vapor phase reaction with hydroxyl radical in air (GEMS 1986; quoted, Howard 1991);

$t_{1/2} = 0.9\text{--}9.1$ 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: $t_{1/2} = 504\text{--}14200$ 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 $t_{1/2}(\text{aerobic}) = 21$ d, $t_{1/2}(\text{anaerobic}) = 1$ d, hydrolysis $t_{1/2} = 760$ d at pH 7 in natural waters (Capel & Larson 1995)

Ground water: $t_{1/2} = 24\text{--}28400$ h, based on estimated aqueous aerobic and anaerobic biodegradation half-lives (Howard et al. 1991).

Sediment:

Soil: $t_{1/2} = 5\text{--}10$ yr persistence in soil (Nash & Woolson 1967);

$t_{1/2} = 504\text{--}14200$ 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 $k = 0.013\text{ d}^{-1}$ with $t_{1/2} = 53.3$ d from biodegradation by soil incubation studies from die-away tests (Rao & Davidson 1980; quoted, Scow 1982);

moderately persistent with a $t_{1/2} = 20\text{--}100$ d (Willis & McDowell 1982; quoted, Howard 1991);

$t_{1/2} = 43\text{--}63$ d in a sandy loam soil incubated in the dark (McLean et al. 1988; quoted, Howard 1991);

selected field $t_{1/2} = 365$ d (Augustijn-Beckers et al. 1994; Hornsby et al. 1996)

$t_{1/2} = 5\text{--}9$ 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							

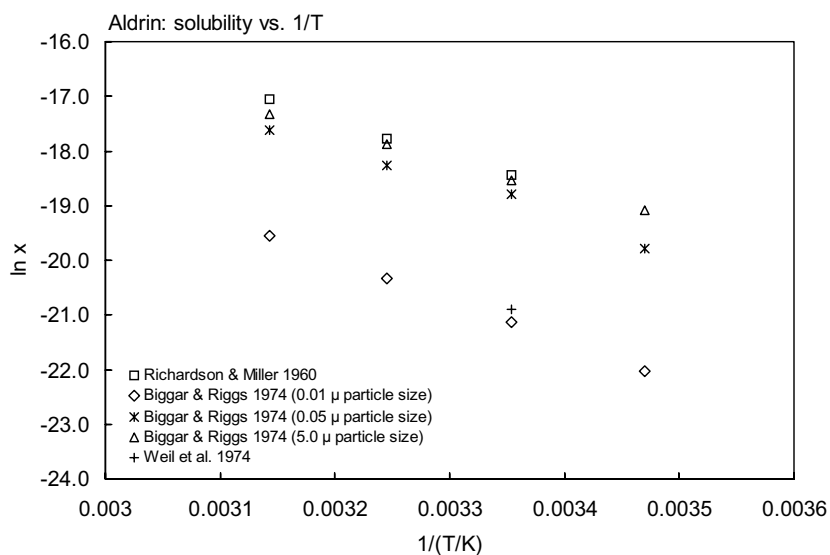


FIGURE 18.1.1.3.1 Logarithm of mole fraction solubility (ln x) versus reciprocal temperature for aldrin.

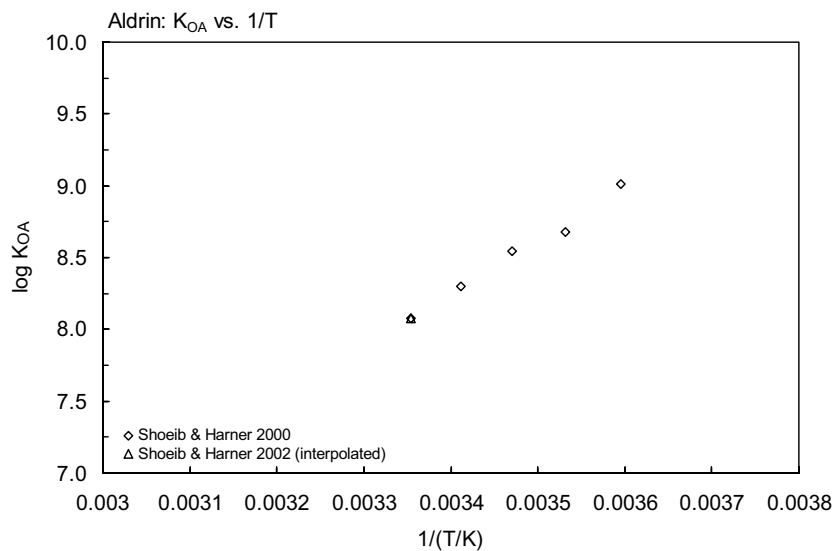


FIGURE 18.1.1.3.2 Logarithm of K_{OA} versus reciprocal temperature for aldrin.

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)
$\log P = A - B/(C + t/^{\circ}C)$		(2)	$\ln P = A - B/(C + t/^{\circ}C)$	(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/^{\circ}C	P/Pa	t/^{\circ}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	

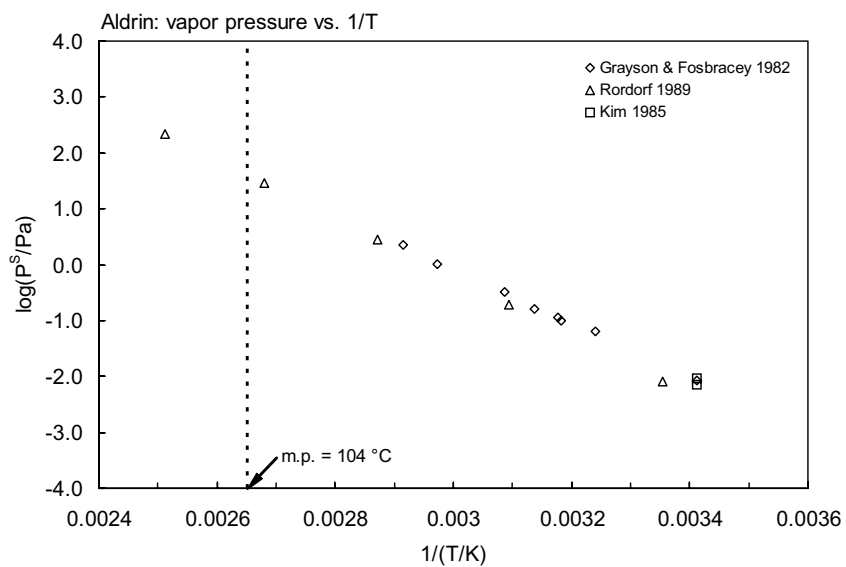
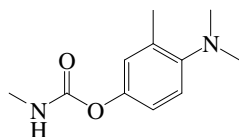


FIGURE 18.1.1.3.3 Logarithm of vapor pressure versus reciprocal temperature for aldrin.

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 ($^{\circ}C$):

94 (Lide 2003)

Boiling Point ($^{\circ}C$):

Density (g/cm^3 at $20^{\circ}C$):

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 $25^{\circ}C$ (assuming $\Delta S_{fus} = 56$ J/mol K), F: 0.210 (mp at $94^{\circ}C$)

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$):

915 ($20^{\circ}C$, shake flask-GC, Bowman & Sans 1983a, b)

915, 1360 ($20^{\circ}C$, $30^{\circ}C$, Montgomery 1993)

915 (20 – $25^{\circ}C$, selected, Augustijn-Beckers et al. 1994; Hornsby et al. 1996)

Vapor Pressure (Pa at $25^{\circ}C$):

0.00227 (20 – $25^{\circ}C$, selected, Augustijn-Beckers et al. 1994; Hornsby et al. 1996)

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

5.17×10^{-4} (20 – $25^{\circ}C$, calculated-P/C, this work)

Octanol/Water Partition Coefficient, $\log K_{ow}$:

1.74 (Zitko & McLeese 1980)

1.73 ($20^{\circ}C$, shake flask-GC, Bowman & Sans 1983b)

1.90 ($22^{\circ}C$, 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 – $25^{\circ}C$, selected, Augustijn-Beckers et al. 1994; Hornsby et al. 1996)

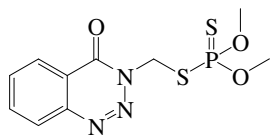
2.52, 1.94 (soil, estimated-class-specific model, estimated-general model, Gramatica et al. 2000)

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

Half-Lives in the Environment:

Soil: selected field $t_{1/2} = 6$ 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 ($^{\circ}C$):

73 (Lide 2003)

Boiling Point ($^{\circ}C$):

> 200 (dec., Montgomery 1993)

Density (g/cm^3 at $20^{\circ}C$):

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 $25^{\circ}C$ (assuming $\Delta S_{fus} = 56$ J/mol K), F : 0.338 (mp at $73^{\circ}C$)

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$ or as indicated):

33 (rm. temp., Spencer 1973; Worthing 1979; Khan 1980; Budavari 1989)

30 ($20^{\circ}C$, Melnikov 1971; Spencer 1982)

33 (20 – $25^{\circ}C$, Willis & McDowell 1982)

20.9 ($20^{\circ}C$, shake flask-GC, Bowman & Sans 1983a, b)

29 (Hartley & Kidd 1987; Lohninger 1994)

28 ($20^{\circ}C$, Worthing & Hance 1991; Tomlin 1994)

29 (20 – $25^{\circ}C$, selected, Wauchope et al. 1992; Hornsby et al. 1996)

30 (Milne 1995)

Vapor Pressure (Pa at $25^{\circ}C$ or as indicated and reported temperature dependence equations):

2.93×10^{-5} ($20^{\circ}C$, Melnikov 1971)

0.0510 ($20^{\circ}C$, Khan 1980)

1.00×10^{-6} ($20^{\circ}C$, Worthing & Walker 1983)

1.11×10^{-5} ($20^{\circ}C$, GC-RT correlation without mp correction, Kim et al. 1984; Kim 1985)

3.10×10^{-6} ($20^{\circ}C$, GC-RT correlation with mp correction, Kim et al. 1984; Kim 1985)

<0.0010 ($20^{\circ}C$, Hartley & Kidd 1987)

3.00×10^{-5} ($20^{\circ}C$, 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, $125^{\circ}C$, gas saturation-GC, Rordorf 1989)

$\log (P_s/P_a) = 14.416 - 6119.2/(T/K)$; measured range 80.3–145°C (solid, gas saturation-GC, Rordorf 1989)
 $\log (P_L/P_a) = 11.327 - 5048.6/(T/K)$; 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 ($\text{Pa}\cdot\text{m}^3/\text{mol}$ 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, $\log \text{BCF}$:

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 χ , 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, $t_{1/2}$:

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, $t_{1/2} = 484, 88, \text{ and } 32$ 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);

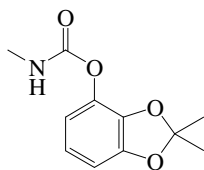
average $t_{1/2} = 40$ d (Dowd et al. 1993);

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 ($^{\circ}C$):

130 (Lide 2003)

Boiling Point ($^{\circ}C$):

Density (g/cm^3 at $20^{\circ}C$):

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 $25^{\circ}C$ (assuming $\Delta S_{fus} = 56 J/mol K$), F: 0.0933 (mp at $130^{\circ}C$)

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$ or as indicated):

40 (Spencer 1973, 1982)

40 (Martin & Worthing 1977; Worthing & Walker 1987; Kenaga 1980;)

40 ($20^{\circ}C$, Hartley & Kidd 1987; Montgomery 1993; Milne 1995)

40 (20 – $25^{\circ}C$, selected, Wauchope et al. 1992; Hornsby et al. 1996)

40 (Lohninger 1994)

280 ($20^{\circ}C$ at pH 7, Tomlin 1994)

Vapor Pressure (Pa at $25^{\circ}C$ or as indicated):

6.6×10^{-4} (Hartley & Kidd 1987)

0.00467 (20 – $25^{\circ}C$, selected, Wauchope et al. 1992; Hornsby et al. 1996)

6.6×10^{-4} ($20^{\circ}C$, Montgomery 1993)

0.0046 (quoted, gas saturation-GC, Tomlin 1994)

Henry's Law Constant ($Pa \cdot m^3/mol$ at $25^{\circ}C$ or as indicated):

0.365 ($20^{\circ}C$, 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)

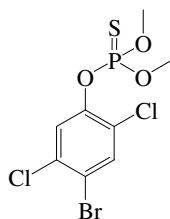
Ground water:

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 ($^{\circ}C$):

54 (Lide 2003)

Boiling Point ($^{\circ}C$):

140–142 at 0.01 mmHg (Hartley & Kidd 1987; Worthing & Walker 1987)

Density (g/cm^3 at $20^{\circ}C$):

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 $25^{\circ}C$ (assuming $\Delta S_{fus} = 56$ J/mol K), F: 0.519 (mp at $54^{\circ}C$)

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$):

40 (Kenaga 1980b; Spencer 1982; Hartley & Kidd 1987)

0.30 ($20^{\circ}C$, shake flask-GC, Bowman & Sans 1979)

0.652 ($20^{\circ}C$, correlated, Bowman & Sans 1983b)

0.70 ($20^{\circ}C$, Worthing & Walker 1987)

Vapor Pressure (Pa at $25^{\circ}C$):

0.017 ($20^{\circ}C$, Hartley & Kidd 1987; Worthing & Walker 1987)

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

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, $t_{1/2}$:

Volatilization:

Photolysis:

Oxidation:

Hydrolysis: hydrolyzed in alkaline media (Worthing 1987).

Biodegradation:

Biotransformation:

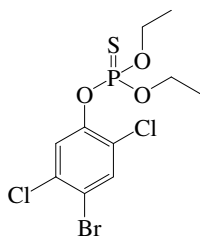
Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants:

$k_1 = 0.01307 \text{ mL g}^{-1} \text{ d}^{-1}$; $k_2 = 0.33 \text{ d}^{-1}$ (guppy, De Bruijn & Hermens 1991)

$k_2 = 12 \text{ d}^{-1}$ (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: C₁₀H₁₂Cl₂O₃PS

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/cm³ at 20°C):

1.52–1.55 (Hartley & Kidd 1987; Worthing & Walker 1987)

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: 1.0

Water Solubility (g/m³ 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·m³/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}:

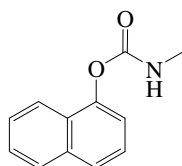
3.48 (soil, calculated-solubility, Kenaga 1980b)

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

Hydrolysis: at room temp., stable in aqueous suspension at $\text{pH} < 9$, hydrolysed at $\text{pH} > 9$, 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: C₁₂H₁₁NO₂

Molecular Weight: 201.221

Melting Point (°C):

145 (Lide 2003)

Boiling Point (°C): dec. on distillation

Density (g/cm³ 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 (cm³/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/m³ 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 m³/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	(<i>Pseudorasbora parva</i> , 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 χ , 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)

$t_{1/2}(\text{air}) = 52\text{--}200$ h in the atmosphere, based on aqueous photolysis data; $t_{1/2}(\text{aq.}) = 52\text{--}200$ h, based on reported photolysis half-life for summer and winter sunlight at 40°N (Howard et al. 1991)

$k(\text{aq.}) = 6.4 \times 10^{-4} \text{ h}^{-1}$ (Armbrust 2000)

$k(\text{aq.}) = (5.6 \pm 0.3) \times 10^{-5} \text{ s}^{-1}$ 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 $t_{1/2} = 4.5\text{--}7.4$ h, based on estimated rate constant for the vapor-phase reaction with hydroxyl radical in air (Howard et al. 1991)

$k_{OH}(\text{aq.}) = 3.40 \times 10^9 \text{ M}^{-1} \text{ s}^{-1}$ 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: $k(\text{alkaline}) = (5.02 \pm 0.03) \text{ M}^{-1} \text{ h}^{-1}$ 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)

$k = 0.066 \text{ d}^{-1}$ at pH 7, $k = 5.2 \text{ d}^{-1}$ 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:

$t_{1/2}(\text{aerobic}) = 40\text{--}720$ h, based on unacclimated aerobic river die-away test data and freshwater grab sample data (Eichelberger & Lichtenberg 1971; quoted, Howard et al. 1991)

$t_{1/2} > 3 \times 10^4$ d, assuming a bacterial population of 0.1 mg/L (Wolfe et al. 1978b)

$k(\text{aq.}) = 2.4 \times 10^{-10} \text{ mL cell}^{-1} \text{ d}^{-1}$ in aquatic system (Scow 1982)

$t_{1/2}(\text{anaerobic}) = 160\text{--}2880$ h, based on unacclimated aerobic biodegradation (Howard et al. 1991)

$t_{1/2}(\text{aerobic}) = 1.7$ d, $t_{1/2}(\text{anaerobic}) = 6.7$ d in natural waters (Capel & Larson 1995)

$k(\text{aerobic}) = 1.70 \times 10^{-3} \text{ h}^{-1}$ (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 $t_{1/2}$ > 3×10^4 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);

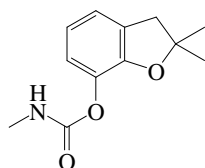
$t_{1/2}$ = 10 d (selected, Halfon et al. 1996)

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 ($^{\circ}C$):

151 (Lide 2003)

Boiling Point ($^{\circ}C$):

Density (g/cm^3 at $20^{\circ}C$):

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 $25^{\circ}C$ (assuming $\Delta S_{fus} = 56 J/mol K$), F: 0.0580 (mp at $151^{\circ}C$)

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$ 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	($19^{\circ}C$, shake flask-GC, Bowman & Sans 1979, 1983b)
700	(Verschuereen 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 – $25^{\circ}C$, selected, Wauchope 1989; Wauchope et al. 1992; Hornsby et al. 1996)
320	($20^{\circ}C$, Montgomery 1993; Tomlin 1994; Milne 1995)
375	($30^{\circ}C$, Montgomery 1993)

Vapor Pressure (Pa at $25^{\circ}C$ 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}	($20^{\circ}C$, Hartley & Graham-Bryce 1980)
2.70×10^{-3}	($33^{\circ}C$, Khan 1980)
2.67×10^{-3}	(20 – $25^{\circ}C$, Weber et al. 1980)
2.70×10^{-4}	(Thomas 1982)
2.20×10^{-3} , 1.08×10^{-4}	($20^{\circ}C$, GC-RT correlation, GC-RT correlation with mp correction, Kim 1985)
2.70×10^{-3}	($33^{\circ}C$, Hartley & Kidd 1987)
8.00×10^{-5}	(20 – $25^{\circ}C$, selected, Wauchope et al. 1992; Hornsby et al. 1996)
3.10×10^{-5} , 7.20×10^{-5}	(20 , $25^{\circ}C$, Tomlin 1994)

Henry's Law Constant (Pa·m³/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 $OC \geq 0.1\%$, $OC \geq 0.5\%$, average, Delle Site 2001)
 1.55 (sediment: organic carbon $OC \geq 0.5\%$, average, Delle Site 2001)

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

Volatilization: initial rate constant $k = 1.2 \times 10^{-3} \text{ h}^{-1}$ and a predicted rate constant $k = 2.9 \times 10^{-4} \text{ h}^{-1}$ from soil with $t_{1/2} = 2390 \text{ h}$ (Thomas 1982).

Photolysis: near surface direct sunlight photolysis rate constant $k = 0.003 \text{ d}^{-1}$ with $t_{1/2} \sim 200 \text{ d}$ (Schnoor & McAvoy 1981; Schnoor 1992);

$t_{1/2} \sim 2, 6, 12 \text{ h}$ for degradation in river, lake and seawater, respectively, from Greece which were irradiated with sunlight (Samanidou et al. 1988; quoted, Howard 1991)

Photodegradation ($\lambda > 290 \text{ nm}$) half-lives in aqueous carbofuran solutions: $t_{1/2} \sim 50 \text{ min}$ with TiO_2 (160 mg/L) + O_2 , $t_{1/2} \sim 40 \text{ min}$ with H_2O_2 ($6 \times 10^{-3} \text{ mg/L}$); $t_{1/2} \sim 30 \text{ min}$ with O_3 (10^{-3} mg/L) and $t_{1/2} \sim 65 \text{ h}$ in water/oil suspension. (Mansour et al. 1997)

Oxidation: photooxidation $t_{1/2} = 4.6 \text{ h}$, based on estimated rate constant for the vapor-phase reaction with hydroxyl radical in air (Atkinson 1987; quoted, Howard et al. 1991)

$k(\text{aq.}) = (620 \pm 60) \text{ M}^{-1} \text{ s}^{-1}$ for direct reaction with ozone in water at pH 3.7 and 21°C , with $t_{1/2} = 54 \text{ s}$ at pH 7 (Yao & Haag 1991).

$k(\text{aq.}) = 7 \times 10^9 \text{ M}^{-1} \text{ s}^{-1}$ for the reaction with hydroxyl radical in aqueous solutions at $24 \pm 1^\circ\text{C}$ (Haag & Yao 1992);

$k_{\text{OH}}(\text{aq.}) = 2.20 \times 10^9 \text{ M}^{-1} \text{ s}^{-1}$ in irradiated field water both in the laboratory and sunlit rice paddies with field dissipation $t_{1/2} = 16.3 \text{ h}$ (Mabury & Crosby 1996).

Hydrolysis: aqueous hydrolysis $t_{1/2} = 5.1 \text{ wk}$ at pH 7.0 and at 27°C and $t_{1/2} = 1.2 \text{ h}$ at pH 10 (Seiber et al. 1978; quoted, Howard 1991);

alkaline chemical hydrolysis rate constant $k = 6 \times 10^{-5} \text{ M}^{-1} \cdot \text{s}^{-1}$ with $t_{1/2} > 10,000 \text{ d}$ (Schnoor & McAvoy 1981; Schnoor 1992);

$t_{1/2} = 690, 8.2, \text{ and } 1.0 \text{ wk}$ in water at 25°C and pH 6.0, 7.0 and 8.0, respectively (Chapman & Cole 1982; quoted, Howard 1991);

hydrolysis rate constants: $k = (30.6 \pm 0.6) \text{ L min}^{-1} \text{ mol}^{-1}$ at 15°C , $k = (67.0 \pm 0.4) \text{ L/min} \cdot \text{mol}$ at 25°C and $k = (163 \pm 1.0) \text{ L min}^{-1} \text{ mol}^{-1}$ at 35°C (Trotter et al. 1991);

$t_{1/2} = 170 \text{ wk}$ at pH 4.5, $t_{1/2} = 690 \text{ wk}$ at pH 5–6, $t_{1/2} = 8.2 \text{ wk}$ at pH 7 and $t_{1/2} = 1 \text{ wk}$ at pH 8.0 at 25°C (Montgomery 1993);

$t_{1/2} > 1 \text{ yr}$ at pH 4, $t_{1/2} = 121 \text{ d}$ at pH 7, and $t_{1/2} = 31 \text{ d}$ at pH 9 at 22°C (Tomlin 1994);

rate constant $k = 5.0 \times 10^{-3} \text{ M}^{-1} \text{ h}^{-1}$ at 24°C ; $t_{1/2} = 737 \text{ h}$ at pH 7.0, $t_{1/2} = 93.7 \text{ h}$ at pH 8.0 and $t_{1/2} = 1.17 \text{ h}$ at pH 10.0 in aqueous solutions; $t_{1/2} = 630 \text{ d}$ at pH 7, $t_{1/2} = 133 \text{ d}$ at pH 8, and $t_{1/2} = 0.87 \text{ d}$ at pH 10 in aqueous solutions with montmorillonite suspensions (23.9 g/L); $t_{1/2} = 937 \text{ d}$ at pH 7, $t_{1/2} = 76.2 \text{ d}$ at pH 8, $t_{1/2} = 0.98 \text{ d}$ at pH 10 in aqueous solutions with beidellite suspensions (4.9 g/L); $t_{1/2} = 889 \text{ d}$ at pH 7, $t_{1/2} = 113 \text{ d}$ at pH 8, $t_{1/2} = 0.78 \text{ d}$ at pH 10 in aqueous solutions with illite suspensions (9.2 g/L); and $t_{1/2} = 753 \text{ d}$ at pH 7, $t_{1/2} = 80.6 \text{ d}$ at pH 8, $t_{1/2} = 0.91 \text{ d}$ at pH 10 in aqueous solutions with vermiculite suspensions (8.5 g/L) with an initial carbofuran concentration of $1.0 \times 10^{-4} \text{ M}$ (Wei et al. 2001).

Biodegradation: rate constants $k = 0.047 \text{ d}^{-1}$ from soil incubation studies and $k = 0.026 \text{ d}^{-1}$ in anaerobic system from flooded soil incubation studies both by die-away test (Rao & Davidson 1980; quoted, Scow 1982);

$t_{1/2} = 40 \text{ d}$ 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: $t_{1/2} = 4.6 \text{ h}$, 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 $t_{1/2} = 57 \text{ h}$ in rice paddy water, but pH dependent, e.g., $t_{1/2} = 1.2 \text{ h}$ at pH 10 and $t_{1/2} = 864 \text{ h}$ at pH 7; $t_{1/2} = 48$ and 55 h for two farm ponds (Seiber et al. 1978);

$t_{1/2} = 2, 6, 12 \text{ h}$ 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 $k = (620 \pm 60) \text{ M}^{-1} \text{ s}^{-1}$ for direct reaction with ozone in water at pH 3.7 and 21°C , with $t_{1/2} = 54 \text{ s}$ at pH 7 (Yao & Haag 1991).

Ground water:

Sediment:

Soil: persistence of less than one month (Wauchope 1978);

$t_{1/2} = 11\text{--}13$ d at pH 6.5, and $t_{1/2} = 60\text{--}75$ 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 $k = 0.047\text{ d}^{-1}$ by die-away test from soil incubation studies and $t_{1/2} = 26$ d from biodegradation rate constant $k = 0.026\text{ d}^{-1}$ in anaerobic system from flooded soil incubation studies by die-away test (Rao & Davidson 1980; quoted, Scow 1982);

moderately persistent in soils with $t_{1/2} = 20\text{--}100$ d (Willis & McDowell 1982);

$t_{1/2} = 1\text{--}2$ 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 $5\text{--}20$ 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);

$t_{1/2} = 30\text{--}60$ d in soil (Tomlin 1994)

Disappearance rate constants $k = (1.33\text{--}5.16) \times 10^{-2}\text{ h}^{-1}$ and $k = (0.36\text{--}1.13) \times 10^{-2}\text{ h}^{-1}$ in non-sterile soil suspensions; $k = (1.20\text{--}5.07) \times 10^{-2}\text{ h}^{-1}$ 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)

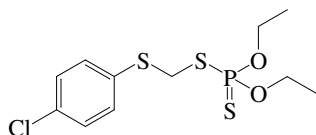
First order rate constants for photolytic decline in sandy soil: $k = 1.88 \times 10^{-3}\text{ h}^{-1}$ with $t_{1/2} = 370$ h irradiated in moisture-maintained soil, $k = 0.86 \times 10^{-3}\text{ h}^{-1}$ with $t_{1/2} = 800$ h, irradiated in air-dried soil, $k = 1.15 \times 10^{-3}\text{ h}^{-1}$ with $t_{1/2} = 600$ h in dark control moist sandy soil, but not degraded in the dark control air-dry system. The photolytic $k = 7.31 \times 10^{-4}\text{ h}^{-1}$ with $t_{1/2} = 950$ h in moist soil and the contribution of moisture to irradiated metabolism $k = 1.02 \times 10^{-3}\text{ h}^{-1}$ 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 ($^{\circ}C$):

colorless liquid (Spencer 1982, Hartley & Kidd 1987, Tomlin 1994)

< 25 (Montgomery 1993)

Boiling Point ($^{\circ}C$):

82 (at 0.01 mmHg, Spencer 1982; Hartley & Kidd 1987; Montgomery 1993; Milne 1995)

Density (g/cm^3):

1.274 (Spencer 1982)

1.271 ($20^{\circ}C$, 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 $25^{\circ}C$, F: 1.0

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$):

< 2.0 (Martin 1961; Spencer 1982)

0.34 (Gunther et al. 1968; Kenaga 1980b; Kenaga & Goring 1980)

< 40 (Verschuere 1983)

0.63 ($20^{\circ}C$, 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, $30^{\circ}C$, Montgomery 1993)

0.34 (selected, Augustijn-Beckers et al. 1994; Hornsby et al. 1996)

40, < 1 (Milne 1995)

Vapor Pressure (Pa at $25^{\circ}C$ or as indicated):

0.40 (Menn et al. 1964)

4.13×10^{-5} ($20^{\circ}C$, Eichler 1965)

4.07×10^{-5} ($20^{\circ}C$, Melnikov 1971)

4.0×10^{-5} ($20^{\circ}C$, Hartley & Graham-Bryce 1980)

1.07 (Spencer 1982)

7.73×10^{-5} ($20^{\circ}C$, 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 ($Pa \cdot m^3/mol$):

0.046 ($20^{\circ}C$, 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 χ , 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, $t_{1/2}$:

Volatilization:

Photolysis:

Photooxidation:

Hydrolysis:

Biodegradation:

Biotransformation: $t_{1/2} \geq 100$ d in soil (Verschuieren 1983; quoted, Montgomery 1993).

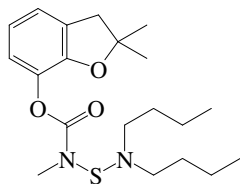
Bioconcentration and Uptake and Elimination Rate Constants (k_1 and k_2):

Half-Lives in the Environment:

Soil: $t_{1/2} \geq 100$ d (Verschuieren 1983; quoted, Montgomery 1993);

field $t_{1/2} = 30$ 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/acaricide/nematicide

CAS Registry No: 55285-14-8

Molecular Formula: $C_{20}H_{32}N_2O_3S$

Molecular Weight: 380.544

Melting Point ($^{\circ}C$):

viscous brown liquid (Hartley & Kidd 1987)

Boiling Point ($^{\circ}C$):

124–128 (Tomlin 1994; Milne 1995)

Density (g/cm^3):

1.056 ($20^{\circ}C$, 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 $25^{\circ}C$, F: 1.0

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$):

0.30 (Hartley & Kidd 1987; Tomlin 1994)

0.03 (Milne 1995)

Vapor Pressure (Pa at $25^{\circ}C$):

0.041×10^{-3} (Hartley & Kidd 1987, Tomlin 1994)

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

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. $t_{1/2}$:

Volatilization:

Photolysis:

Oxidation:

Hydrolysis: hydrolyzed in aqueous media with $t_{1/2} < 1$ h in pure water at pH 4; $t_{1/2} = 22$ h at pH 6, $t_{1/2} = 7.6$ d at pH 7, $t_{1/2} = 14.2$ d at pH 8 and $t_{1/2} > 58.3$ d at pH 9 (Hartley & Kidd 1987; Tomlin 1994)

Biodegradation: in soil, rapidly degraded under both aerobic and anaerobic conditions with $t_{1/2} = 2-3$ 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, $t_{1/2} < 1$ h in pure water at pH 4; $t_{1/2} = 22$ h at pH 6, $t_{1/2} = 7.6$ d at pH 7, $t_{1/2} = 14.2$ d at pH 8 and $t_{1/2} > 58.3$ d at pH 9 (Hartley & Kidd 1987; Tomlin 1994)

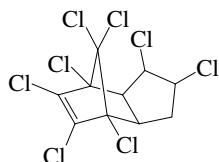
Ground water:

Sediment:

Soil: rapidly degraded under both aerobic and anaerobic conditions with $t_{1/2} = 2-3$ 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-3a,4,7,7a-tetrahydro-4,7-methano-1*H*-indane; 1,2,4,5,6,7,8,8-octa-chloro-3a,4,7,7a-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 ($^{\circ}C$):

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 ($^{\circ}C$):

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 $20^{\circ}C$):

1.59–1.63 ($25^{\circ}C$, 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 $25^{\circ}C$, F :

0.162 (assuming $\Delta S_{fus} = 56$ J/mol K, Mackay et al. 1986)

0.140 ($20^{\circ}C$, assuming $\Delta S_{fus} = 56$ J/mol K, Suntio et al. 1988)

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$ 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 ($20^{\circ}C$, 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 – $25^{\circ}C$, 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)
 $\log [S_L/(\text{mol/L})] = -0.880 - 1124/(T/K)$ (liquid, *cis*-isomer, Passivirta et al. 1999)
 $\log [S_L/(\text{mol/L})] = -0.880 - 1118/(T/K)$ (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)
 $\log (P_L/\text{Pa}) = 11.968 - 4033.7/(T/K)$; 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)
 $\log (P_L/\text{Pa}) = 12.435 - 4332.5/(T/K)$; 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)
 $\log (P_S/\text{Pa}) = 12.318 - 4235.5/(T/K)$; measured range 50/1–135°C (β -chlordane, liquid, gas saturation-GC, Rordorf 1989)
 $\log (P_L/\text{Pa}) = 13.396 - 4803.6/(T/K)$; 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)
 $\log (P_L/\text{Pa}) = 12.04 - 4284/(T/K)$ (*cis*-chlordane, supercooled liquid P_L , GC-RT correlation, Hinckley et al. 1990; quoted, Passivirta et al. 1999)
 $\log (P_L/\text{Pa}) = 11.95 - 4216/(T/K)$ (*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)
 $\log (P_S/\text{Pa}) = 14.99 - 5407/(T/K)$ (*cis*-chlordane, solid, Passivirta et al. 1999)
 $\log (P_S/\text{Pa}) = 14.91 - 5333/(T/K)$ (*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)

$\log(P_L/\text{Pa}) = -4238/(T/K) + 12.32$ (*cis*-chlordane, supercooled liquid P_L : linear regression, Shen & Wania 2005)

Henry's Law Constant ($\text{Pa}\cdot\text{m}^3/\text{mol}$ 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)
 $\log[H/(\text{Pa}\cdot\text{m}^3/\text{mol})] = 12.92 - 3160/(T/K)$ (*cis*-chlordane, Passivirta et al. 1999)
 $\log[H/(\text{Pa}\cdot\text{m}^3/\text{mol})] = 12.84 - 3098/(T/K)$ (*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*-chlordanes, 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*-chlordanes, gas saturation-GC, Shoeib & Harner 2002)
 8.967*, 8.872 (*trans*-chlordanes, 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*-chlordanes, gas saturation-GC, Shoeib & Harner 2002)
 8.3887*, 8.387 (oxychlordanes, 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 (oxychlordanes, gas saturation-GC, Shoeib & Harner 2002)
 8.91, 8.85 (*cis*-chlordanes, LDV literature-derived value, FAV final-adjusted value, Shen & Wania 2005)
 8.86, 8.85 (*trans*-chlordanes, 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*-chlordanes, Schimmel et al. 1976)
 3.57–4.23 (96 h exposures of *trans*-chlordanes to whole marine fish, Schimmel et al. 1976)
 4.11–4.34 (186-d chronic exposures, *trans*-chlordanes to sheephead minnow, Parrish et al. 1978)
 3.85–4.46 (exposures *trans*-chlordanes 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 -chlordanes, 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 -chlordanes, 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 -chlordanes, 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 -chlordanes, rainbow trout, steady-state BCF-concentration ratio., Oliver & Niimi 1985)
 4.45, 4.20 (α -, γ -chlordanes, rainbow trout, kinetic state BCF-ratio of rate const., Oliver & Niimi 1985)
 6.15, 4.88 (α -, γ -chlordanes, rainbow trout, Lake Ontario field BCF., Oliver & Niimi 1985)
 4.58; 4.33, 4.40 (measured for fathead minnow; calculated- K_{OW} for sheephead 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 sheephead 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 redbreast, Roberts et al. 1977)
 2.03, 2.51, 3.0 (frogs, bluegills, goldfish, Verschuere 1983)
 6.73, 7.89, 6.99 (total chlordanes: 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 $t_{1/2} \sim 7.3$ 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 $t_{1/2} \sim 18$ –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); $t_{1/2} \sim 43$ 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 $k = 0.3 \text{ d}^{-1}$ (Glottfelty et al. 1984; Glottfelty et al. 1989);
 calculated rate constant $k = 1.0 \text{ d}^{-1}$ (Glottfelty 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);

$k_{OH}(aq.) = 8 \times 10^8 \text{ M}^{-1} \text{ s}^{-1}$ for the reaction (photo-Fenton with reference to lindane) with hydroxyl radical in aqueous solutions at pH 3.3 and at $24 \pm 1^\circ\text{C}$ (Buxton et al. 1988; quoted, Faust & Hoigné 1990; Haag & Yao 1992)

$k(aq.) < 0.04$ – $> 300 \text{ M}^{-1} \text{ s}^{-1}$ for direct reaction with ozone in water at pH 6.2–6.4 and $19 \pm 2^\circ\text{C}$, with 2 min $> t_{1/2} > 10$ d at pH 7 (Yao & Haag 1991).

$k(aq.) = (6$ – $170) \times 10^8 \text{ M}^{-1} \text{ s}^{-1}$ for the reaction (photo-Fenton with reference to acetophenone) with hydroxyl radicals in aqueous solutions at pH 3.3 and at $24 \pm 1^\circ\text{C}$ (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 $k = 4.3 \times 10^{-3} \text{ M}^{-1} \text{ h}^{-1}$ 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);

$k = 0.0024 \text{ d}^{-1}$ 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 1985)

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 \pm 5.7 yr at Eagle Harbor, 10 \pm 2.3 yr at Sleeping Bear Dunes and 6.8 \pm 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- > 300 M⁻¹ s⁻¹ for direct reaction with ozone in water at pH 6.2–6.4 and 19 \pm 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 10⁷ 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 daphnids 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);

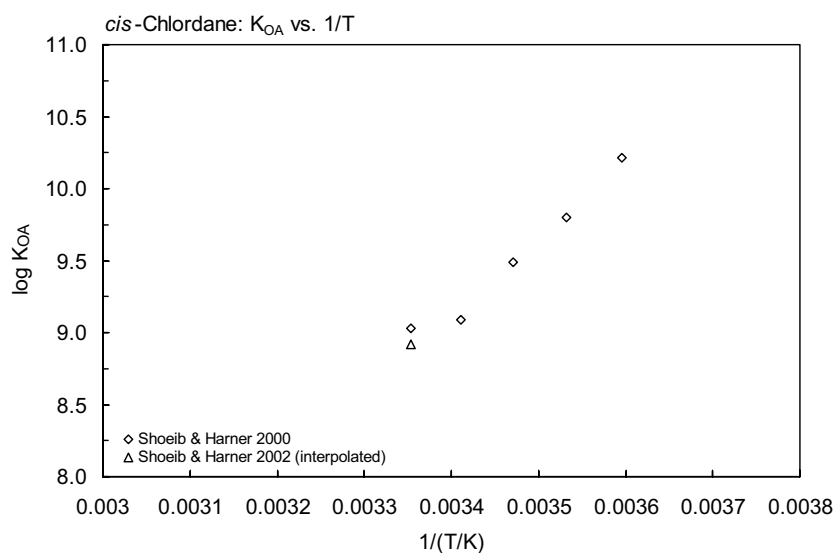
depuration $t_{1/2}$ = 7.1 d for γ -chlordane, and $t_{1/2}$ = 5.9 d for α -chlordane (rats, Dearth & Hites 1991);

$t_{1/2}$ = 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

<i>cis</i> -chlordane		<i>trans</i> -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.

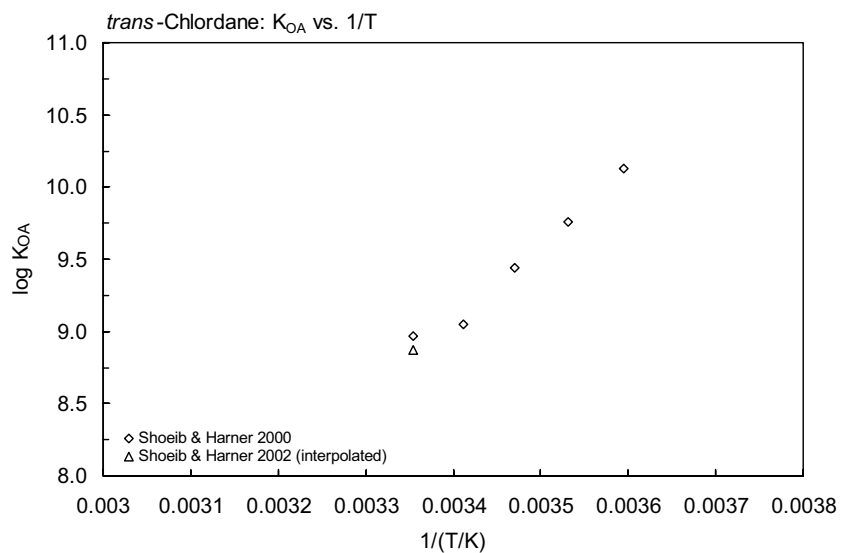


FIGURE 18.1.1.13.1B Logarithm of K_{OA} versus reciprocal temperature for *trans*-chlordane.

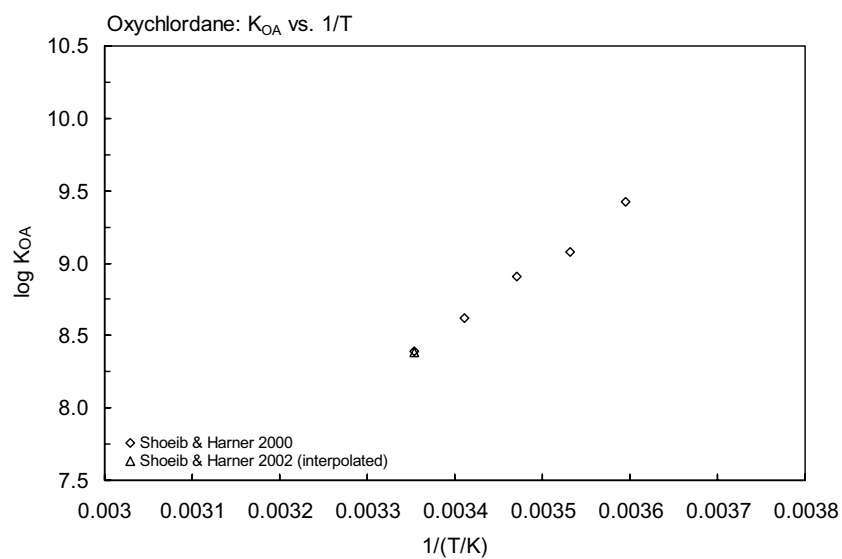
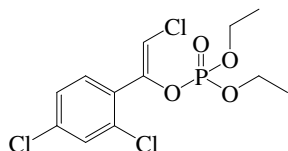


FIGURE 18.1.1.13.1C Logarithm of K_{OA} versus reciprocal temperature for oxychlordane.

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 ($^{\circ}C$):

-19 (Lide 2003)

Boiling Point ($^{\circ}C$):

167–170 (at 0.5 mmHg, Hartley & Kidd 1987; Tomlin 1994)

Density (g/cm^3 at $20^{\circ}C$):

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 $25^{\circ}C$ (assuming $\Delta S_{fus} = 56$ J/mol K), F: 1.0

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$ or as indicated):

145 ($20^{\circ}C$, Melnikov 1971)

145 (Martin & Worthing 1977; Milne 1995)

145 ($23^{\circ}C$, Khan 1980)

146 ($20^{\circ}C$, Briggs 1981)

124 ($20^{\circ}C$, shake flask-GC, Bowman & Sans 1983a, b)

145 ($23^{\circ}C$, Hartley & Kidd 1987; Worthing & Walker 1987, 1991; Tomlin 1994)

130 ($20^{\circ}C$, selected, Suntio et al. 1988)

Vapor Pressure (Pa at $25^{\circ}C$ or as indicated and reported temperature dependence equations):

0.00053 ($20^{\circ}C$, Khan 1980)

2.7×10^{-5} (Verschuereen 1983)

0.0010 (Hartley & Kidd 1987; Tomlin 1994)

0.00010 ($20^{\circ}C$, selected, Suntio et al. 1988)

8.20×10^{-4} , 1.70×10^{-2} , 0.22, 2.0, 14.0 (25, 50, 70, 100, $125^{\circ}C$, gas saturation-GC, Rordorf 1989)

$\log(P_L/Pa) = 13.794 - 5032.8/(T/K)$; measured range 36.9 – $129^{\circ}C$ (liquid, gas saturation-GC, Rordorf 1989)

0.00053 ($20^{\circ}C$, 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 ($\text{Pa}\cdot\text{m}^3/\text{mol}$ 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)
- $\log K_{\text{AW}} = 0.173 - 1187/(T/K)$ (van't Hoff eq. derived from literature data, Staudinger & Roberts 2001)

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

- 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, $\log \text{BCF}$:

- 1.57 (calculated-S, Kenaga 1980)
- 2.30 (earthworms, Lord et al. 1980; quoted, Connell & Markwell 1990)

Sorption Partition Coefficient, $\log K_{\text{OC}}$:

- 2.45 (calculated-S, Kenaga 1980)
- 2.47 (soil, sorption isotherm, converted from reported $\log K_{\text{OM}}$ 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)

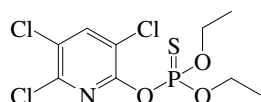
Environmental Fate Rate Constants, k , or Half-Lives, $t_{1/2}$:

Hydrolysis: at 38°C : $t_{1/2} > 700$ h at pH 1.1 and $t_{1/2} > 400$ h at pH 9.1; $t_{1/2} = 1.28$ h at pH 13 and 20°C (Tomlin 1994).

Half-Lives in the Environment:

Soil: $t_{1/2} > 24$ wk in sterile sandy loam and $t_{1/2} < 1.0$ wk in nonsterile sandy loam; $t_{1/2} > 24$ wk in sterile organic soil and $t_{1/2} = 1.0$ 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 ($^{\circ}C$):

42 (Lide 2003)

Boiling Point ($^{\circ}C$):

Density (g/cm^3 at $20^{\circ}C$):

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 $25^{\circ}C$ (assuming $\Delta S_{fus} = 56$ J/mol K), F: 0.681 (mp at $42^{\circ}C$)

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$ or as indicated):

0.40, 0.47 (23, $25^{\circ}C$, 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, $20^{\circ}C$, shake flask-GC, Bowman & Sans 1979)

0.30 ($23^{\circ}C$, Kenaga 1980a, b)

0.30 (Dow Chemical Data, Kenaga & Goring 1980)

2.00 ($35^{\circ}C$, Khan 1980)

2.00 (20 – $25^{\circ}C$, Willis & McDowell 1982)

0.40 (Verschueren 1983)

0.73 ($20^{\circ}C$, 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 – $25^{\circ}C$, selected, Wauchope et al. 1992; Hornsby et al. 1996)

1.93 (Racke 1993)

0.73, 1.30 ($20^{\circ}C$, $30^{\circ}C$, 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 $25^{\circ}C$ at $25^{\circ}C$ or as indicated):

0.00145 ($20^{\circ}C$, Eichler 1965; Wolfdietrich 1965)

0.0025 (Brust 1966; Neely & Blau 1977)

0.0037 (Hamaker 1975)

0.00253 (Melnikov 1971)

0.0104 ($30^{\circ}C$, NIEHS 1975)

0.0012 ($20^{\circ}C$, 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 ($\text{Pa}\cdot\text{m}^3/\text{mol}$ 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 χ , 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 $\geq 0.1\%$, OC $\geq 0.5\%$, 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, $t_{1/2} \sim 9.0$ d for a model river 1 m deep, flowing 1 m/s with a wind velocity of 3 m/s (Howard 1991);
 initial $k = 8.8 \times 10^{-2} \text{ h}^{-1}$ and predicted $k = 1.3 \times 10^{-3} \text{ h}^{-1}$ from soil with $t_{1/2} = 533$ h (Thomas 1982);
 $t_{1/2} = 0.3\text{--}3.2$ d for disappearance from an inert surface at 25°C (Meikle et al. 1983).

Photolysis: $t_{1/2}(\text{exptl}) = 22$ d determined under midday summer sunlight in California (Meikle et al. 1983; quoted, Howard 1991)

$k_p = (2.19 \pm 0.17) \times 10^{-2} \text{ h}^{-1}$, $(2.09 \pm 0.17) \times 10^{-2} \text{ h}^{-1}$ 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)
 $k(\text{alkaline}) = 0.1 \text{ M}^{-1} \text{ s}^{-1}$, $k(\text{neutral}) = 1 \times 10^{-7} \text{ s}^{-1}$, $10^{-7}\text{--}10^{-9} \text{ M}$ in aqueous buffer at 20°C (Harris 1982)
 $k = (1.08 - 2.0) \times 10^{-3} \text{ h}^{-1}$ 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 $k(\text{acidic}) < 0.008 \text{ d}^{-1}$ in acidic soils with pH ≤ 7.0 , corresponding to $t_{1/2} = 92\text{--}341$ d and $k(\text{alkaline}) = (0.006 - 0.063) \text{ d}^{-1}$ in alkaline soils corresponding to $t_{1/2} = 11\text{--}200$ d in abiotic hydrolysis in 37 different soils with pH 3.8–8.5. (Racke et al. 1996)

$k = 0.0009 \text{ d}^{-1}$ at pH 5, $k = 0.023 \text{ d}^{-1}$ at pH 7, $k = 0.044 \text{ d}^{-1}$ at pH 9; measured hydroxy radical rate constant for chlorpyrifos $1.3 \times 10^{13} \text{ M}^{-1} \text{ h}^{-1}$ (Armbrust 2000).

Biodegradation:

$k = 0.014 \text{ d}^{-1}$ in soil at 28°C (Miles et al. 1979; quoted, Klečka 1985)
 $k = 0.008\text{--}0.025 \text{ d}^{-1}$ in soil at 25°C (Getzin 1981; quoted, Klečka 1985)
 $k = (-0.000945 \text{ to } -0.00243) \text{ h}^{-1}$ in nonsterile sediment and $k = (-0.000562 \text{ to } -0.00151) \text{ h}^{-1}$ in sterile sediment by shake-tests at Range Point and also $k = (-0.00109 \text{ to } -0.00231) \text{ h}^{-1}$ in nonsterile water and $k = (-0.00144 \text{ to } -0.00197) \text{ h}^{-1}$ in sterile water by shake-tests at Range Point (Walker et al. 1988)
 $t_{1/2} = 39\text{--}51$ d in loamy and clay soils under anaerobic conditions, $t_{1/2} = 150\text{--}200$ d in anaerobic pond sediments (Racke 1993)
 $k(\text{aerobic}) = 9.47 \times 10^{-4} \text{ h}^{-1}$ for exposure analysis (Armbrust 2000).

Biotransformation:

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

elimination $t_{1/2} = 3.3$ d in channel catfish (Barron et al. 1991)

$k_1 = 7000 \pm 2000$ L kg⁻¹ d⁻¹ (guppy, lipid-based modeling data, Deneer 1993)

$k_2 = (0.40 \pm 0.11)$ d⁻¹ (guppy, lipid-based modeling data, Deneer 1993)

$k_1 = (26 \pm 8.0) \times 10^3$ L kg⁻¹ d⁻¹ (stickleback, lipid-based lab data, Deneer 1994).

$k_2 = (1.2 \pm 0.4)$ d⁻¹ (stickleback, lipid-based lab data, Deneer 1994).

Half-Lives in the Environment:

Air: $t_{1/2} = 6.34$ h for the vapor phase reaction with hydroxyl radicals in air (Atkinson 1987; quoted, Howard 1991);
reaction rate $k = 4.77 \times 10^{-4}$ min⁻¹ in air (Paraiba et al. 1999).

Surface water: based on Henry's law constant, volatilization $t_{1/2} \sim 9.0$ 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: $t_{1/2} < 2.0$ d, indoor at 25°C with 12-h photo-period white fluorescent light, $t_{1/2} = 4.6$ d, outdoor-light (stoppered, Pyrex flasks exposed to ambient sunlight with temperature 22–45°C), $t_{1/2} = 7.1$ d, outdoor-dark (foil-covered flasks) and $t_{1/2} = 24$ d in an estuary (Schimmel et al. 1983; quoted, Montgomery 1993)

$t_{1/2} = 120$ d in water at pH 6.1, 20°C (quoted, Lartiges & Garrigues 1995);

reaction rate $k = 3.80 \times 10^{-4}$ min⁻¹ in water (Paraiba et al. 1999).

Ground water:

Sediment: $t_{1/2} = 24$ d in 10 g untreated sediment/100 mL of a pesticide-seawater solution and $t_{1/2} > 28$ d in 10 g sterile sediment/100 mL of a pesticide-seawater solution (Schimmel et al. 1983)

$t_{1/2} = 150$ –200 d in anaerobic pond sediments (Racke 1993)

reaction rate $k = 2.85 \times 10^{-5}$ min⁻¹ in sediment (Paraiba et al. 1999)

First-order degradation $k = 0.034$ d⁻¹ with $t_{1/2} = 20.3$ d under aerobic conditions, $k = 0.003$ d⁻¹ with $t_{1/2} = 223$ d under anaerobic conditions in sediment from San Diego Creek, Orange County, CA; first-order degradation $k = 0.029$ d⁻¹ with $t_{1/2} = 23.7$ d under aerobic conditions, $k = 0.012$ d⁻¹ with $t_{1/2} = 57.6$ d under anaerobic conditions in sediment from Bonita Creek, Orange County, CA (Bondarendo & Gan 2004)

Soil: $t_{1/2} = 17.0$ wk in sterile sandy loam and $t_{1/2} < 1.0$ wk in nonsterile sandy loam; $t_{1/2} > 24$ wk in sterile organic soil and $t_{1/2} = 2.5$ wk in nonsterile organic soil (Miles et al. 1979);

$t_{1/2} = 12$ and 24 wk in a silt loam and clay loam, $t_{1/2} = 24$ wk while in sterilized soils; however, temperature also had noticeable effects on decomposition as $t_{1/2} = 25$, 13, and 6 wk for soil samples incubated at 15, 25, and 35°C, respectively (Getzin 1981a; quoted, Montgomery 1993);

hydrolysis $t_{1/2} = 8$ d in Sultan silt loam (Getzin 1981b; quoted, Montgomery 1993);

$t_{1/2} = 80$ –100 d slowly degraded in soil (Hartley & Kidd 1987; quoted, Montgomery 1993);

$t_{1/2} = 63$ d from screening model calculations (Jury 1987b);

persists in soil for 60–120 d (Worthing & Hance 1991);

Selected field $t_{1/2} = 30$ d (Wauchope et al. 1992; quoted, Dowd et al. 1993; Richards & Baker 1993; Hornsby et al. 1996);

$t_{1/2} = 30$ d (Pait et al. 1992);

Field dissipation $t_{1/2} = 39$ –51 d in loamy and clay soils under anaerobic conditions; and aerobic solid degradation $t_{1/2} = 5$ –141 d (Racke 1993)

$t_{1/2}$ = of 60–120 d (Tomlin 1994)

Dissipation $t_{1/2} \leq 7$ d when applied to dry soils or the soil surface ($t_{1/2} = 7$ –14 d); and $t_{1/2} = 30$ –60 d when incorporated into the soil profile (Racke et al. 1996)

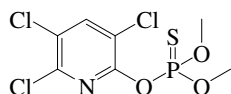
First order rate constants for photolytic decline in sandy soil: $k = 2.91 \times 10^{-3}$ h⁻¹ with $t_{1/2} = 240$ h irradiated in moisture-maintained, $k = 2.06 \times 10^{-3}$ h⁻¹ with $t_{1/2} = 340$ h, irradiated in air-dried $k = 1.67 \times 10^{-3}$ h⁻¹ with $t_{1/2} = 420$ h in dark control moist and $k = 0.99 \times 10^{-3}$ h⁻¹ with $t_{1/2} = 700$ h in dark control air-dried sandy soil from Sauk County, WI. The photolytic $k = 8.43 \times 10^{-4}$ h⁻¹ with $t_{1/2} = 820$ h in moist soil, $k = 1.07 \times 10^{-3}$ h⁻¹ with $t_{1/2} = 650$ h in dry soil. The contribution of moisture to irradiated metabolism $k = 1.24 \times 10^{-3}$ h⁻¹ with $t_{1/2} = 560$ h, but for dark control system for $k = 6.78 \times 10^{-4}$ h⁻¹ with $t_{1/2} = 1020$ h (Graebing & Chib 2004)

Biota: $t_{1/2} = 335$ h clearance from fish (Neely 1980);

biochemical $t_{1/2} = 63$ d from screening model calculations (Jury et al. 1987b);

elimination $t_{1/2} \sim 3.3$ 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 ($^{\circ}C$):

43 (Lide 2003)

Boiling Point ($^{\circ}C$):

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 $25^{\circ}C$ (assuming $\Delta S_{fus} = 56 J/mol K$), F : 0.666 (mp at $43^{\circ}C$)

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$):

4.76	($20^{\circ}C$, shake flask-GC, Chiou et al. 1977)
0.40	(Spencer 1982)
4.0	(Kenaga 1980a, b, Kenaga & Goring 1980)
3.2	($20^{\circ}C$, shake flask, Bowman & Sans 1983b)
4.0	($24^{\circ}C$, Hartley & Kidd 1987; Tomlin 1994)
4.0	(selected, 20 – $25^{\circ}C$, Augustijn-Beckers et al. 1994; Hornsby et al. 1996)

Vapor Pressure (Pa at $25^{\circ}C$):

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 ($Pa \cdot m^3/mol$ at $25^{\circ}C$):

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, $t_{1/2}$:

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), $t_{1/2} = 3$ 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 $t_{1/2} \sim 38$ 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), $t_{1/2} = 3$ d at pH 8 (Tomlin 1994).

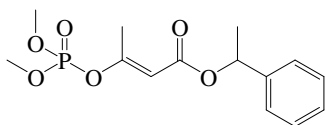
Ground water:

Sediment:

Soil: field $t_{1/2} = 7$ d (Augustijn-Beckers et al. 1994; Hornsby et al. 1996); $t_{1/2} = 1.5$ 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: C₁₄H₁₉O₆P

Molecular Weight: 314.271

Melting Point (°C): liquid

Boiling Point (°C):

135 (at 0.03 mmHg, Montgomery 1993)

Density (g/cm³ at 20°C):

1.2 (Spencer 1982)

1.19 (25°C, Montgomery 1993)

Molar Volume (cm³/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/m³ 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·m³/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 al. 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)

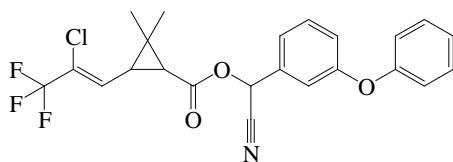
2.00; 2.07, 2.59 (soil, quoted obs.; estimated-class-specific model, estimated-general model using molecular descriptors, Gramatica et al. 2000)

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

Half-Lives in the Environment:

Surface water: biodegradation $t_{1/2} = 7.5$ d at pH 9 and $t_{1/2} = 22.5$ 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-trifluoroprop-1-en-1-yl)-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 ($^{\circ}C$):

yellow to brown viscous oil (technical, Hartley & Kidd 1987; Tomlin 1994)

Boiling Point ($^{\circ}C$):

187–190/0.2 mmHg (Hartley & Kidd 1987; Tomlin 1994)

Density (g/cm^3):

1.25 (25 $^{\circ}C$, 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 $^{\circ}C$, F: 1.0

Water Solubility (g/m^3 or mg/L at 25 $^{\circ}C$ or as indicated):

< 1.0 (Worthing & Walker 1983)

0.003 (20 $^{\circ}C$, Hartley & Kidd 1987; Worthing & Walker 1987)

0.004 (20 $^{\circ}C$, Tomlin 1994)

Vapor Pressure (Pa at 25 $^{\circ}C$ or as indicated):

$\sim 1.0 \times 10^{-6}$ (20 $^{\circ}C$, Hartley & Kidd 1987)

0.001×10^{-3} (20 $^{\circ}C$, Tomlin 1994)

1.90×10^{-5} (40 $^{\circ}C$, Knudsen effusion method, Goodman 1997)

$\log(P/Pa) = 13.47 - 5723/(T/K)$ (Antoine eq., measured range 45–85 $^{\circ}C$, Goodman 1997)

1.51×10^{-5} (P^S , GC-RT correlation, Tsuzuki 2001)

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

Octanol/Water Partition Coefficient, $\log K_{ow}$:

6.02 (HPLC-RT correlation, Hu & Leng 1992)

6.80 (20 $^{\circ}C$, Tomlin 1994)

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

Bioconcentration Factor, $\log BCF$ or $\log K_B$:

Sorption Partition Coefficient, $\log K_{OC}$:

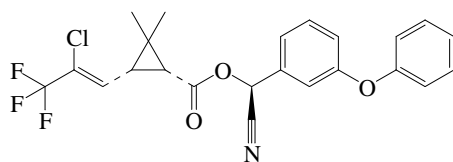
Environmental Fate Rate Constants, k , and Half-Lives, $t_{1/2}$:

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*)-(*1R,3R*)-3-(2-chloro-3,3,3-trifluoropropyl)-2,2-dimethylcyclopropanecarboxylate and (*S*)- α -cyano-3-phenoxybenzyl(*Z*)-(*1S,3S*)-3-(2-chloro-3,3,3-trifluoropropyl)-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 ($^{\circ}C$):

49.2 (Hartley & Kidd 1987; Tomlin 1994; Lide 2003)

Boiling Point ($^{\circ}C$):

Density (g/cm^3):

1.33 ($25^{\circ}C$, 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 $25^{\circ}C$ (assuming $\Delta S_{fus} = 56\ J/mol\ K$), F : 0.579 (mp at $49.2^{\circ}C$)

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$ or as indicated):

0.005 ($20^{\circ}C$, 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 $25^{\circ}C$ 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} ($20^{\circ}C$, Hartley & Kidd 1987)

2.0×10^{-7} , 2.0×10^{-4} (20 , $60^{\circ}C$, Tomlin 1994)

$7.80 \times 10^{-6*}$ ($40^{\circ}C$, Wollerton & Husband 1988, quoted in Goodman 1997)

$19 \times 10^{-6*}$ ($40^{\circ}C$, Knudsen effusion method, measured range 40 – $80^{\circ}C$, Goodman 1997)

1.88 (extrapolated-Antoine eq., Goodman 1997)

$\log(P/kPa) = 13.47 - 5723/(T/K)$; temp range 40 – $80^{\circ}C$ (Antoine eq., Knudsen effusion, Goodman 1997)

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

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

7.0 ($20^{\circ}C$, 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}:

Half-Lives in the Environment:

- Air:
- Surface water:
- Ground water:
- Sediment: t_{1/2} ~ 20 d in water-sediment mixture in sunlight (Tomlin 1994).
- Soil: t_{1/2} ~ 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)
$\log P = A - B/(C + t/^{\circ}C)$		(2)	$\ln P = A - B/(C + t/^{\circ}C)$	(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	

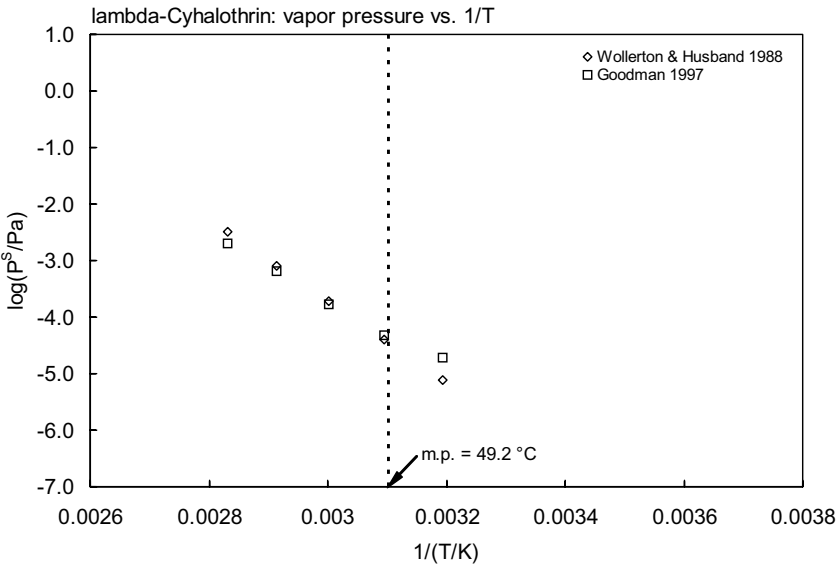
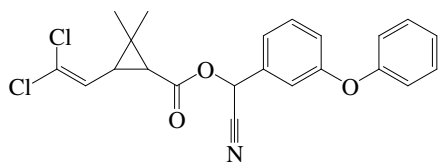


FIGURE 18.1.1.19.1 Logarithm of vapor pressure versus reciprocal temperature for lambda-cyhalothrin.

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 ($^{\circ}C$):

70 (Lide 2003)

Boiling Point ($^{\circ}C$):

Density (g/cm^3 at $20^{\circ}C$):

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 $25^{\circ}C$ (assuming $\Delta S_{fus} = 56$ J/mol K), F: 0.362 (mp at $70^{\circ}C$)

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$ or as indicated):

0.041 (shake flask-GC, Coats & O'Donnell-Jefferey 1979)

0.005–0.01 (Stephenson 1982)

0.010 ($20^{\circ}C$, Hartley & Kidd 1987)

0.01–0.2 ($21^{\circ}C$, Worthing & Walker 1987)

0.004 (20 – $25^{\circ}C$, selected, Wauchope 1989; Wauchope et al. 1992; Hornsby et al. 1996)

0.004 (Montgomery 1993)

0.004 (at pH 7, Tomlin 1994)

0.009 ($20^{\circ}C$, selected, Siebers & Mattusch 1996)

Vapor Pressure (Pa at $25^{\circ}C$ 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} ($70^{\circ}C$, Hartley & Kidd 1987)

2.4×10^{-6} (GC-RT correlation, supercooled liquid P_L , Hinckley et al. 1990)

1.9×10^{-7} (20 – $25^{\circ}C$, selected, Wauchope et al. 1992; Hornsby et al. 1996)

1.9×10^{-7} ($20^{\circ}C$, extrapolated, Montgomery 1993)

2.3×10^{-7} ($20^{\circ}C$, 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} ($20^{\circ}C$, 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 ($\text{Pa}\cdot\text{m}^3/\text{mol}$) 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	(<i>cis</i> -form, HPLC-RT correlation, Muir et al. 1985)
5.0 ± 0.6	(<i>trans</i> -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, $\log \text{BCF}$:

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	(<i>trans</i> -form on sediment, 24 h BCF for chironomid larvae in water, Muir et al. 1985)
1.63–2.39	(<i>trans</i> -form on sediment, 24 h BCF for chironomid larvae in sediment, Muir et al. 1985)
1.49–2.05	(<i>trans</i> -form on sediment, 24 h BCF for chironomid larvae in sediment/pore water, Muir et al. 1985)
1.53–2.38	(<i>cis</i> -form on sediment, 24 h BCF for chironomid larvae in water, Muir et al. 1985)
1.84–2.59	(<i>cis</i> -form on sediment, 24 h BCF for chironomid larvae in sediment, Muir et al. 1985)
1.68–2.02	(<i>cis</i> -form on sediment, 24 h BCF for chironomid larvae in sediment/pore water, Muir et al. 1985)
2.89	(<i>Oncorhynchus mykiss</i> , Muir et al. 1994; quoted, Devillers et al. 1996)
2.92	(<i>Oncorhynchus mykiss</i> , Muir et al. 1994; quoted, Devillers et al. 1996)

Sorption Partition Coefficient, $\log K_{oc}$:

2.36	(<i>cis</i> -form, silt, K_p on 24% DOC, Muir et al. 1985)
2.57	(<i>cis</i> -form, clay, K_p on 56% DOC, Muir et al. 1985)
2.59	(<i>trans</i> -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).

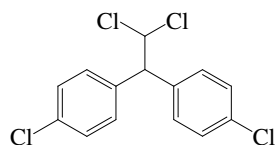
Ground water:

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: C₁₄H₁₀Cl₄

Molecular Weight: 321.041

Melting Point (°C):

109.5 (Ballschmiter & Wittlinger 1991; Kühne et al. 1995; Lide 2003)

Boiling Point (°C):

Density (g/cm³ at 20°C):

Molar Volume (cm³/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/m³ 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/(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·m³/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)
 $\log[H/(Pa \text{ m}^3/\text{mol})] = 12.20 - 3168/(T/K)$ (*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 $t_{1/2} = 13.3\text{--}133$ 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 $(2.8 \pm 0.9) \times 10^{-6} \text{ h}^{-1}$ and $5.2 \text{ M}^{-1} \text{ h}^{-1}$ (Ellington et al. 1987, 1988, 1989; quoted, Howard et al. 1991);
 rate constant $k = 2.5 \times 10^{-2} \text{ yr}^{-1}$ at pH 7 and 25°C (Kollig 1993).

Biodegradation: aqueous aerobic $t_{1/2} = 2\text{--}15.6$ 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 $t_{1/2} = 70\text{--}294$ 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:

$k_1 = 52.9 \text{ h}^{-1}$; $k_2 = 0.0058 \text{ h}^{-1}$ (mussel, Ernst 1977; quoted, Hawker & Connell 1986)

Half-Lives in the Environment:

Air: $t_{1/2} = 17.7\text{--}177$ h, based on estimated photooxidation half-life in air (Howard et al. 1991).

Surface water: $t_{1/2} = 2\text{--}15.6$ 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 $k = 5.0 \times 10^{-2} \text{ h}^{-1}$ with $t_{1/2} = 13.9$ h for 1.0 ppm *p,p'*-DDD and $k = 0.76 \times 10^{-2} \text{ h}^{-1}$ with $t_{1/2} = 96.3$ h for *o,p'*-DDD both at $21 \pm 2^\circ\text{C}$ 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: $t_{1/2} = 1680\text{--}270,000$ 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: $t_{1/2} = 2\text{--}15.6$ 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);

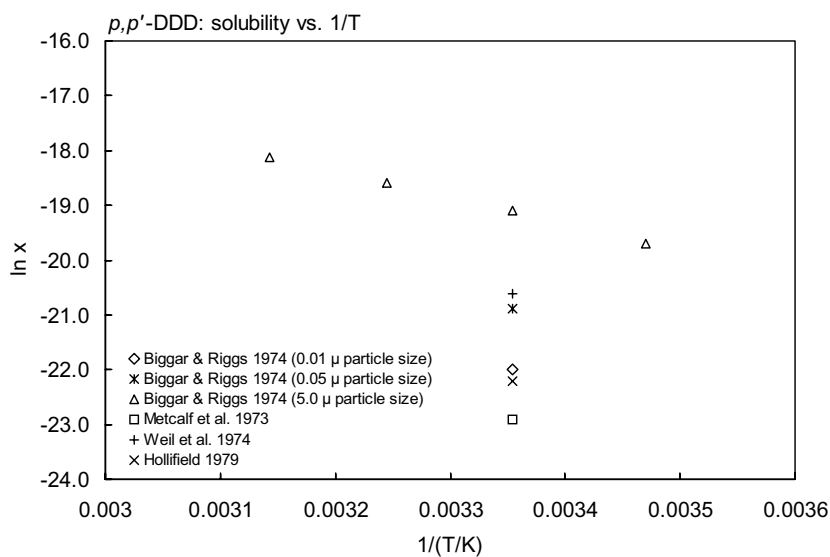
estimated field $t_{1/2} \sim 1000$ d (20–25°C, Hornsby et al. 1996).

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}	
<i>p,p'</i> -DDD			<i>o,p</i> -DDD			<i>p,p'</i> -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.

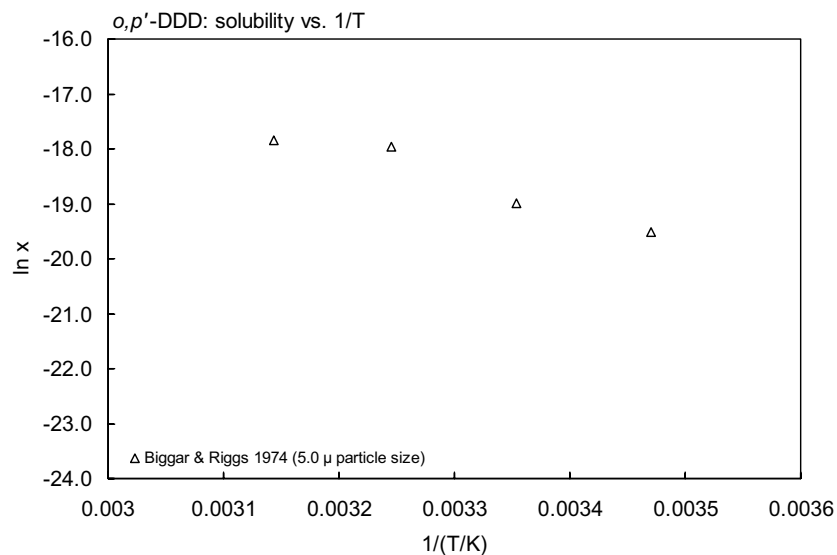


FIGURE 18.1.1.21.1B Logarithm of mole fraction solubility ($\ln x$) versus reciprocal temperature for *o,p'*-DDD.

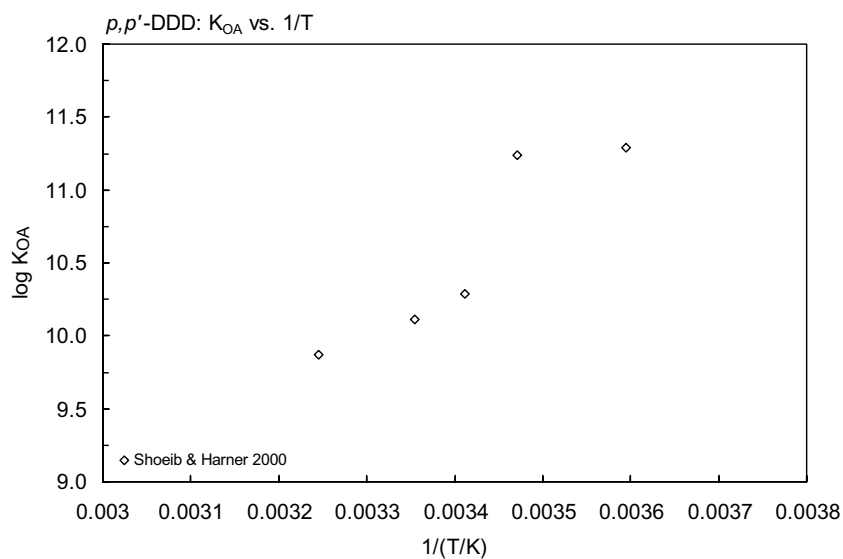
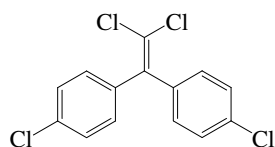


FIGURE 18.1.1.21.2 Logarithm of K_{OA} versus reciprocal temperature for *p,p'*-DDD.

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 ($^{\circ}C$):

89 (Lide 2003)

Boiling Point ($^{\circ}C$):

Density (g/cm^3 at $20^{\circ}C$):

Molar Volume (cm^3/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 $25^{\circ}C$ (assuming $\Delta S_{fus} = 56$ J/mol K, F: 0.236 (mp at $89^{\circ}C$))

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$ 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 $15-45^{\circ}C$, Biggar & Riggs 1974)

0.014 (generator column-GC/ECD, Weil et al. 1974)

0.040 ($20^{\circ}C$, 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 ($30^{\circ}C$, semimicro gas-saturation method, Westcott et al. 1981)

0.0011, 0.006 (generator column-GC, HPLC-RT correlation, Swann et al. 1983)

$\log [S_L/(mol/L)] = 0.173 - 1263/(T/K)$ (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 $25^{\circ}C$ or as indicated and reported temperature dependence equations):

p,p'-DDE

8.65×10^{-4} ($30^{\circ}C$, gas saturation-vapor density-GC, Spencer & Cliath 1972)

9.87×10^{-4} (GC-RT correlation, Westcott & Bidleman 1981)

1.73×10^{-4} ($30^{\circ}C$, 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)
 $\log(H/(Pa \text{ m}^3/\text{mol})) = 12.62 - 3291/(T/K)$ (*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, $t_{1/2}$:

Volatilization:

Photolysis: midday $t_{1/2} = 5$ h in hydrocarbon media (Zepp et al. 1976)

$t_{1/2} = 1.5$ d under sunlight in water (Mansour & Feicht 1994).

Oxidation:

Hydrolysis: the first-order rate constant $k = 1.4 \times 10^{-9} \text{ M}^{-1} \text{ s}^{-1}$ and the hydrolytic $t_{1/2} > 120$ yr in water at 27°C (Wolfe et al. 1977);

hydrolytic $t_{1/2} = 120$ yr at pH 7 and 25°C of 120 yr and a rate constant $k = 6.6 \times 10^{-7} \text{ h}^{-1}$ (Callahan et al. 1979, Mabey et al. 1982).

Biodegradation:

Biotransformation:

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

$k_1 = 170.0 \text{ d}^{-1}$; $k_2 = 0.021 \text{ d}^{-1}$ (*p,p'*-DDE, rainbow trout, Oliver & Niimi 1985)

$k_2 = 0.950 \text{ yr}^{-1}$ (*Larus argentatus*, Norstrom et al. 1986)
 $k_1 = 20800 \text{ d}^{-1}$; $k_2 = 0.020 \text{ d}^{-1}$ (*Oligochaetes*, Connell et al. 1988)
 $k_2 = 0.0004 \text{ h}^{-1}$ (azalea leaves, Paterson et al. 1991)
 $k_2 = 0.0030 \text{ h}^{-1}$ (midge *C. riparius*, water only system, Lydy et al. 1992)
 $k_2 = 0.0046 \text{ h}^{-1}$ (midge *C. riparius*, screened, Lydy et al. 1992)
 $k_2 = 0.0080 \text{ h}^{-1}$ (midge *C. riparius*, 3% organic carbon, Lydy et al. 1992)
 $k_2 = 0.0046 \text{ h}^{-1}$ (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 $t_{1/2} = 5 \text{ h}$ in hydrocarbon media (Zepp et al. 1976)

hydrolytic $t_{1/2} > 120 \text{ yr}$ in water at 27°C (Wolfe et al. 1977);

estimated $t_{1/2} = 690 \text{ d}$ in surface waters in case of first order reduction process, and estimated $t_{1/2} > 300 \text{ d}$ in lakes in the Netherlands (Zoeteman et al. 1980);

photolysis $t_{1/2} = 1.5 \text{ d}$ under sunlight in water (Mansour & Feicht 1994).

Ground water:

Sediment:

Soil: field $t_{1/2} = 1000 \text{ d}$ (estimated, Hornsby et al. 1996);

$t_{1/2} > 20 \text{ yr}$, 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 $t_{1/2} = 340 \text{ d}$ (*p,p'*-DDE, rainbow trout, Oliver & Niimi 1985);

$t_{1/2} = 264 \text{ d}$ in herring gulls compared to literature average $t_{1/2} = 300 \text{ d}$ for birds (Norstrom et al. 1986);

elimination $t_{1/2} = 2230 \text{ h}$ (Azalea leaves, Bacci & Gaggi 1987);

$t_{1/2} = 231 \text{ h}$ in the midge (*Chironomus riparius*) under varying sediment conditions (water only system with no sediment), $t_{1/2} = 150 \text{ h}$ (midge screened from the sediment), $t_{1/2} = 87 \text{ h}$ (midge screened from 3% organic carbon sediment), $t_{1/2} = 99 \text{ h}$ (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

<i>p,p'</i> -DDE				<i>o,p'</i> -DDE			
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	S/g·m ⁻³	S/g·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			

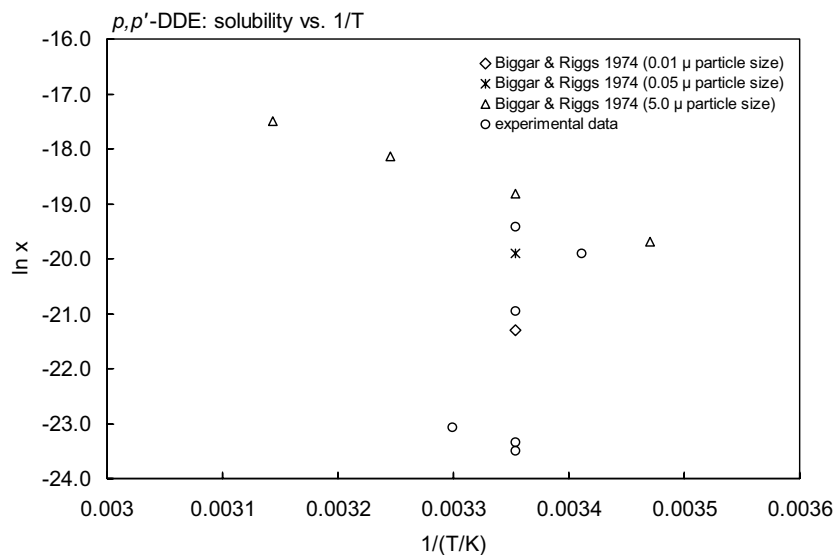


FIGURE 18.1.1.22.1A Logarithm of mole fraction solubility ($\ln x$) versus reciprocal temperature for *p,p'*-DDE.

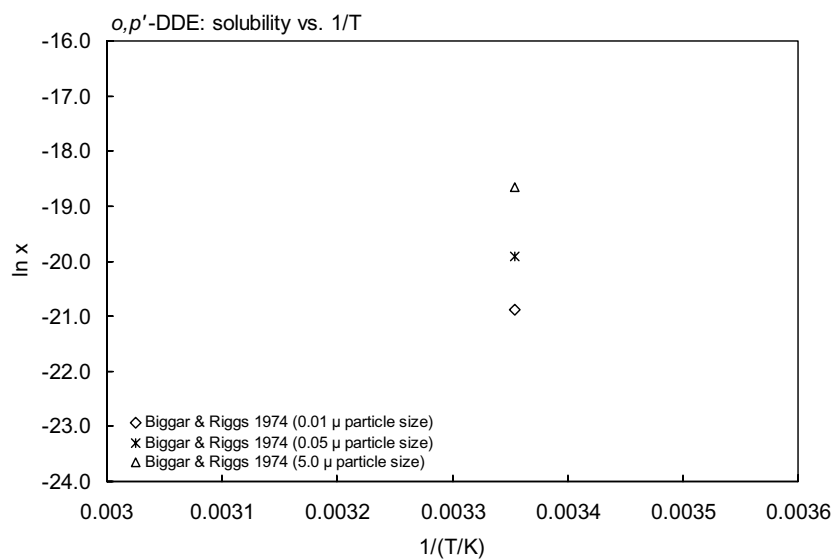
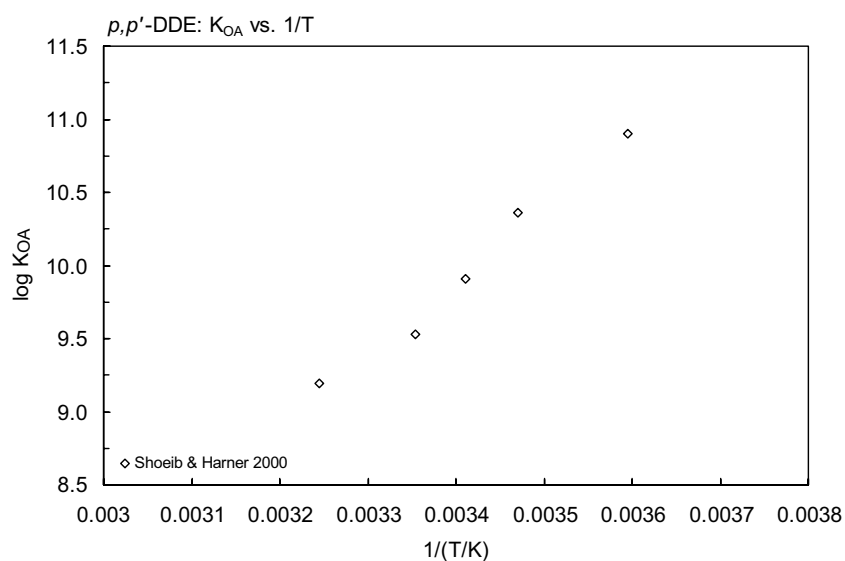


FIGURE 18.1.1.22.1B Logarithm of mole fraction solubility ($\ln x$) versus reciprocal temperature for *o,p'*-DDE.

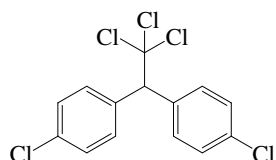
TABLE 18.1.1.22.2

Reported octanol-air partition coefficient of *p,p'*-DDE at various temperaturesShoeib & 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 ($^{\circ}C$):

108.5 (Lide 2003)

Boiling Point ($^{\circ}C$):

260 (Lide 2003)

Density (g/cm^3 at $20^{\circ}C$):

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 $25^{\circ}C$, F:

0.147 (assuming $\Delta S_{fus} = 56$ J/mol K., Mackay et al. 1986)

0.130 ($20^{\circ}C$, assuming $\Delta S_{fus} = 56$ J/mol K, Suntio et al. 1988)

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$ 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 ($15^{\circ}C$, shake flask-bioassay, Richards & Cutkomp 1946)

0.0374 (shake flask-radiometric method, measured range 2 – $37.5^{\circ}C$, 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, 5.0 μ 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 (Verschuere 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)
 $\log [S_L/(\text{mol/L})] = -0.195 - 1454/(T/K)$ (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)
 $\log (P/\text{mmHg}) = 14.191 - 6160/(T/K)$, temp range 66–100°C (Antoine eq., effusion, Balson 1947)
 $\log (P/\text{mmHg}) = 13.778 - 6010/(T/K)$; 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)
 $\log (P/\text{mmHg}) = 14.24 - 6176/(T/K)$; 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)
 $\log (P_L/Pa) = (12.38 \pm 0.48) - (4665 \pm 166)/(T/K)$; $\Delta S_{fus} = 70.9 \text{ J mol}^{-1} \text{ K}^{-1}$ (*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 ($\text{Pa} \cdot \text{m}^3/\text{mol}$ 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)
 $\log (H/(\text{Pa m}^3/\text{mol})) = 13.02 - 3369/(T/K)$ (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 \pm 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 \pm 0.030 (p,p' -, shake flask/slow-stirring method, De Bruijn et al. 1989; received highest ranking from Pontolillo & Eganhouse 2001)
- 6.307 \pm 0.045; 6.914 \pm 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*; *Amphidarium 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 \pm 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 \geq 0.5%, Delle Site 2001)
 5.63, 5.54 (*p,p'*-DDT, soils: organic carbon OC \geq 0.1%, OC \geq 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, $t_{1/2}$:

Volatilization: $t_{1/2} = 3.7$ d for water depth of 1 m (Mackay & Wolkoff 1973);

$t_{1/2} = 73.9$ h (Mackay & Leinonen 1975, Branson 1978);

initial rate constant $k = 6.9 \times 10^{-4} \text{ h}^{-1}$ and predicted rate constant $k = 1.2 \times 10^{-3} \text{ h}^{-1}$ from soil with $t_{1/2} = 578$ h;

$t_{1/2}(\text{calc}) = 45$ 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 $k = 8.5 \times 10^{-8} \text{ s}^{-1}$ with $t_{1/2} > 227000$ h in water, $t_{1/2} = 280000$ h in hydrocarbon media; midday $t_{1/2} > 460000$ h (52.5 yr) average over all seasons in water at latitude 40°N , daily average direct photolysis $t_{1/2} > 150$ 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: $t_{1/2} = 22$ yr, estimated first-order half-life in aquatic environment (Callahan et al. 1979)

$k < 3600 \text{ M}^{-1} \text{ h}^{-1}$ for singlet oxygen, $k = 3600 \text{ M}^{-1} \text{ h}^{-1}$ for RO_2 (Mabey et al., 1982)

photooxidation $t_{1/2} = 17.7$ –177 h in air, based on estimated rate constant for the reaction with hydroxyl radicals in air (Howard et al. 1991).

photooxidation $t_{1/2} = 168$ –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: $k(\text{alkaline}) = 9.90 \times 10^{-3} \text{ M}^{-1} \text{ s}^{-1}$ at 27°C corresponds to $t_{1/2} = 81$ d at pH 9, $k(\text{neutral}) = 1.9 \times 10^{-9} \text{ s}^{-1}$ corresponds to $t_{1/2} = 12$ yr in 5% acetonitrile-water at pH 5 and 27°C (Wolfe et al. 1977b)

$k(\text{alkaline}) = 9.90 \times 10^{-3} \text{ M}^{-1} \text{ s}^{-1}$ at pH 9, $k(\text{neutral}) = 1.9 \times 10^{-9} \text{ s}^{-1}$ for $1 \times 10^{-8} \text{ M}$ in water at 27°C (Harris 1982)

$k = 1.57 \times 10^{-4} \text{ h}^{-1}$ at pH 7 (Neely & Blau 1985)

$k = 6.0 \times 10^{-2} \text{ yr}^{-1}$ at pH 7.0 and 25°C (Kollig 1993).

Biodegradation: $t_{1/2}(\text{aq. aerobic}) = 2$ –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)

$t_{1/2}(\text{aq. anaerobic}) = 16$ –100 d, based on anaerobic flooded soil die-away data for two flooded soils (Castro & Yoshida 1971; quoted, Howard et al. 1991)

$t_{1/2} = 3837$ d (Hamaker 1972; quoted, Jury et al. 1983, 1984, 1987a, b, Jury & Ghodrati 1989)

$k = 0.00013 \text{ d}^{-1}$ from soil incubation studies, and $k = 0.0035 \text{ d}^{-1}$ from flooded soil incubation studies in anaerobic system both by die-away test (Rao & Davidson 1980; quoted, Scow 1982)

$t_{1/2}(\text{aq. aerobic}) = 2$ –15.6 yr, based on aerobic degradation in soil; $t_{1/2}(\text{aq. anaerobic}) = 16$ –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:

$k_2 = 0.002, 0.0007 \text{ h}^{-1}$ (algae, daphnids, Ellgehausen et al. 1980)

$k_2 = 0.052 \text{ d}^{-1}$ (catfish, Ellgehausen et al. 1980)

$k_1 = 170 \text{ d}^{-1}$; $k_2 = 0.0021 \text{ d}^{-1}$ (rainbow trout, Oliver & Niimi 1985)

$k_1 = 818 \text{ d}^{-1}$; $k_2 = 0.009 \text{ d}^{-1}$ (rainbow trout, Muir et al. 1985)

$k_2 = 8.60 \text{ yr}^{-1}$; $k_2 = 4.50 \text{ yr}^{-1}$ (*P. hoyi*, Evans et al. 1991)

$k_1 = 20609 \text{ d}^{-1}$; $k_2 = 1.845 \text{ d}^{-1}$ (algae *Selenastrum capricornutum*, Wang et al. 1996)

$k_1 = 135.6 \text{ d}^{-1}$; $k_2 = 0.191 \text{ d}^{-1}$ (water flea *Daphnia magna*, Wang et al. 1996)

$k_1 = 9.761 \text{ d}^{-1}$; $k_2 = 0.002 \text{ d}^{-1}$ (catfish *Ictalurus melas*, Wang et al. 1996)

Half-Lives in the Environment:

Air: $t_{1/2} = 17.7$ –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. $t_{1/2} = 17.0 \pm 6.8$ yr at Eagle Harbor, $t_{1/2} = 8.2 \pm 1.4$ yr at Sleeping Bear Dunes and $t_{1/2} = 7.1 \pm 1.0$ yr at Sturgeon Point (Buehler et al. 2004).

Surface water: dehydrochlorination rate constant $k = 1.75 \times 10^{-2} \text{ h}^{-1}$ for 1 ppm *p,p'*-DDT and $k = 1.65 \times 10^{-2} \text{ h}^{-1}$ for 1 ppm *o,p'*-DDT both at $21 \pm 2^\circ\text{C}$ and pH 12.8, in 0.1 N NaOH solution (Choi & Chen 1976);

degradation $t_{1/2} = 8$ yr in water at 27°C (Wolfe et al. 1977);

midsummer direct photolysis $t_{1/2} > 227000$ h in water, $t_{1/2} = 280000$ h in hydrocarbon media; midday $t_{1/2} > 460000$ h (52.5 yr) average over all seasons in water at latitude 40°N , daily average direct photolysis $t_{1/2} > 150$ yr (12-h days) in water in the Central U.S. (Zepp et al. 1976)

- $t_{1/2} = 73.9$ h for a pond 1 m deep (Branson 1978);
 $t_{1/2} = 168$ –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 $t_{1/2} = 110$ 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 $t_{1/2} \sim 10$ yr average from the loss rates in Lake Michigan (Bierman & Swain 1982).
 Ground water: $t_{1/2} = 16$ 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: $t_{1/2} = 3$ to 5 yr (Bierman & Swain 1982); $t_{1/2} = 21$ yr (conversion of *p,p'*-DDT to *p,p'*-DDE in sediment, Oliver et al. 1989); $t_{1/2} = 78800$ h (quoted mean value from Howard et al. 1991, Mortimer & Connell 1995).
 Soil: $t_{1/2} = 2$ –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 $t_{1/2} \sim 12$ 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 $t_{1/2} = 173$ d when incorporated into soil (Willis et al. 1971; quoted, Nash 1983);
 microagroecosystem $t_{1/2} > 50$ d with open cotton canopy (quoted, Nash 1983);
 persistence of more than 36 months (Wauchope 1978);
 $t_{1/2} > 50$ d and subject to plant uptake via volatilization (Callahan et al. 1979; quoted, Ryan et al. 1988);
 estimated first-order $t_{1/2} = 14.6$ yr from biodegradation rate constant $k = 0.00013$ d⁻¹ from soil incubation studies and $t_{1/2} = 198$ 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 $t_{1/2} > 100$ d (Willis & McDowell 1982);
 microagroecosystem $t_{1/2} > 50$ d in moist fallow soil (Nash 1983);
 $t_{1/2} = 3837$ d from screening model calculations (Jury et al. 1984, 1987a, b; Jury & Ghorati 1989);
 $t_{1/2} = 173$ d from field study, $t_{1/2} > 50$ d from microagroecosystem, $t_{1/2} = 116$ d from laboratory data (Nash 1985);
 $t_{1/2} = 3800$ d (Jury et al. 1987; quoted, Montgomery 1993);
 reaction $t_{1/2} = 3837$ d and overall $t_{1/2} =$ in soil 9.4 yr (Mackay & Stiver 1991);
 estimated field $t_{1/2} = 2000$ d (Augustijn-Beckers et al. 1994; Hornsby et al. 1996);
 $t_{1/2} = 14.0$ and 12.0 yr for control and sludge-amended Luddington soils, respectively, for *o,p'*-DDT, and $t_{1/2} = 11.8$ and 10.5 yr for control and sludge-amended Luddington soils, respectively, for *p,p'*-DDT (Meijer et al. 2001).
 Biota: field $t_{1/2} = 15$ d in fruit leaves (Decker et al. 1950; quoted, Nash 1983);
 microagroecosystem $t_{1/2} = 29$ d in cotton leaves (Nash & Harris 1977; quoted, Nash 1983);
 $t_{1/2} = 915$ h from fish compared with calculated value of $t_{1/2} = 517$ h from regression (Neely 1980);
 $t_{1/2} = 0.70$ h in algae, $t_{1/2} = 3.65$ d in catfish and $t_{1/2} = 315$ h in daphnids (Ellgehausen et al. 1980);
 $t_{1/2} = 340$ d in rainbow trout (Oliver & Niimi 1985);
 biochemical $t_{1/2} = 3837$ d (Jury et al. 1987a, b; Jury & Ghodrati 1989);
 biological $t_{1/2} = 77$ d for trout, $t_{1/2} = 31$ d for salmon, $t_{1/2} = 4$ d for catfish (Niimi 1987).

TABLE 18.1.1.23.1
Reported aqueous solubilities of DDT at various temperatures

<i>p,p'</i> -DDT				<i>o,p'</i> -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

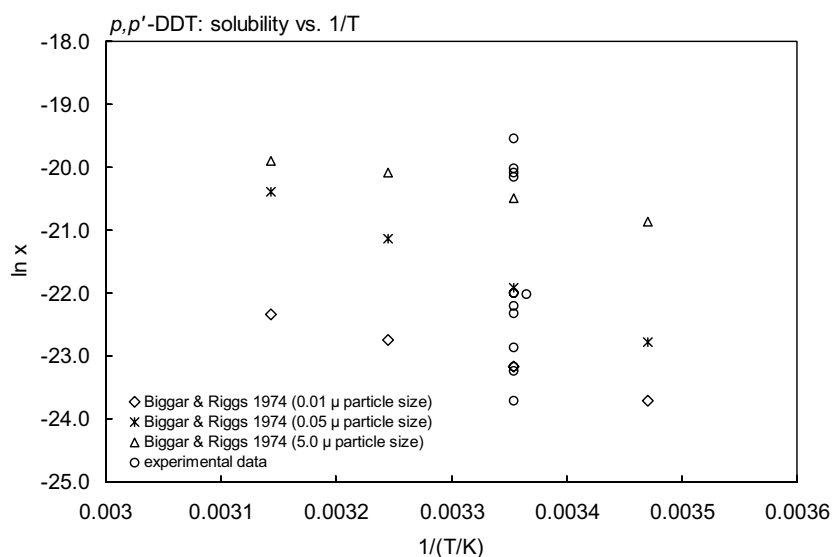


FIGURE 18.1.1.23.1A Logarithm of mole fraction solubility ($\ln x$) versus reciprocal temperature for *p,p'*-DDT.

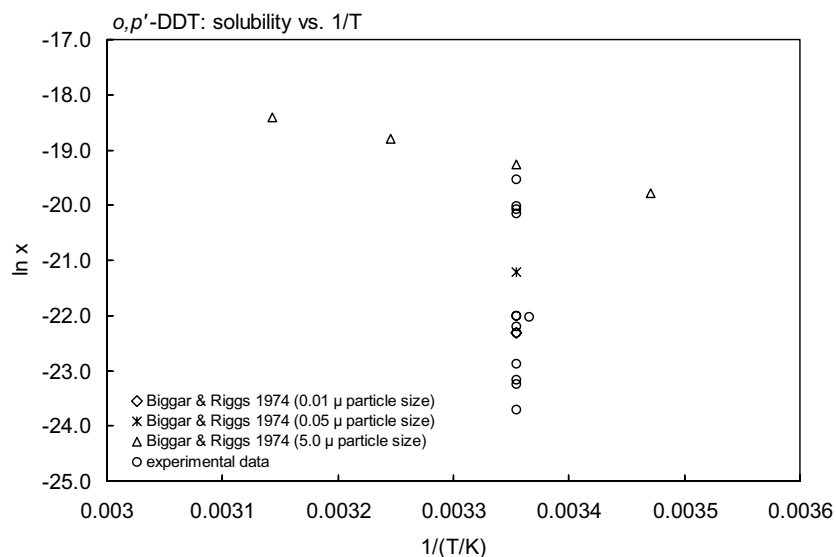


FIGURE 18.1.1.23.1B Logarithm of mole fraction solubility ($\ln x$) versus reciprocal temperature for *o,p'*-DDT.

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)
$\log P = A - B/(C + t/^{\circ}\text{C})$	(2)	$\ln P = A - B/(C + t/^{\circ}\text{C})$	(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/ $^{\circ}\text{C}$	P/Pa	t/ $^{\circ}\text{C}$	P/Pa	t/ $^{\circ}\text{C}$	P/Pa	t/ $^{\circ}\text{C}$	P/Pa
<i>p,p'</i> -DDT		<i>p,p'</i> -DDT		<i>p,p'</i> -DDT		<i>p,p'</i> -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	<i>o,p'</i> -DDT			
90	0.224	50.1	0.002027	30	7.37×10^{-4}	$\Delta H_{\text{sub}} = 100.6 \text{ kJ/mol}$	
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 $^{\circ}\text{C}$		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
<i>o,p'</i> -DDT					
30	1.17 × 10 ⁻³	<i>o,p'</i> -DDT		<i>p,p'</i> -DDT	
		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
		<i>p,p'</i> -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	

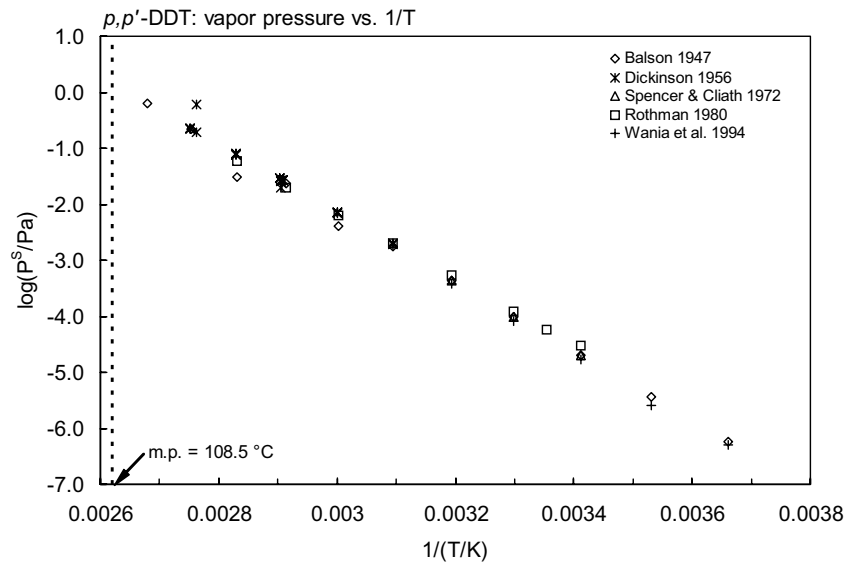
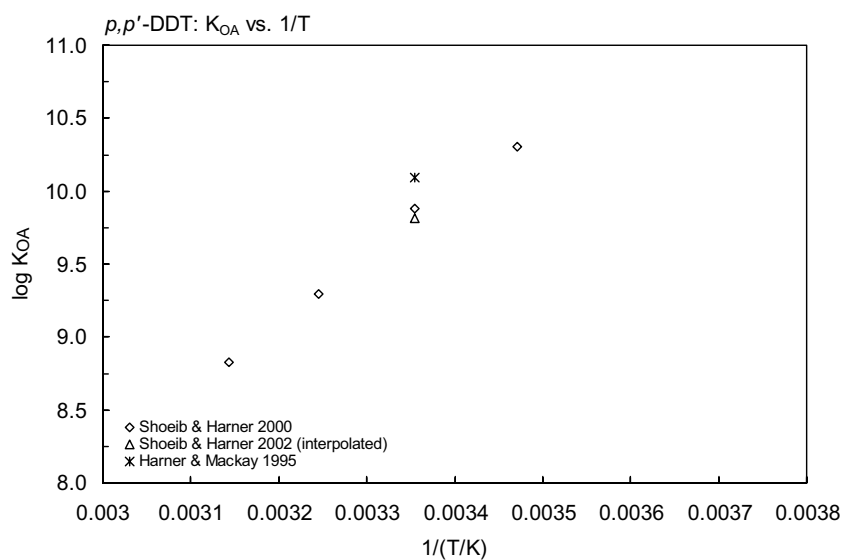


FIGURE 18.1.1.23.2 Logarithm of vapor pressure versus reciprocal temperature for *p,p'*-DDT.

TABLE 18.1.1.23.3

Reported octanol-air partition coefficients of DDT at various temperatures

<i>p,p'</i> -DDT				<i>o,p'</i> -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		$\Delta H_{OA}/(\text{kJ mol}^{-1}) = 88.1$		$\Delta H_{OA}/(\text{kJ mol}^{-1}) = 87.9$	
$\Delta H_{OA}/(\text{kJ mol}^{-1}) = 75.7$					

FIGURE 18.1.1.23.3A Logarithm of K_{OA} versus reciprocal temperature for *p,p'*-DDT.

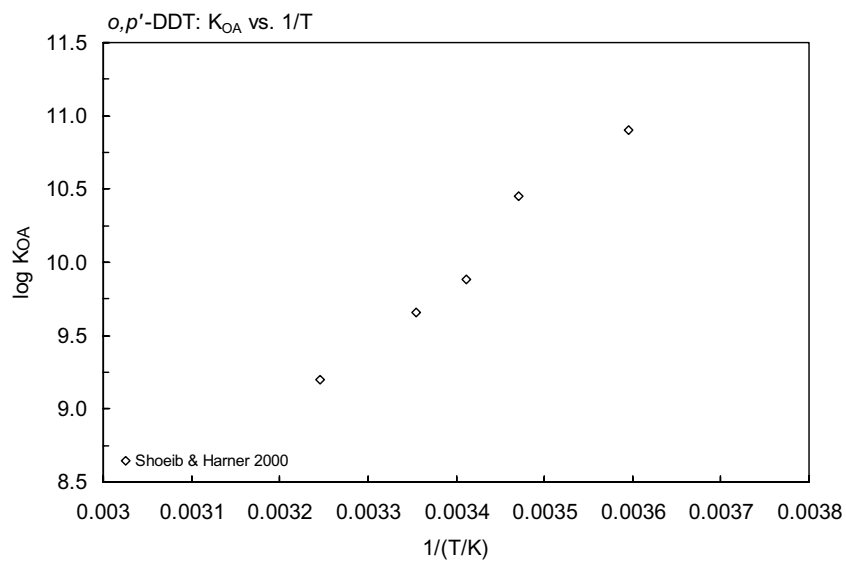
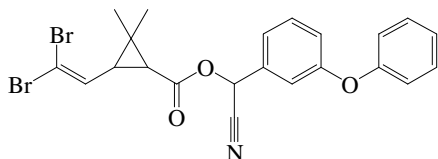


FIGURE 18.1.1.23.3B Logarithm of K_{OA} versus reciprocal temperature for *o,p'*-DDT.

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 ($^{\circ}C$):

98–101 (Hartley & Kidd 1987)

98–102 (Tomlin 1994)

Boiling Point ($^{\circ}C$):

Density (g/cm^3 at $20^{\circ}C$):

0.55 ($25^{\circ}C$, 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 $25^{\circ}C$ (assuming $\Delta S_{fus} = 56\ J/mol\ K$), F :

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$):

<0.002 ($20^{\circ}C$, Hartley & Kidd 1987)

<0.0002 (Tomlin 1994)

Vapor Pressure (Pa at $25^{\circ}C$):

2.0×10^{-6} (Hartley & Kidd 1987)

$<1.33 \times 10^{-5}$ (Tomlin 1994)

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

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, $t_{1/2}$:

Volatilization:

Photolysis: $t_{1/2} = 9$ d in soil (Tomlin 1994).

Oxidation:

Hydrolysis: more stable in acidic than in alkaline media with $t_{1/2} = 2.5$ d at pH 9 and 25°C (Tomlin 1994).

Biodegradation: microbial degradation half-life are, $t_{1/2}(\text{aerobic}) = 21\text{--}25$ d, $t_{1/2}(\text{anaerobic}) = 31\text{--}36$ d in laboratory;
 $t_{1/2} < 23$ d in field (Tomlin 1994)

Biotransformation:

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

Half-Lives in the Environment:

Air:

Surface water: $t_{1/2} = 2\text{--}4$ d in water of small outdoor ponds (Muir et al. 1985);

more stable in acidic than in alkaline media with $t_{1/2} = 2.5$ d at pH 9 and 25°C (Tomlin 1994).

Ground water:

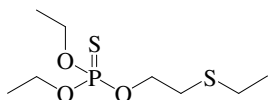
Sediment:

Soil: undergoes microbial degradation within 1–2 wk (Hartley & Kidd 1987)

microbial degradation half-life are, $t_{1/2}(\text{aerobic}) = 21\text{--}25$ d, $t_{1/2}(\text{anaerobic}) = 31\text{--}36$ d in laboratory; $t_{1/2} < 23$ d in field; photolysis $t_{1/2} = 9$ 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 demeton-S, systox-S

Molecular Formula: $C_8H_{19}O_3PS_2$

Molecular Weight: 258.339

Melting Point ($^{\circ}C$):

pale yellow oil (Hartley & Kidd 1987)

Boiling Point ($^{\circ}C$):

123 (Khan 1980)

92–93 (at 0.15 mmHg, Hartley & Kidd 1987)

Density (g/cm^3 at $20^{\circ}C$):

1.119 ($25^{\circ}C$, 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 $25^{\circ}C$ (assuming $\Delta S_{fus} = 56$ J/mol K), F: 1.0

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$ or as indicated):

60 ($20^{\circ}C$, Kenaga 1980a)

60 ($22^{\circ}C$, Khan 1980; Worthing & Walker 1983)

100 (20 – $25^{\circ}C$, Willis & McDowell 1982)

60 (rm. temp., Spencer 1982; Hartley & Kidd 1987)

60 (20 – $25^{\circ}C$, selected, Augustijn-Beckers et al. 1994; Hornsby et al. 1996)

Vapor Pressure (Pa at $25^{\circ}C$ or as indicated):

0.0973, 0.0987 ($30^{\circ}C$, demeton-O, demeton-S, Eichler 1965)

0.00331, 0.0347 ($20^{\circ}C$, demeton-O, demeton-S, Melnikov 1971)

0.00373, 0.0347 ($20^{\circ}C$, demeton-O, demeton-S, Hartley & Graham-Bryce 1980)

0.0331 (Khan 1980)

0.033 ($20^{\circ}C$, Spencer 1982)

0.0167, 0.00707 ($20^{\circ}C$, demeton-O, demeton-S, GC-RT correlation, Kim 1985)

0.034 ($20^{\circ}C$, Hartley & Kidd 1987)

0.030 ($20^{\circ}C$, selected, Suntio et al. 1988)

0.1333 (20 – $25^{\circ}C$, selected, Augustijn-Beckers et al. 1994; Hornsby et al. 1996)

Henry's Law Constant ($Pa \cdot m^3/mol$ at $25^{\circ}C$ or as indicated):

0.130 ($20^{\circ}C$, 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)

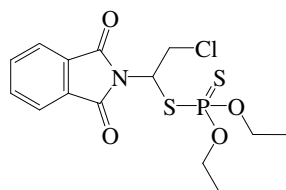
Environmental Fate Rate Constants, k, or Half-Lives, $t_{1/2}$:

Oxidation: calculated rate constant $k = 128 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ for the vapor phase reaction with hydroxyl radical in air (Winer & Atkinson 1990).

Half-Lives in the Environment:

Soil: selected field $t_{1/2} = 15 \text{ d}$ (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-yl)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 ($^{\circ}C$):

68 (Lide 2003)

Boiling Point ($^{\circ}C$):

Density (g/cm^3 at $20^{\circ}C$):

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 $25^{\circ}C$ (assuming $\Delta S_{fus} = 56\ J/mol\ K$), F : 0.379 (mp at $68^{\circ}C$)

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$):

0.18 (Chiou et al. 1977; Kenaga 1980b)

< 1.0 (Hartley & Kidd 1987)

0.18 (room temp., Montgomery 1993)

Vapor Pressure (Pa at $25^{\circ}C$):

0.133 ($35^{\circ}C$, Hartley & Kidd 1987)

1.08×10^{-7} ($20^{\circ}C$, Montgomery 1993)

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

0.142 ($20^{\circ}C$, 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 $20^{\circ}C$ and pH 7.4, $t_{1/2} = 1.8\ h$ at $37.5^{\circ}C$ 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).

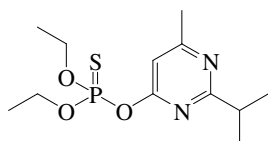
Ground water:

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, Dacid, 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 ($^{\circ}C$):

colorless oil (Hartley & Kidd 1987; Tomlin 1994)

Boiling Point ($^{\circ}C$):

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 $20^{\circ}C$):

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 $25^{\circ}C$ (assuming $\Delta S_{fus} = 56$ J/mol K), F: 1.0

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$):

40 (Spencer 1973, 1982; Martin & Worthing 1977; Worthing 1979, Worthing & Walker 1987)

40 (Wauchope 1978; Briggs 1981; Burkhard & Guth 1981; Kanazawa 1989)

68.8 ($22^{\circ}C$, shake flask-GC, Bowman & Sans 1979, 1983a, b)

40 (Hartley & Graham-Bryce 1980)

40 ($22^{\circ}C$, Khan 1980)

40.5 (20 – $25^{\circ}C$, shake flask-GC, Kanazawa 1981)

40 ($20^{\circ}C$, Windholz 1983)

40 ($20^{\circ}C$, Hartley & Kidd 1987; Worthing & Hance 1991; Tomlin 1994; Milne 1995)

60 (20 – $25^{\circ}C$, selected, Wauchope et al. 1992; Hornsby et al. 1996)

53.5, 43.7 ($20^{\circ}C$, $30^{\circ}C$, 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 $25^{\circ}C$ 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 & Stambach 1964)

0.0111 ($20^{\circ}C$, Wolfdietrich 1965)

0.0112 ($20^{\circ}C$, Melnikov 1971)

- 0.0161 (gas saturation, Heiber & Szelagiewicz 1976)
 0.020 (gas saturation method, measured range 32–73°C, Marti 1976)
 $\log(P/\text{mmHg}) = 11.46 - 4569.55/(T/K)$, 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)
 $\log(P/\text{mmHg}) = 9.3871 - 4014.67/(T/K)$; 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)
 $\log(P_L/\text{Pa}) = 13.482 - 4571.2/(T/K)$; 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 ($\text{Pa m}^3/\text{mol}$ 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)
 $H'/(M \text{ atm}^{-1}) = (7.2 \pm 0.5) \times 10^{-15} \exp[(11900 \pm 700)/(T/K)]$; 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 gudgeon, 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, Zarogian 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 (Glottfelty 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: $t_{1/2} \sim 1$ d river water exposed to sunlight, $t_{1/2} \sim 5$ d lake water exposed to sunlight and $t_{1/2} \sim 5.5$ d with humic acid exposed to sunlight (Mansour et al. 1997)

photolytic $k = 2.39 \times 10^{-3} \text{ h}^{-1}$ with $t_{1/2} = 290$ h in moist sandy soil, $k = 6.62 \times 10^{-5} \text{ h}^{-1}$ with $t_{1/2} = 10500$ h in dry sandy soil; $k = 2.55 \times 10^{-3} \text{ h}^{-1}$ 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).

$k_{\text{OH}} = 9.7 \times 10^{-11} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 298 K in gas phase with atmospheric lifetime of 4.1 h but reduced to .19 h at 283 K; $\log k_{\text{OH}}(\text{aq.}) = 8.2 \times 10^9 \text{ M}^{-1} \text{ s}^{-1}$ in aqueous phase (Feigenbrugel et al. 2004)

Hydrolysis:

$k(\text{acid}) = 2.1 \times 10^{-2} \text{ M}^{-1} \text{ s}^{-1}$ for acid catalyzed hydrolysis, $k(\text{neutral}) = 4.3 \times 10^{-8} \text{ M}^{-1} \text{ s}^{-1}$ for neutral hydrolysis and $k(\text{alkaline}) = 5.3 \times 10^{-3} \text{ M}^{-1} \text{ s}^{-1}$ 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)

$k = 0.023 \text{ d}^{-1}$ with estimated first-order $t_{1/2} = 30$ d in soil incubation studies by soil die-away test (Rao & Davidson 1980; quoted, Scow 1982)

$k(\text{av.}) = 0.0193 \text{ d}^{-1}$ in silty clay with $t_{1/2} = 36$ d; and $k(\text{av.}) = 0.0245 \text{ d}^{-1}$ in sandy clay with $t_{1/2} = 28$ d (Sattar 1990)

Biotransformation:

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

$k_2 = 0.070 \text{ h}^{-1}$ (willow shiner, Tsuda et al. 1989)

$k_2 = 0.023 \text{ h}^{-1}$ (eel's liver, Sancho et al. 1993)

$k_2 = 0.019 \text{ h}^{-1}$ (eel's muscle, Sancho et al. 1993)

$k_2 = 0.21 \text{ h}^{-1}$ (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 $k = 0.048 \text{ d}^{-1}$ with $t_{1/2} = 14.4$ d under aerobic conditions, $k = 0.022 \text{ d}^{-1}$ with $t_{1/2} = 31.7$ d under anaerobic conditions in sediment from San Diego Creek, Orange County, CA; first-order degradation $k = 0.033 \text{ d}^{-1}$ with $t_{1/2} = 21.1$ d under aerobic conditions, $k = 0.029 \text{ d}^{-1}$ 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
				293.05	0.0281
log P = A – B/(T/K)		log P = A – B/(T/K)		293.05	0.0390
	P/mmHg		P/Pa	293.15	0.0349
A	9.3871	A	13.482	293.15	0.0375
B	4014.67	B	4571.2	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

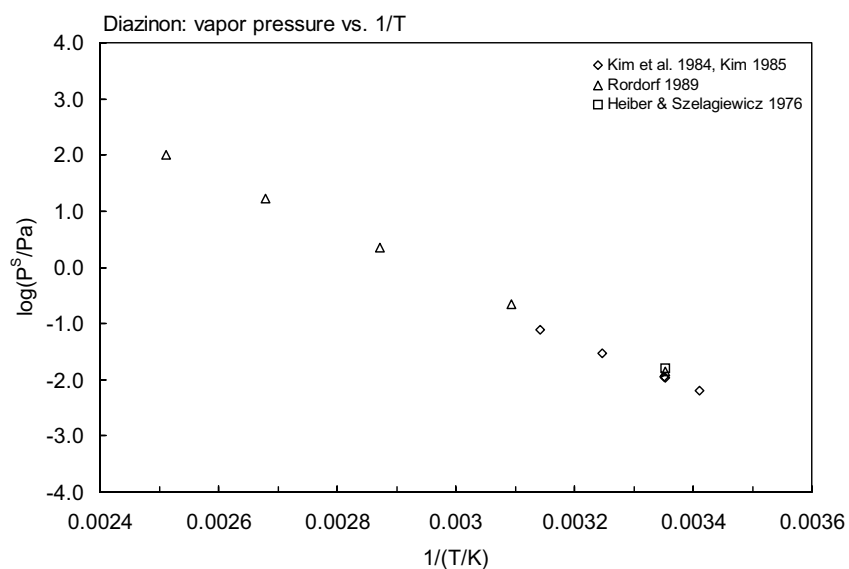


FIGURE 18.1.1.27.1 Logarithm of vapor pressure versus reciprocal temperature for diazinon.

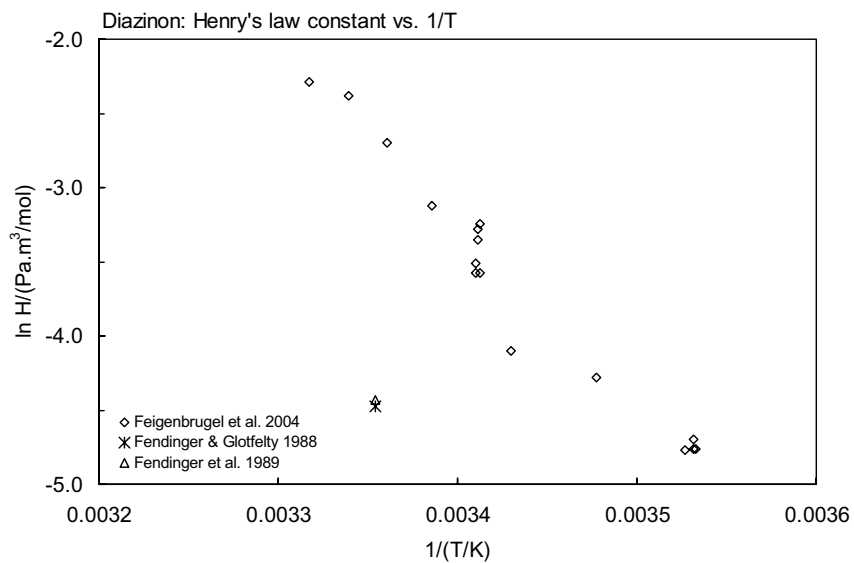
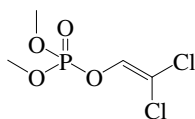


FIGURE 18.1.1.27.2 Logarithm of Henry's law constant versus reciprocal temperature for diazinon.

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 ($^{\circ}C$):

colorless to amber liquid (Hartley & Kidd 1987)

Boiling Point ($^{\circ}C$):

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 $20^{\circ}C$):

1.415 ($25^{\circ}C$, Spencer 1982; Hartley & Kidd 1987; Montgomery 1993; Milne 1995)

1.420 ($25^{\circ}C$, 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 $25^{\circ}C$ (assuming $\Delta S_{fus} = 56$ J/mol K), F: 1.0

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$ 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 ($20^{\circ}C$, Hartley & Kidd 1987; Worthing & Hance 1991; Milne 1995)

16000 (Kawamoto & Urano 1989)

16000 ($20^{\circ}C$, Montgomery 1993)

10000 (20 – $25^{\circ}C$, estimated, Augustijn-Beckers et al. 1994; Hornsby et al. 1996)

8000 (Tomlin 1994)

Vapor Pressure (Pa at $25^{\circ}C$ or as indicated. Additional data at other temperatures designated * are compiled at the end of this section):

1.60 ($20^{\circ}C$, Eichler 1965; Wolfdietrich 1965)

1.60 ($20^{\circ}C$, Melnikov 1971; Hartley & Graham-Bryce 1980; Spencer 1982; Montgomery 1993)

1.60* ($20^{\circ}C$, 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* ($20^{\circ}C$, evaporate rate-gravimetric method, measured range 20 – $60^{\circ}C$, Gückel et al. 1982)

7.026 (gas saturation-GC, Kim et al. 1984)

4.011 (20 , $25^{\circ}C$, 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 ($\text{Pa}\cdot\text{m}^3/\text{mol}$ 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)
- $\ln [H'/(M \text{ atm}^{-1})] = -28.904 + 11100/(T/K)$; 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, $t_{1/2} \sim 57$ d from a model river (Lyman et al. 1982; quoted, Howard 1991);

$t_{1/2} \sim 400$ 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_{NO_3} with NO_3 radical and k_{O_3} with O_3 or as indicated, *data at other temperatures see reference:

atmospheric $t_{1/2} = 320$ d, based on an estimated rate constant $k_{O_3} = 3.58 \times 10^{-20} \text{ cm}^3\cdot\text{molecule}^{-1} \text{ s}^{-1}$ at 25°C for the vapor-phase reaction with ozone of concn $7 \times 10^{11}/\text{cm}^3$ in air (Atkinson & Carter 1984; quoted, Howard 1991)

atmospheric $t_{1/2} = 2$ d, based on an estimated rate constant $k_{OH} = 9.24 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 25°C for the vapor-phase reaction with hydroxyl radical of $5 \times 10^5/\text{cm}^3$ in air (Atkinson 1987; quoted, Howard 1991).

$k_{OH} = 9.4 \times 10^{-12} \text{ cm}^3 \cdot \text{molecule}^{-1} \text{ s}^{-1}$ with calculated tropospheric lifetime about 1.2 d at 298 K assuming an average OH concn of $1 \times 10^6 \text{ molecule/cm}^3$ (Gautier et al. 2003)

Hydrolysis: $t_{1/2} = 462$ min at pH 7 and $t_{1/2} = 30$ min at pH 8 (Montgomery 1993);

$t_{1/2} \sim 31.9$ d at pH 4, $t_{1/2} \sim 2.9$ d at pH 7, and $t_{1/2} \sim 2.0$ 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 $k(\text{aerobic}) = 0.20 \text{ d}^{-1}$ with $t_{1/2} = 3.5$ d at 20°C by aerobic activated sludge, and $k(\text{anaerobic}) = 0.20 \text{ d}^{-1}$ with $t_{1/2} = 3.5$ d at 20°C by anaerobic microorganisms (batch contacting method, Kawamoto & Urano 1990).

$t_{1/2}(\text{aerobic}) = 180$ d, $t_{1/2}(\text{anaerobic}) = 1$ 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 $k = 3.58 \times 10^{-20} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 25°C for the vapor-phase reaction with ozone of $7 \times 10^{11}/\text{cm}^3$ in air (Atkinson & Carter 1984; quoted, Howard 1991)

atmospheric $t_{1/2} = 2$ d, based on an estimated rate constant $k = .24 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 25°C for the vapor-phase reaction with hydroxyl radical of $5 \times 10^5/\text{cm}^3$ 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 $t_{1/2}(\text{aerobic}) = 180$ d, $t_{1/2}(\text{anaerobic}) = 1$ d, hydrolysis $t_{1/2} = 3800$ d at pH 7 in natural waters (Capel & Larson 1995)

Ground water:

Sediment:

Soil: average degradation rate constant $k = 0.0423 \text{ d}^{-1}$ in silty clay with $t_{1/2} = 16$ d and average degradation rate constant $k = 0.0444 \text{ d}^{-1}$ 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:
 $\ln H = \ln(M \text{ atm}^{-1}) = -A + B/(T/K)$
A 28.904
B 11100

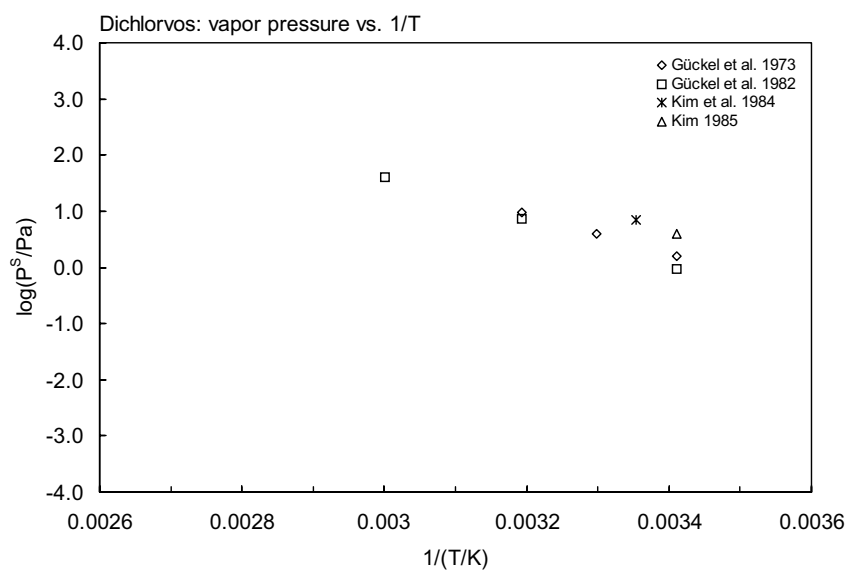


FIGURE 18.1.1.28.1 Logarithm of vapor pressure versus reciprocal temperature for dichlorvos.

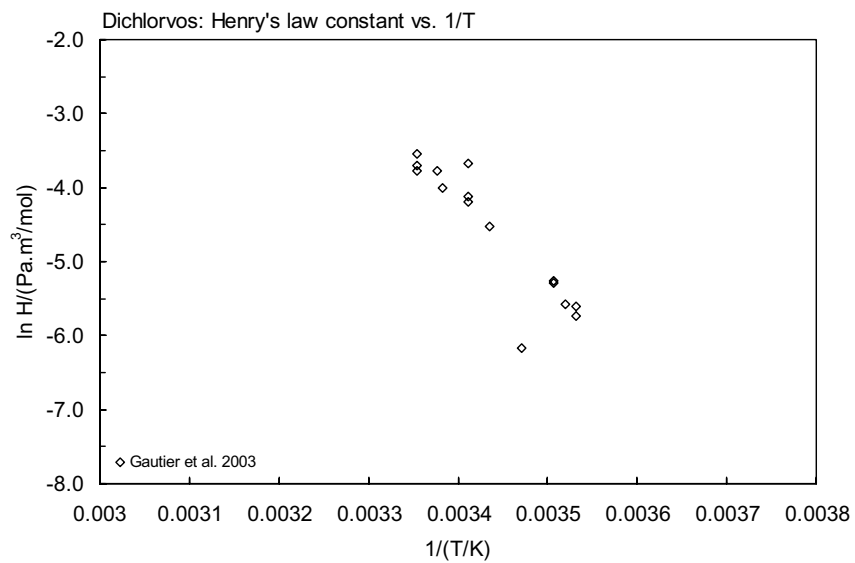
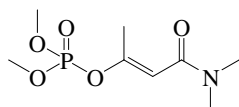


FIGURE 18.1.1.28.2 Logarithm of Henry's law constant versus reciprocal temperature for dichlorvos.

18.1.1.29 Dicrotophos



Common Name: Dicrotophos

Synonym: Bidirl, Bidrin, C 709, Cabicron, Carbomicron, CIBA 709, Diapadrin, Dicrotofos, Ektafos, ENT 24,482, Karbicon, 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: C₈H₁₆NO₅P

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/cm³ 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 (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: 1.0

Water Solubility (g/m³ 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°C or 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·m³/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, $t_{1/2}$:

- Hydrolysis: $t_{1/2}$ = 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 $t_{1/2}$ = 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: $t_{1/2}$ = 3 d in sandy loam soil (Lee et al. 1989; quoted, Montgomery 1993);
- selected field $t_{1/2}$ = 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

$t/^{\circ}\text{C}$	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

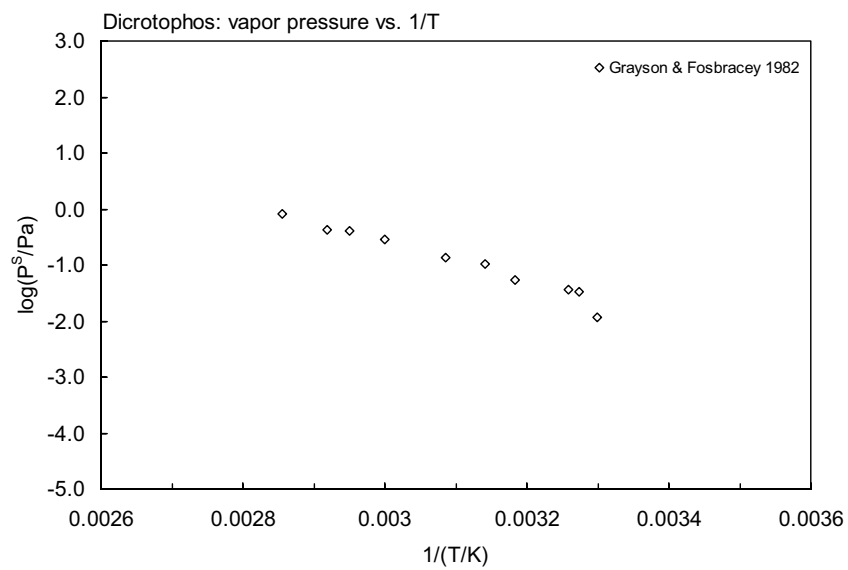
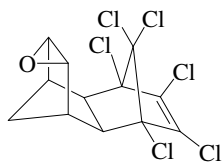


FIGURE 18.1.1.29.1 Logarithm of vapor pressure versus reciprocal temperature for dicrotophos.

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-1,4,4a,5,6,7,8, 8a-octahydroendo-1,4-*exo*-5,8-dimethano-naphthalene; 3,4,5,6,9,9-hexachloro-1a,2,2a,3,6,6a,7,7a-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: C₁₂H₈Cl₆O

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/cm³ at 20°C):

1.75 (Hartley & Kidd 1987; Montgomery 1993)

Molar Volume (cm³/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/m³ 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)
$4.20 \times 10^{-4*}$	(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)
$7.90 \times 10^{-4*}$	(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 ($\text{Pa} \cdot \text{m}^3/\text{mol}$ 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*, Schauburger & Wildman 1977)
- 2.70; 3.26 (*Anacystis nidulans*, *Nostoc muscorum*, Schauburger & 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	(<i>Trienodes tardus</i> , Belluck & Felsot 1981)
3.65	(<i>Pseudorasbora parva</i> , 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 <i>Chlorella</i> : wet wt basis, dry wt basis, Geyer et al. 2000)
3.49, 5.49	(mussel <i>Mytilus edulis</i> : wet wt basis, lipid wt basis, Geyer et al. 2000)
3.54, 5.57	(<i>Daphnia</i> : wet wt basis, lipid wt basis, Geyer et al. 2000)
3.46, 5.54	(oyster <i>Crassostrea virginica</i> : wet wt basis, lipid wt basis, Geyer et al. 2000)
3.32, 5.34	(oyster <i>Crassostrea virginica</i> : wet wt basis, lipid wt basis, Geyer et al. 2000)
3.70, 5.62	(oyster <i>Crassostrea virginica</i> : 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 <i>Crassostrea virginica</i> : 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	(<i>Oncorhynchus mykiss</i> , 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, $t_{1/2}$:

Volatilization: $t_{1/2} \sim 1.4$ 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 $k = 4.8 \times 10^{-4} \text{ h}^{-1}$ 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, $k < 3600 \text{ M}^{-1} \text{ h}^{-1}$ and for RO_2 radicals $k < 30 \text{ M}^{-1} \text{ h}^{-1}$ (Mabey et al. 1982); photooxidation $t_{1/2} = 4\text{--}40.5$ 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 $t_{1/2} = 10.5$ yr based on a first-order rate constant $k = 7.5 \times 10^{-6} \text{ h}^{-1}$ at pH 7.0 and 25°C (Ellington et al. 1986, 1987, 1988; quoted, Howard et al. 1991; Montgomery 1993); rate constant $k = 6.3 \times 10^{-2} \text{ yr}^{-1}$ at pH 7 and 25°C (Kollig 1993).

Biodegradation: aqueous aerobic $t_{1/2} = 4200\text{--}25,920$ 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);

$t_{1/2} = 868$ d (Nash 1980; quoted, Jury et al. 1983);

rate constant $k = 0.013 \text{ d}^{-1}$ from soil incubation studies by die-away tests (Rao & Davidson 1980; quoted, Scow 1982);

aqueous anaerobic $t_{1/2} = 24\text{--}168$ h, based on soil and freshwater mud grab sample data (Maule et al. 1987; quoted, Howard et al. 1991);

$t_{1/2} = 870$ 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:

$k_1 = 20.40 \text{ h}^{-1}$; $k_2 = 0.013 \text{ h}^{-1}$ (Ernst 1977; quoted, Hawker & Connell 1986)

$k_2 = 0.017 \text{ d}^{-1}$ (fish, Fordham & Reagan 1991)

$k_2 = 0.014 \text{ d}^{-1}$ (birds, Fordham & Reagan 1991)

Half-Lives in the Environment:

Air: $t_{1/2} = 4\text{--}40.5$ 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 $t_{1/2} \geq 300$ d in lake waters (Zoeteman et al. 1980);

$t_{1/2} = 4200\text{--}25920$ h, based on estimated aqueous aerobic biodegradation half-life (Howard et al. 1991; quoted, Mortimer & Connell 1995).

Ground water: $t_{1/2} = 24\text{--}51840$ h, based on estimated aqueous aerobic and anaerobic biodegradation half-lives (Howard et al. 1991).

Sediment: $t_{1/2} = 15100$ h (mean value quoted from Howard et al. 1991).

Soil: field $t_{1/2} = 49$ d in nondisked soil (Nash 1983);

$t_{1/2} \sim 7$ 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);

$t_{1/2} = 4200\text{--}25920$ 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 $t_{1/2} \sim 53.3$ d from rate constant $k = 0.013 \text{ d}^{-1}$ from soil incubation studies by die-away tests (Rao & Davidson 1980; quoted, Scow 1982);

moderately persistent in soils with $t_{1/2} = 20\text{--}100$ d (Willis & McDowell 1982);

microagroecosystem $t_{1/2} = 19\text{--}26$ d in moist fallow soil (Nash 1983);

measured dissipation rate $k = 0.055 \text{ d}^{-1}$ (Nash 1983; quoted, Nash 1988);

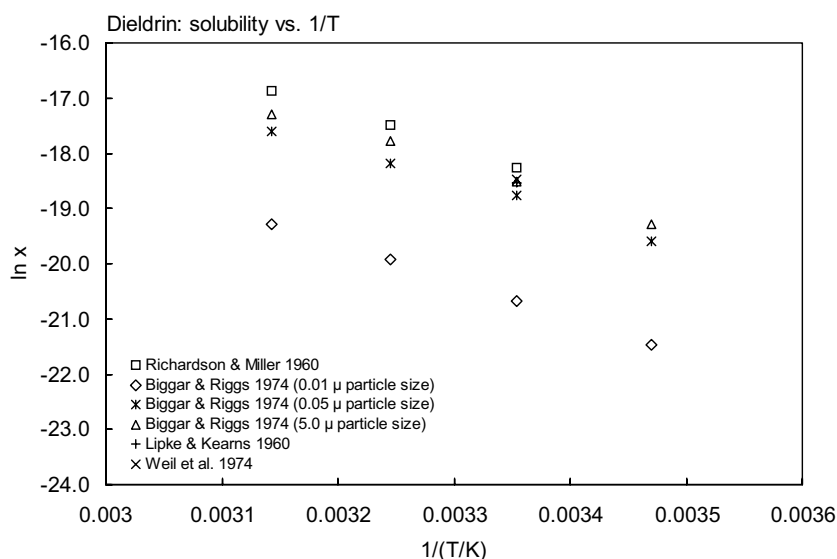
estimated dissipation rate $k = 0.034$ and 0.049 d^{-1} (Nash 1988);

biodegradation $t_{1/2} = 868$ d (Jury et al. 1984, 1987a, b; Jury & Ghodrati 1989; quoted, Montgomery 1993);
 $t_{1/2} > 50$ d and subject to plant uptake via volatilization (Ryan et al. 1988);
 estimated field $t_{1/2} = 1000$ d (Augustijn-Beckers et al. 1994; Hornsby et al. 1996);
 $t_{1/2} = 5 - 9$ yr in soil (Geyer et al. 2000)
 $t_{1/2} = 21.7$ and 25 yr for control and sludge-amended Luddington soils, respectively (Meijer et al. 2001).
 Biota: estimated $t_{1/2} \sim 1.3$ and 10.2 d in rat's liver, and similar values estimated $t_{1/2} = 10.3$ d for the blood in rat
 and $t_{1/2} = 3$ d in adipose tissue of rat (Robinson et al. 1969);
 $t_{1/2} = 53.1$ h in mussels (Ernst 1977; quoted, Hawker & Connell 1986);
 biochemical $t_{1/2} = 868$ 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	
$t/^{\circ}\text{C}$	$S/\text{g}\cdot\text{m}^{-3}$	$t/^{\circ}\text{C}$	$S/\text{g}\cdot\text{m}^{-3}$	$S/\text{g}\cdot\text{m}^{-3}$	$S/\text{g}\cdot\text{m}^{-3}$	$t/^{\circ}\text{C}$	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							
$\Delta H_{OA}/(\text{kJ mol}^{-1}) = 72.6$							

FIGURE 18.1.1.30.1 Logarithm of mole fraction solubility ($\ln x$) versus reciprocal temperature for dieldrin.

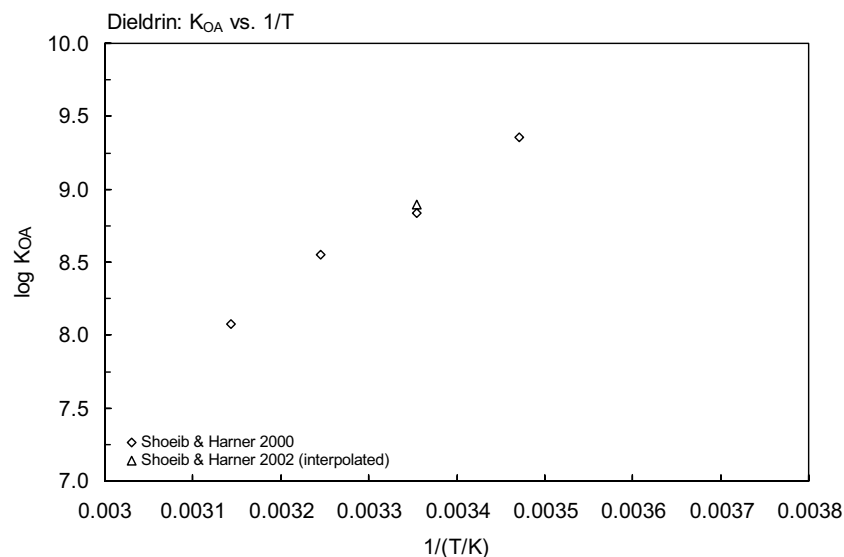


FIGURE 18.1.1.30.2 Logarithm of K_{OA} versus reciprocal temperature for dieldrin.

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)		$\ln P = A - B/(T/K)$		(1a)	
$\log P = A - B/(C + t/^{\circ}C)$		(2)		$\ln P = A - B/(C + t/^{\circ}C)$		(2a)	
$\log P = A - B/(C + T/K)$		(3)					
$\log P = A - B/(T/K) - C \cdot \log (T/K)$		(4)					
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
				B	5210.07	B	4220.71
eq.1	P/mmHg	eq. 1a	P/Pa	eq. 1	P _L /Pa	eq. 1	PL/Pa
A	12.07	A	11285	A	11.6603	A	9.519590
B	5178	B	30.7	B	4001.62	B	3280.59
				$\Delta H_v = 76.6 \text{ kJ/mol}$		$\Delta H_v = 62.8 \text{ kJ/mol}$	

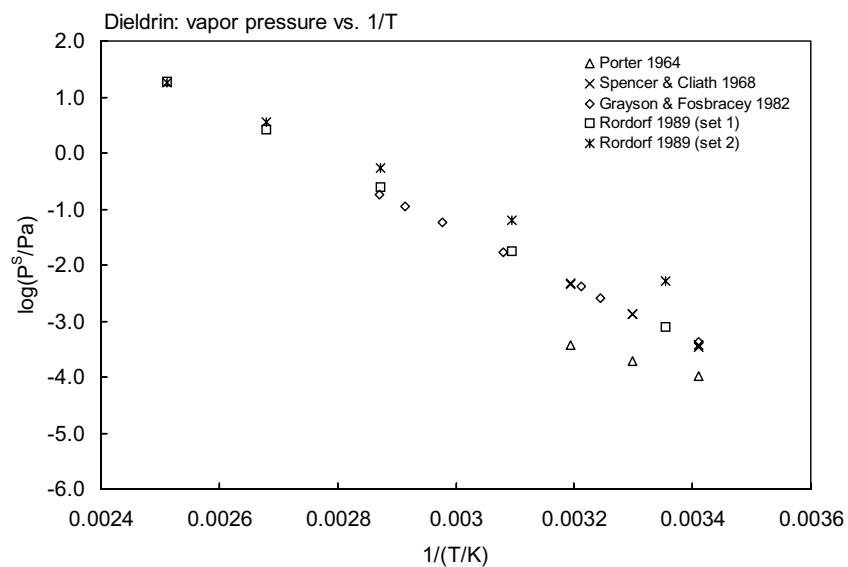
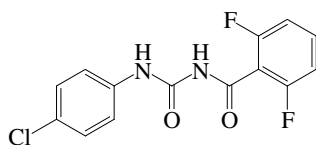


FIGURE 18.1.1.30.3 Logarithm of vapor pressure versus reciprocal temperature for dieldrin.

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 ($^{\circ}C$):

230–232 (pure, Hartley & Kidd 1987; Montgomery 1993; Milne 1995)

230–232 (dec., Tomlin 1994)

239 (Lide 2003)

Boiling Point ($^{\circ}C$):

dec. on distillation (Montgomery 1993)

Density (g/cm^3 at $20^{\circ}C$):

288.3 (calculated-Le Bas method at normal boiling point)

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 $25^{\circ}C$ (assuming $\Delta S_{fus} = 56 J/mol K$), F : 0.00795 (mp at $239^{\circ}C$)

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$ or as indicated):

0.25 (Ivie et al. 1980; quoted, Belluck & Felsot 1981)

0.20 (Spencer 1982; Wauchope 1989)

0.14 ($20^{\circ}C$, Hartley & Kidd 1987; Milne 1995)

0.10 ($20^{\circ}C$, Worthing & Walker 1987, 1991)

14.0 (Montgomery 1993)

0.30 (Milne 1995)

0.08 (selected, Lohninger 1994)

0.08 (20 – $25^{\circ}C$, selected, Hornsby et al. 1996)

Vapor Pressure (Pa at $25^{\circ}C$ or as indicated):

$< 3.3 \times 10^{-5}$ ($50^{\circ}C$, Hartley & Kidd 1987)

$< 1.3 \times 10^{-5}$ (Worthing & Hance 1991)

3.33×10^{-5} ($20^{\circ}C$, Montgomery 1993)

1.20×10^{-7} (gas saturation method, Tomlin 1994)

1.20×10^{-7} (20 – $25^{\circ}C$, selected, Hornsby et al. 1996)

Henry's Law Constant ($Pa \cdot m^3/mol$ at $25^{\circ}C$ or as indicated):

7.40×10^{-4} (20 – $25^{\circ}C$, calculated-P/C, Montgomery 1993)

4.70×10^{-4} (20 – $25^{\circ}C$, 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:

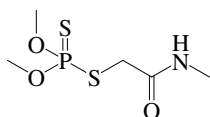
Soil: $t_{1/2} < 7$ d (Hartley & Kidd 1987; quoted, Montgomery 1993; Tomlin 1994);

$t_{1/2} = 10$ 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, Trimeton

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: C₅H₁₂NO₃PS₂

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/cm³ 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 (cm³/mol):

205.6	(calculated-Le Bas method at normal boiling point)
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Dissociation Constant, pK_a:

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

23.43	(DSC method, Plato & Glasgow 1969)
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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/m³ 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·m³/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, $t_{1/2}$:

Volatilization:

Photolysis:

Oxidation: photooxidation $t_{1/2} = 0.469\text{--}4.69$ h in air, based on estimated rate constant for the reaction with hydroxyl radical in air (Atkinson 1987; quoted, Howard et al. 1991).Hydrolysis: $t_{1/2} = 0.8$ h at pH 9 and $t_{1/2} = 21$ h at pH 2 both at 70°C (Melnikov 1971; quoted, Freed et al. 1977) neutral rate constant $k = 1.7 \times 10^{-4} \text{ h}^{-1}$ with a calculated $t_{1/2} = 118$ h at pH 7 and 25°C (Ellington et al. 1987, 1988; quoted, Montgomery 1993);first-order $t_{1/2} = 2822$ h, based on measured neutral and base catalyzed hydrolysis rate constants (Ellington et al. 1987; quoted, Howard et al. 1991);rate constant $k = 1.68 \text{ yr}^{-1}$ at pH 7.0 and 25°C (Kollig 1993); $t_{1/2} = 12$ d at pH 9 (Tomlin 1994) $t_{1/2} = 120$ d at pH 2, $t_{1/2} = 120$ d at pH 7 and $t_{1/2} = 0.0038$ d at pH 12 in natural waters (Capel & Larson 1995)Biodegradation: aqueous aerobic $t_{1/2} = 264\text{--}1344$ 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 $t_{1/2} = 1056\text{--}5376$ h, based on estimated unacclimated aqueous aerobic biodegradation half-life (Howard et al. 1991) $t_{1/2}(\text{aerobic}) = 11$ d, $t_{1/2}(\text{anaerobic}) = 44$ d in natural waters (Capel & Larson 1995)

Biotransformation:

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

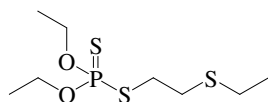
Half-Lives in the Environment:

Air: $t_{1/2} = 0.469\text{--}4.69$ h, based on estimated rate constant for the reaction with hydroxyl radical in air (Atkinson 1987; quoted, Howard et al. 1991).Surface water: $t_{1/2} = 264\text{--}1344$ h, based on estimated unacclimated aqueous aerobic biodegradation half-life (Howard et al. 1991)Biodegradation $t_{1/2}(\text{aerobic}) = 11$ d, $t_{1/2}(\text{anaerobic}) = 44$ d, hydrolysis $t_{1/2} = 120$ d at pH 2, $t_{1/2} = 120$ d at pH 7 and $t_{1/2} = 0.0038$ d at pH 12 in natural waters (Capel & Larson 1995) $t_{1/2} = 423$ d at 6°C, 193h at 23°C in darkness for Milli-Q water; $t_{1/2} = 171$ d at 6°C, $t_{1/2} = 43$ d at 22°C in darkness, $t_{1/2} = 29$ d under sunlight conditions for river water at pH 7.3; $t_{1/2} = 173$ d at 6°C, $t_{1/2} = 29$ d at 22°C in darkness for filtered river water, pH 7.3; $t_{1/2} = 219$ d at 6°C, $t_{1/2} = 36$ d at 22°C in darkness, $t_{1/2} = 74$ d under sunlight conditions for seawater, pH 8.1 (Lartiges & Garrigues 1995).Ground water: $t_{1/2} = 528\text{--}2688$ h, based on estimated unacclimated aqueous aerobic biodegradation half-life (Howard et al. 1991).

Sediment:

Soil: $t_{1/2} = 264\text{--}888$ h, based on soil die-away test data for two soils (Bro-Rasmussen et al. 1970; quoted, Howard et al. 1991);selected $t_{1/2} = 7.0$ d (Wauchope et al. 1992; Hornsby et al. 1996);aerobic $t_{1/2} = 2\text{--}4.1$ d in soil and photolytic $t_{1/2} = 7\text{--}16$ d on soil surface (Tomlin 1994); $t_{1/2} = 7.0$ d (selected, Halfon et al. 1996).Biota: disappearance rate and half-life from treated plants: $t_{1/2} = 2.95$ d for cabbage, $t_{1/2} = 3.40$ d for tomato leaves and $t_{1/2} = 2.40$ 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 ($^{\circ}C$):

-25 (Milne 1995; Lide 2003)

Boiling Point ($^{\circ}C$):

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 $20^{\circ}C$):

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 $25^{\circ}C$ (assuming $\Delta S_{fus} = 56$ J/mol K), F: 1.0

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$ or as indicated):

66 (Günther 1968)

25 ($20^{\circ}C$, Melnikov 1971; Spencer 1973)

25 (Martin & Worthing 1977)

16.3 ($19.5^{\circ}C$, shake flask-GC, Bowman & Sans 1979, 1983b)

25 ($22^{\circ}C$, Khan 1980; Worthing & Walker 1983)

15–66 (20 – $25^{\circ}C$, selected, Willis & McDowell 1982)

25 ($22^{\circ}C$, Hartley & Kidd 1987)

12 ($22^{\circ}C$, Worthing & Hance 1991)

25 (20 – $25^{\circ}C$, selected, Wauchope et al. 1992; Hornsby et al. 1996)

12 ($20^{\circ}C$, Tomlin 1994)

12 ($22^{\circ}C$, 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 $25^{\circ}C$ or as indicated):

0.024 ($20^{\circ}C$, vapor density, MacDougall & Archer 1964)

$\log(P/mmHg) = 10.20 - 4084.80/(T/K)$; temp range 10 – $40^{\circ}C$ (vapor density, MacDougall & Archer 1964)

0.024 ($20^{\circ}C$, Eichler 1965)

0.024 ($20^{\circ}C$, Melnikov 1971; Khan 1980)

0.024 (Worthing 1983)

0.0041 ($20^{\circ}C$, GC-Rt correlation, Kim et al. 1984; Kim 1985)

0.024 ($20^{\circ}C$, Hartley & Kidd 1987)

0.020 ($20^{\circ}C$, 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 ($\text{Pa}\cdot\text{m}^3/\text{mol}$ 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 χ , 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, $t_{1/2}$:

Volatilization: gas exchange $t_{1/2}$ = of 900 d for winter and $t_{1/2}$ = 360 d for summer in Rhine River (Wanner et al. 1989).

Photolysis: photolytic $t_{1/2}$ = 1000 d for winter and $t_{1/2}$ = 100 d for summer in the Rhine River (Wanner et al. 1989); $t_{1/2}$ = 1–4 d (Tomlin 1994)

Apparent first-order rate constant phototransformation at $\lambda > 285$ nm, $k = (1.38 \pm 0.12) \times 10^{-2} \text{ h}^{-1}$ in purified water, and $k = (1.68 \pm 0.12) \times 10^{-2} \text{ h}^{-1}$ in Capot river water with $t_{1/2} \sim 40$ h (Zamy et al. 2004)

Oxidation: half-life ranged from $t_{1/2} \sim 5$ h of midday sunlight during summer to $t_{1/2} = 12$ h during winter estimated from kinetic data for oxygenation reactions photosensitized by humic substances in water exposed to sunlight (Zepp et al. 1981);

photooxidation $t_{1/2} = 0.50$ –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 $t_{1/2} = 103$ d, based on measured overall rate constant $k = 2.8 \times 10^{-4} \text{ h}^{-1}$ at pH 7, 25°C (Ellington et al. 1986, 1987, 1988; quoted, Howard et al. 1991);

abiotic hydrolysis $k = 1.3 \times 10^{-7} \text{ s}^{-1}$ under neutral condition, $k = 2.0 \times 10^{-3} \text{ s}^{-1}$ under base-catalyzed condition at 20°C and hydrolysis $t_{1/2} = 170$ d at 11°C, pH 9 and $t_{1/2} = 62$ d in summer were predicted in Rhine River (Wanner et al. 1989);

$t_{1/2} = 3.04$ yr in water at pH 1–5 and at 20°C; 1.2 d at pH 7 and $t_{1/2} = 7.2$ h at pH 9 both at 70°C (Worthing & Hance 1991);

rate constant $k = 3.23 \text{ yr}^{-1}$ at pH 7.0 and 25°C (Kollig 1993);

$t_{1/2} = 133$ d at pH 4, $t_{1/2} = 169$ d at pH 7, and $t_{1/2} = 131$ d at pH 9 at 22°C (Tomlin 1994).

Biodegradation: $t_{1/2} < 14$ d, rapidly oxidized in soil (Szeto et al. 1983)

primary biodegradation rate constant $k = 0.2 \mu\text{g}^2 \text{ L}^2 \text{ d}^{-1}$ with $t_{1/2} = 41$ d, and the degradation $t_{1/2} = 7$ –41 d for winter and $t_{1/2} = 4$ –28 d for summer in Rhine River (Wanner et al. 1989);

aqueous aerobic $t_{1/2} = 72$ –504 h, based on aerobic soil field data and reported half-lives for soil (Howard et al. 1991);

aqueous anaerobic $t_{1/2} = 288$ –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: $t_{1/2} = 0.50$ –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 $t_{1/2} = 900$ d for winter, $t_{1/2} = 360$ d for summer; abiotic hydrolysis half-lives of 170 d for winter, 62 d for summer; photolytic transformation $t_{1/2} = 1000$ d for winter, $t_{1/2} = 200$ d for summer and primary biodegradation $t_{1/2} = 7$ –41 d for winter, $t_{1/2} = 8$ –28 d for summer in Rhine River under environmental conditions (Wanner et al. 1989);

overall $t_{1/2} = 72$ –504 h, based on estimated unacclimated aqueous aerobic biodegradation half-life (Howard et al. 1991).

$t_{1/2} \sim 40$ h upon photolysis in Capot river water (Zamy et al. 2004)

Ground water: $t_{1/2} = 144$ –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);

$t_{1/2} = 72$ –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);

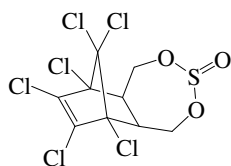
$t_{1/2} = 5$ d from screening model calculations (Jury et al. 1987b);

estimated $t_{1/2} = 30$ d (Wauchope et al. 1992; Hornsby et al. 1996);

soil $t_{1/2} = 9$ d (Pait et al. 1992).

Biota: biochemical $t_{1/2}$ = 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-1,5,5a,6,9,9a-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: C₉H₆Cl₆O₃S

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)
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Density (g/cm³ at 20°C):

1.80	(tech. grade, Tomlin 1994)
1.745	(Milne 1995; Montgomery 1993)

Molar Volume (cm³/mol):

312.8	(calculated-Le Bas method at normal boiling point.)
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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 $\Delta S_{\text{fus}} = 56$ J/mol K), F:

0.22. 0.13	(20°C, α -, β -endosulfan, Suntio et al. 1988)
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Water Solubility (g/m³ 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·m³/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 33.31%, 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 33.31%, 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 171‰ 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 161‰ 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 121‰, 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 $k = (3.2 \pm 2.0) \times 10^{-3} \text{ h}^{-1}$ 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 $k = (3.7 \pm 2.0) \times 10^{-3} \text{ h}^{-1}$ for β -endosulfan at pH 7 and 25°C (Ellington et al. 1987, 1988; quoted, Howard et al. 1991; Montgomery

1993); rate constant $k = 6.1 \times 10^{-2} \text{ yr}^{-1}$ for α -endosulfan at pH 7 and 25°C and rate constant $k = 8.9 \times 10^{-2} \text{ yr}^{-1}$ for β -endosulfan at pH 7 and 25°C (Kollig 1993).

$t_{1/2} = 360 \text{ d}$ at pH 2, $t_{1/2} = 9.1 \text{ d}$ at pH 7 and $t_{1/2} = 0.00029 \text{ d}$ at pH 12 in natural waters (Capel & Larson 1995)

Biodegradation: aqueous aerobic $t_{1/2} = 48\text{--}336 \text{ h}$, 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 $k = -0.00502 \text{ h}^{-1}$ in nonsterile sediment, $k = -0.00796 \text{ h}^{-1}$ in sterile sediment by shake-tests at Range Point, first-order $k = -0.0157 \text{ h}^{-1}$ in nonsterile water, and $k = -0.0325 \text{ h}^{-1}$ 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)

$t_{1/2}(\text{aerobic}) = 2 \text{ d}$, $t_{1/2}(\text{anaerobic}) = 8 \text{ d}$ in natural waters (Capel & Larson 1995).

Biotransformation:

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

$k_1 = 12.3 \text{ h}^{-1}$; $k_2 = 0.0205 \text{ h}^{-1}$ (mussel from α -endosulfan, Ernst 1977; quoted, Hawker & Connell 1986)

Half-Lives in the Environment:

Air: $t_{1/2} = 2.5\text{--}24.8 \text{ h}$, 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);

$t_{1/2} = 9.2 \pm 4 \text{ yr}$ 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);

$t_{1/2} = 30 \text{ d}$ and 45 d for α - and β -endosulfan respectively for surface waters in case of first order reduction process may be assumed and estimated $t_{1/2} \sim 30\text{--}300 \text{ d}$ for β -endosulfan in lakes in the Netherlands (Zoeteman et al. 1980);

$t_{1/2} = 4.5\text{--}218 \text{ h}$, 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)

$t_{1/2} = 1.3 \text{ d}$ in rice paddy water (Tejada et al. 1993; quoted, Abdullah et al. 1997)

$t_{1/2}(\text{aerobic}) = 2 \text{ d}$, $t_{1/2}(\text{anaerobic}) = 8 \text{ d}$, hydrolysis $t_{1/2} = 360 \text{ d}$ at pH 2, $t_{1/2} = 9.1 \text{ d}$ at pH 7 and $t_{1/2} = 0.00029 \text{ d}$ at pH 12 in natural waters (Capel & Larson 1995)

Ground water: estimated $t_{1/2} = 30\text{--}300 \text{ d}$ in lakes and Ground water (β -Endosulfan, Zoeteman et al. 1980);

$t_{1/2} = 4.5\text{--}218 \text{ h}$, 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: $t_{1/2} = 4.5\text{--}218 \text{ h}$, 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);

$t_{1/2} > 50 \text{ d}$ and subject to plant uptake via volatilization (Ryan et al. 1988);

selected $t_{1/2} = 50 \text{ d}$ (Wauchope et al. 1992; Hornsby et al. 1996);

$t_{1/2} = 1.2 \text{ d}$ in rice soil (Tejada et al. 1993; quoted, Abdullah et al. 1997);

soil $t_{1/2} = 120 \text{ d}$ (Pait et al. 1992);

degraded in soil with $t_{1/2} = 30\text{--}70 \text{ d}$ (Tomlin 1994); 50 d (selected, Halfon et al. 1996)

$t_{1/2} = 5\text{--}7 \text{ yr}$ in soil (Geyer et al. 2000)

Biota: $t_{1/2} = 33.8 \text{ h}$ in mussels (α -endosulfan, Ernst 1977);

$t_{1/2} = 1.0 \text{ d}$ 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
 $\Delta H_{OA}/(\text{kJ mol}^{-1}) = 83.0$

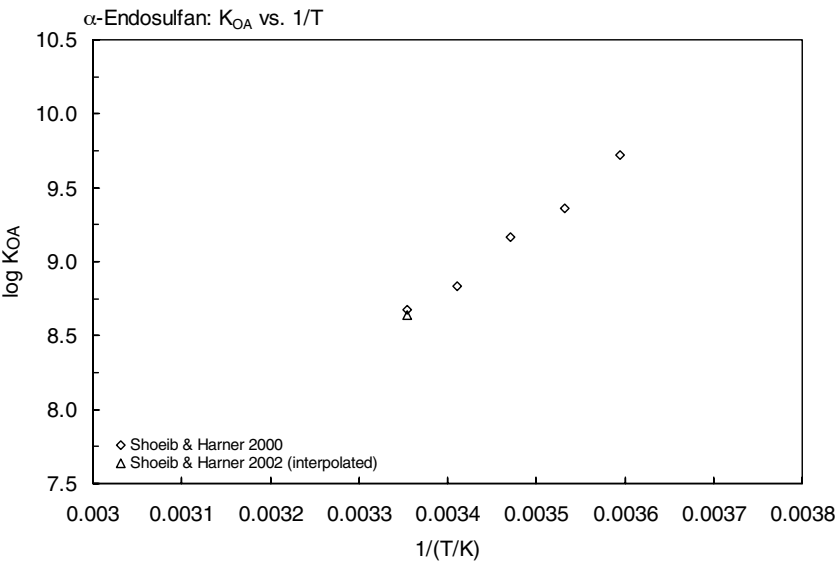
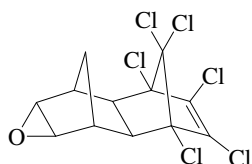


FIGURE 18.1.1.34.1 Logarithm of K_{OA} versus reciprocal temperature for α -endosulfan.

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-1,4,4a,5,6,7,8,8a-octahydro-*exo*-1,4-*exo*-5,8-dimethano-naphthalene

Uses: Insecticide/Avicide/Rodenticide

CAS Registry No: 72-20-8

Molecular Formula: C₁₂H₈Cl₆O

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/cm³ at 20°C):

1.70, 1.65 (pure, technical, at 25°C, Montgomery 1993)

Molar Volume (cm³/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/m³ 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 5.0 μm, 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/(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 ($\text{Pa}\cdot\text{m}^3/\text{mol}$ 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 *Crassostrea virginica*: wet wt basis, lipid wt basis, Geyer et al. 2000)
 3.44, 5.37 (oyster *Crassostrea 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: $t_{1/2} \sim 9.6$ 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:

$k(aq.) = (2.7 \pm 0.7) \times 10^8 \text{ M}^{-1} \text{ s}^{-1}$ for the reaction with OH radical in aqueous solution (Fenton reaction) at $24 \pm 1^\circ\text{C}$ and pH 2.8 (Haag & Yao 1992) with reference to $4.2 \times 10^8 \text{ M}^{-1} \text{ s}^{-1}$ for the reaction of DPCP with OH radical in aqueous solution (Buxton et al. 1988; quoted, Haag & Yao 1992);

$k(aq.) = (1.3 \pm 0.4) \times 10^9 \text{ M}^{-1} \text{ s}^{-1}$ (Fenton reaction) and $k = (1.1 \pm 0.2) \times 10^9 \text{ M}^{-1} \text{ s}^{-1}$ (photo-Fenton reaction) for the reaction with OH radical in aqueous solution at $24 \pm 1^\circ\text{C}$ and pH 3.4 (Haag & Yao 1992) with reference to $8 \times 10^8 \text{ M}^{-1} \text{ s}^{-1}$ for the reaction of lindane with OH radical in aqueous solution (Buxton et al. 1988; quoted, Haag & Yao 1992)

$k(aq.) < 0.02 \text{ M}^{-1} \text{ s}^{-1}$ for direct reaction with ozone in water at pH 2.7–6.4 and $23 \pm 3^\circ\text{C}$, 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)

$\log k_1 = 1.5 \text{ h}^{-1}$; $-\log k_2 = 1.78$ 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 $k_{O_3}(aq.) < 0.02 \text{ M}^{-1} \text{ s}^{-1}$ for direct reaction with ozone in water at pH 2.7–6.4 and $23 \pm 3^\circ\text{C}$, with $t_{1/2} > 20$ d at pH 7 (Yao & Haag 1991).

Ground water:

Sediment:

Soil: $t_{1/2} \sim 12$ 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 $t_{1/2} = 20\text{--}100$ 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)
 $t_{1/2} \sim 12$ 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							

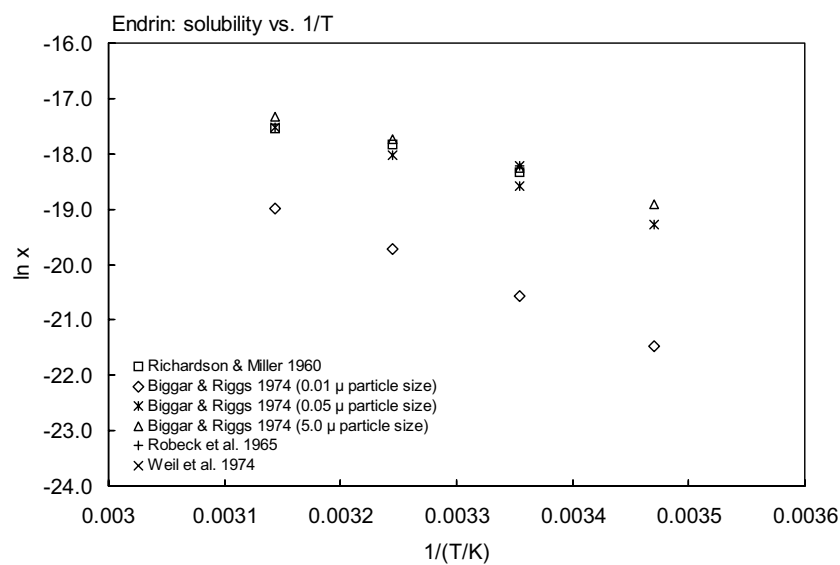


FIGURE 18.1.1.35.1 Logarithm of mole fraction solubility (ln x) versus reciprocal temperature for endrin.

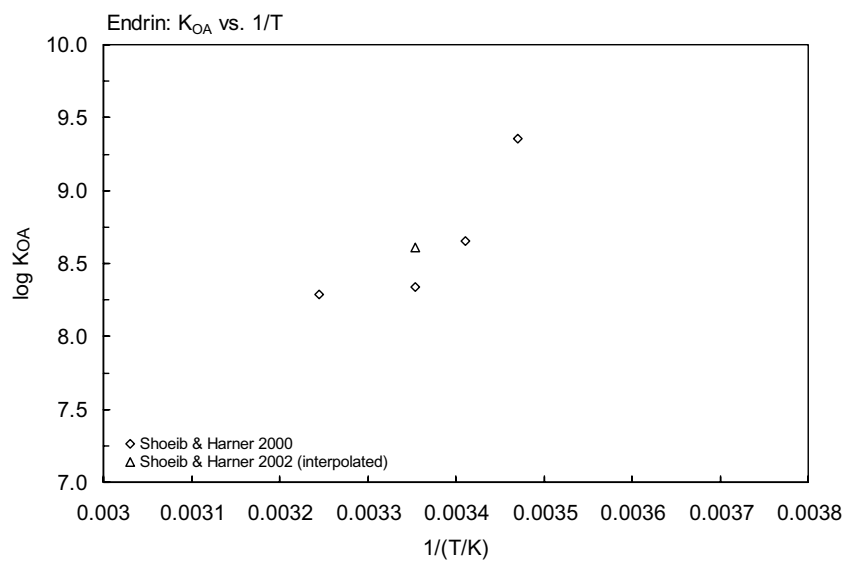
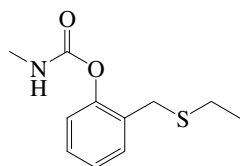


FIGURE 18.1.1.35.2 Logarithm of K_{OA} versus reciprocal temperature for endrin.

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 ($^{\circ}C$):

33.4 (Spencer 1982; Hartley & Kidd 1987, Montgomery 1993, Tomlin 1994)

Boiling Point ($^{\circ}C$):

decomposes on distillation (Hartley & Kidd 1987, Tomlin 1994)

Density (g/cm^3 at $20^{\circ}C$):

1.1473 (Hartley & Kidd 1987, Worthing & Walker 1987; Montgomery 1993)

1.231 ($20^{\circ}C$, 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 $25^{\circ}C$ (assuming $\Delta S_{fus} = 56 J/mol K$), F : 0.827 (mp at $33.4^{\circ}C$)

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$):

1900 ($20^{\circ}C$, Spencer 1982, Hartley & Kidd 1987, Montgomery 1993)

1820 ($20^{\circ}C$, Worthing & Walker 1987)

1800 ($20^{\circ}C$, Tomlin 1994)

Vapor Pressure (Pa at $25^{\circ}C$):

6.67×10^{-4} (Spencer 1982)

0.013 ($30^{\circ}C$, Hartley & Kidd 1987; Worthing & Walker 1987)

4.506×10^{-4} ($20^{\circ}C$, Montgomery 1993)

0.00045, 0.00094, 0.026 (20, 25, $50^{\circ}C$, Tomlin 1994)

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

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:

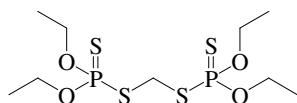
Biotransformation:

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 $t_{1/2} = 300$ d at pH 2, $t_{1/2} = 45$ h at pH 7 and $t_{1/2} = 5$ 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 ($^{\circ}C$):

−12 to −15 (Montgomery 1993; Tomlin 1994; Milne 1995)

−13 (Lide 2003)

Boiling Point ($^{\circ}C$):

164–165 (at 0.3 mmHg, Hartley & Kidd 1987; Howard 1991; Tomlin 1994; Milne 1995)

Density (g/cm^3 at $20^{\circ}C$):

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 $25^{\circ}C$ (assuming $\Delta S_{fus} = 56$ J/mol K), F: 1.0

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$ or as indicated):

2.0 (Metcalf 1971, 1974)

0.60 (Miles 1976; Miles & Harris 1978)

1.0 (20 – $25^{\circ}C$, selected, Willis & McDowell 1982; Gerstl & Helling 1987)

1.1 ($19.5^{\circ}C$, shake flask-GC, Bowman & Sans 1983b)

1.1 (20 – $25^{\circ}C$, selected, Wauchope et al. 1992; Hornsby et al. 1996)

0.68, 0.76 ($20^{\circ}C$, $30^{\circ}C$, Montgomery 1993)

2.0 (Tomlin 1994)

Vapor Pressure (Pa at $25^{\circ}C$):

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} ($20^{\circ}C$, selected, Suntio et al. 1988)

3.20×10^{-4} (20 – $25^{\circ}C$, 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·m³/mol at $25^{\circ}C$ or as indicated):

0.0699 (calculated-P/C, Lyman et al. 1982; quoted, Howard 1991)

0.032 ($20^{\circ}C$, 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 χ , 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, $t_{1/2}$:

Volatilization: using Henry's law constant, $t_{1/2} \sim 102$ 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 $t_{1/2} \sim 6.95$ 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);

$t_{1/2}$ (exptl) = 20.8 wk was determined in buffered distilled water at 30°C between pH 4 and 7, $t_{1/2} = 8.9$ wk at pH 8 and $t_{1/2} = 1$ d at pH 10 (Dierberg & Pfeuffer 1983; quoted, Howard 1991);

$t_{1/2} = 390$ d at pH 9 (Tomlin 1994).

Biodegradation: $t_{1/2} > 24$ wk in sterile sandy loam and $t_{1/2} = 7$ wk in nonsterile sandy loam; $t_{1/2} > 24$ wk in sterile organic soil and $t_{1/2} = 8.0$ wk in nonsterile organic soil (Miles et al. 1979; quoted, Howard 1991);

$t_{1/2} = 24$ –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: $t_{1/2} \sim 6.95$ h for the vapor-phase reaction with hydroxyl radical in air (Howard 1991).

Surface water: $t_{1/2} = 4$ wk in river water (Eichelberger & Lichtenberg 1971).

Ground water:

Sediment:

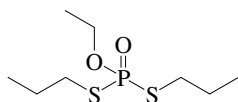
Soil: $t_{1/2} > 24$ wk in sterile sandy loam and $t_{1/2} = 7$ wk in nonsterile sandy loam; $t_{1/2} > 24$ wk in sterile organic soil and $t_{1/2} = 8.0$ wk in nonsterile organic soil (Miles et al. 1979; quoted, Howard 1991);

selected field $t_{1/2} = 150$ d (Wauchope et al. 1992; Hornsby et al. 1996);

$t_{1/2} = 90$ 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 ($^{\circ}C$): liquid

20 (Montgomery 1993)

Boiling Point ($^{\circ}C$):

86–91/0.2 mmHg (Spencer 1982; Hartley & Kidd 1987; Worthing & Walker 1987; Montgomery 1993; Tomlin 1994)

Density (g/cm^3 at $20^{\circ}C$):

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 $25^{\circ}C$ (assuming $\Delta S_{fus} = 56\ J/mol\ K$), F: 1.0

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$):

700 ($20^{\circ}C$, 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 $25^{\circ}C$):

0.0465 ($26^{\circ}C$, Hartley & Kidd 1987)

0.0465 ($20^{\circ}C$, Montgomery 1993)

0.0507 (selected, Wauchope et al. 1992; Hornsby et al. 1996)

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

0.0161 (calculated-P/C, Montgomery 1993; Majewski & Capel 1995)

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

3.59 ($21^{\circ}C$, 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, $t_{1/2}$:

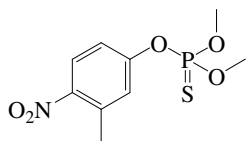
Hydrolysis: stable in water up to 100°C at pH 7, but rapidly hydrolyzed at 25°C at pH 7 (Worthing 1987; Tomlin 1994).

Half-Lives in the Environment:

Soil: $t_{1/2} \sim 87$ d in humus-containing soil at pH 4.5 and $t_{1/2} = 14\text{--}28$ d in sandy loam at pH 7.2–7.3 (Hartley & Kidd 1987; Montgomery 1993; Tomlin 1994);

field $t_{1/2} = 87$ d in organic soil, $t_{1/2} = 1\text{--}28$ d in sandy soil; others $t_{1/2} = 3\text{--}63$ d; recommended $t_{1/2} = 25$ 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 ($^{\circ}C$):

3.4 (Tomlin 1994)

Boiling Point ($^{\circ}C$):

164 (at 1 mmHg, Worthing & Hance 1991; Milne 1995)

140–145 (at 0.1 mmHg, dec., Tomlin 1994)

Density (g/cm^3 at $20^{\circ}C$):

1.328 (Worthing & Hance 1991; Tomlin 1994)

1.3227 ($25^{\circ}C$, 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 $25^{\circ}C$ (assuming $\Delta S_{fus} = 56 J/mol K$, F: 1.0)

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$ or as indicated):

30 (Macy 1948; Hamaker 1975; Kenaga 1980; Kenaga & Goring 1980)

30 ($20^{\circ}C$, Bright et al. 1950; Melnikov 1971; Hamaker 1975)

25.2 ($20^{\circ}C$, shake flask-GC, Bowman & Sans 1979)

38.7 (20 – $25^{\circ}C$, shake flask-GC, Kanazawa 1981)

21 ($20^{\circ}C$, Worthing & Hance 1991; Tomlin 1994)

30 (20 – $25^{\circ}C$, selected, Augustijn-Beckers et al. 1994; Hornsby et al. 1996)

30 ($21^{\circ}C$, Milne 1995)

Vapor Pressure (Pa at $25^{\circ}C$ or as indicated):

8.0×10^{-3} ($20^{\circ}C$, Melnikov 1971)

7.2×10^{-3} ($20^{\circ}C$, Freed et al. 1979)

8.0×10^{-4} ($20^{\circ}C$, 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} ($20^{\circ}C$, Worthing & Hance 1991)

1.3×10^{-4} (20 – $25^{\circ}C$, estimated, Augustijn-Beckers et al. 1994; Hornsby et al. 1996)

0.0180 ($20^{\circ}C$, 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 ($\text{Pa}\cdot\text{m}^3/\text{mol}$ 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, $\log K_{\text{OW}}$:

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, $\log \text{BCF}$:

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, $\log K_{\text{OC}}$:

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, $t_{1/2}$:

Volatilization: $t_{1/2} = 6.3$ d from the bottom of Palfrey Lake and $t_{1/2} = 7.2$ d from the surface of Palfrey Lake vs. a calculated $t_{1/2} = 20.6$ d; 0.9 d from Palfrey Brook vs. a calculated $t_{1/2} = 5.40$ d (Metcalf et al. 1980).

Photolysis: disappearance rate constant $k = 0.053 \text{ h}^{-1}$ with calculated first-order $t_{1/2} = 13 \text{ h}$ (Lacorte & Barcelo 1994).

Oxidation:

Hydrolysis: second-order alkaline hydrolysis rate constant $k = 4.2 \times 10^{-3} \text{ M}^{-1} \text{ s}^{-1}$ at 27°C (Maquire & Hale 1980; quoted, Wolfe 1980);

estimated half-lives at 22°C : $t_{1/2} \sim 108.8 \text{ d}$ at pH 4, $t_{1/2} \sim 84.3 \text{ d}$ at pH 7, and $t_{1/2} \sim 75 \text{ d}$ at pH 9 (Tomlin 1994).

Biodegradation: aerobic degradation $k = 2.3 \times 10^{-3} \text{ h}^{-1}$ with $t_{1/2} = 13.0 \text{ d}$ for control system, $k = 0.4 \times 10^{-3} \text{ h}^{-1}$ with $t_{1/2} = 73.0 \text{ d}$ for metabolism, $k = 5.3 \times 10^{-3} \text{ h}^{-1}$ with $t_{1/2} = 8.50 \text{ d}$ for co-metabolism; anaerobic degradation $k = 1.7 \times 10^{-3} \text{ h}^{-1}$ with $t_{1/2} = 17.0 \text{ d}$ for control system, $k = 3.9 \times 10^{-3} \text{ h}^{-1}$ with $t_{1/2} = 9.6 \text{ d}$ for metabolism, $k = 38.0 \times 10^{-3} \text{ h}^{-1}$ with $t_{1/2} = 1.0 \text{ d}$ 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:

$k_1 = 88 \text{ d}^{-1}$ (rainbow trout, Takimoto & Miyamoto 1976; quoted, McLeese et al. 1976)

$k_2 = 0.4 \text{ d}^{-1}$ (rainbow trout, Takimoto & Miyamoto 1976; quoted, McLeese et al. 1976)

$k_2 = 0.070 \text{ h}^{-1}$ (willow shiner, Tsuda et al. 1989)

$k_1 = (3.89 \pm 1.39) \times 10^{-3} \text{ mL g}^{-1} \text{ d}^{-1}$ (guppy, De Bruijn & Hermens 1991)

$k_2 = (1.13 \pm 0.07) \text{ d}^{-1}$ (guppy, De Bruijn & Hermens 1991)

$k_2 = 1.01 \text{ d}^{-1}$ (guppy, calculated- K_{OW} , De Bruijn & Hermens 1991)

$k_2 = (0.28 \pm 0.02) \times 10^{-3} \text{ (NADPH) min}^{-1} \cdot \text{mg protein}^{-1}$ (rainbow trout, De Bruijn et al. 1993)

$k_2 = (0.15 \pm 0.02) \times 10^{-3} \text{ (GSH) min}^{-1} \cdot \text{mg protein}^{-1}$ (rainbow trout, De Bruijn et al. 1993)

Half-Lives in the Environment:

Air:

Surface water: $t_{1/2} = 15\text{--}168 \text{ h}$ in summer, Palfrey Lake, Canada at pH 6.7, 11°C under sunlight conditions (Metcalf et al. 1980);

$t_{1/2} = 36\text{--}48 \text{ h}$ at pH 7.0–7.5, $19\text{--}23^\circ\text{C}$ under sunlight conditions, $t_{1/2} = 518\text{--}1188 \text{ h}$ at pH 7.5, 23°C under dark conditions in Lac Bourgeois, Quebec (Greenhalgh et al. 1980);

$t_{1/2} = 5.5 \text{ d}$ and 1.0 d under aerobic and anaerobic co-metabolism conditions, $t_{1/2} = 73 \text{ d}$ under aerobic metabolism condition (Liu et al. 1981)

$t_{1/2} = 13 \text{ h}$ in winter, irrigation ditch from Ebre Delta, Spain under sunlight conditions, at pH 7.8, 11°C (Lacorte & Barcelo 1994);

$t_{1/2} = 202 \text{ d}$ at 6°C , $t_{1/2} = 62 \text{ d}$ at 22°C in darkness for Milli-Q water at pH 6.1; $t_{1/2} = 103 \text{ d}$ at 6°C , $t_{1/2} = 31 \text{ d}$ at 22°C in darkness, $t_{1/2} = 4 \text{ d}$ under sunlight conditions for river water at pH 7.3; $t_{1/2} = 143 \text{ d}$ at 6°C , $t_{1/2} = 27 \text{ d}$ at 22°C in darkness for filtered water at pH 7.3; $t_{1/2} = 224 \text{ d}$ at 6°C , $t_{1/2} = 34 \text{ d}$ at 22°C in darkness, $t_{1/2} = 3 \text{ d}$ under sunlight conditions in seawater (Arcachon Bay, France) at pH 8.1, $22\text{--}25^\circ\text{C}$ (Lartiges & Garri gues 1995);

$t_{1/2} = 11\text{--}19.3 \text{ h}$ at pH 7.8–8.2, $25\text{--}20^\circ\text{C}$ under sunlight conditions in rice crop field; $t_{1/2} = 70\text{--}74 \text{ h}$ at pH 8.2, $15\text{--}18^\circ\text{C}$ under dark conditions from Ebre Delta, Spain (Oubina et al. 1996).

Ground water:

Sediment:

Soil: selected field $t_{1/2} = 4 \text{ d}$ (Augustijn-Beckers et al. 1994; Hornsby et al. 1996);

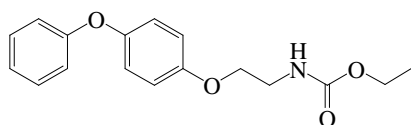
$t_{1/2} = 12\text{--}28 \text{ d}$ under upland conditions and $t_{1/2} = 4\text{--}20 \text{ d}$ under submerged conditions (Tomlin 1994).

Biota: excretion $t_{1/2} = 9.9 \text{ h}$ (willow shiner, Tsuda et al. 1989);

elimination rate constants $k = (0.28 \pm 0.02) \times 10^3 \text{ (NADPH)}$ and $(0.15 \pm 0.02) \times 10^3 \text{ (GSH) min}^{-1} \cdot \text{mg protein}^{-1}$ (rainbow trout, De Bruijn et al. 1993);

degradation $t_{1/2} = 4 \text{ d}$ 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: C₁₇H₁₉NO₄

Molecular Weight: 301.338

Melting Point (°C):

53 (Lide 2003)

Boiling Point (°C):

Density (g/cm³ at 20°C):

1.23 (Tomlin 1994)

Molar Volume (cm³/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/m³ 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·m³/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}:

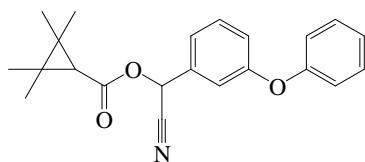
3.00 (20–25°C, estimated, Hornsby et al. 1996)

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

Half-Lives in the Environment:

Soil: t_{1/2} = 1.7–2.5 months in laboratory soil and water and t_{1/2} = few days to 31 d in field soil and water (Tomlin 1994);
field t_{1/2} = 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 ($^{\circ}C$):

47 (Lide 2003)

Boiling Point ($^{\circ}C$):

Density (g/cm^3 at $20^{\circ}C$):

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 $25^{\circ}C$ (assuming $\Delta S_{fus} = 56 J/mol K$), F : 0.608 (mp at $47^{\circ}C$)

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$):

0.33 (Hartley & Kidd 1987)

0.0141 (Tomlin 1994)

0.33 (selected, Augustijn-Beckers et al. 1994)

Vapor Pressure (Pa at $25^{\circ}C$):

0.00073 ($20^{\circ}C$, 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 ($Pa \cdot m^3/mol$ at $25^{\circ}C$):

Octanol/Water Partition Coefficient, $\log K_{ow}$:

6.0 ($20^{\circ}C$, 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, $t_{1/2} = 2.7$ wk in river water (Hartley & Kidd 1987; Tomlin 1994).

Ground water:

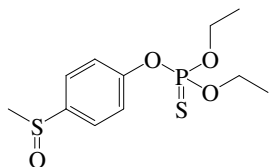
Sediment:

Soil: duration of activity in soil 1–5 d (Hartley & Kidd 1987; Tomlin 1994);

reported field $t_{1/2} = 8$ –144 d, recommended field $t_{1/2} = 5$ 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-methylsulphonylphenyl 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 ($^{\circ}C$):

yellow-brown oil (Spencer 1982; Hartley & Kidd 1987)

< 25 (Montgomery 1993)

Boiling Point ($^{\circ}C$):

138–141/0.01 mmHg (Hartley & Kidd 1987, Worthing & Walker 1987; Howard 1991)

Density (g/cm^3):

1.202 ($20^{\circ}C$, 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 $25^{\circ}C$, F : 1.0

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$):

1600 (Spencer 1982)

2000 ($20^{\circ}C$, 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 $25^{\circ}C$):

9.09×10^{-5} (Howard 1991)

6.67×10^{-3} (selected, Augustijn-Beckers et al. 1994; Hornsby et al. 1996)

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

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 EUROSOLS 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 EUROSOLS 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 EUROSOLS 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: $t_{1/2} = 58\text{--}87$ d over pH range of 4.5–8.0 at 25°C in pure water (Howard 1991).

Biodegradation: field $t_{1/2} \sim 30$ d (estimated, Augustijn-Becker et al. 1994).

Biotransformation:

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

$k_2 = 0.17 \text{ h}^{-1}$ (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: $t_{1/2} = 58\text{--}87$ d in pure water at 25°C over the pH range of 4.5–8.0 (Howard 1991).

Ground water:

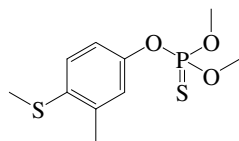
Sediment:

Soil: $t_{1/2} < 1$ wk to several weeks in soil (Howard 1991);

field $t_{1/2} = 3$ to 182 d and $t_{1/2} \sim 30$ 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: $C_{10}H_{15}O_3PS_2$

Molecular Weight: 278.328

Melting Point ($^{\circ}C$):

7.0 (Montgomery 1993)

7.5 (Tomlin 1994; Milne 1995)

Boiling Point ($^{\circ}C$):

87.0 (at 0.01 mmHg, Hartley & Kidd 1987; Worthing & Hance 1991; Montgomery 1993; Tomlin 1994; Milne 1995)

Density (g/cm^3 at $20^{\circ}C$):

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 $25^{\circ}C$ (assuming $\Delta S_{fus} = 56$ J/mol K), F: 1.0

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$ or as indicated):

55 (Günther et al. 1968; Martin & Worthing 1977; Budavari 1989)

54–56 (rm. temp., Spencer 1973, 1980)

56 ($22^{\circ}C$, Khan 1980)

55 ($22^{\circ}C$, Verschueren 1983)

7.51 ($20^{\circ}C$, shake flask-GC, Bowman & Sans 1983a, b)

9.3 ($20^{\circ}C$, shake flask-GC, Bowman & Sans 1985)

54–56 ($20^{\circ}C$, Hartley & Kidd 1987)

2.0 ($20^{\circ}C$, Worthing & Walker 1987; Worthing & Hance 1991; Milne 1995)

2.0, 4.2, 7.51, 9.3, 50 ($20^{\circ}C$, literature data variability, Heller et al. 1989)

4.2 (20 – $25^{\circ}C$, selected, Wauchope et al. 1992; Lohninger 1994; Hornsby et al. 1996)

9.30, 11.3 ($20^{\circ}C$, $30^{\circ}C$, Montgomery 1993)

4.2 ($20^{\circ}C$, Tomlin 1994)

Vapor Pressure (Pa at $25^{\circ}C$ or as indicated and reported temperature dependence equations):

4.0×10^{-3} ($20^{\circ}C$, Eichler 1965)

4.0×10^{-3} ($20^{\circ}C$, Melnikov 1971)

4.0×10^{-3} ($20^{\circ}C$, Hartley & Graham-Bryce 1980)

4.0×10^{-3} ($20^{\circ}C$, Khan 1980; Budavari 1989; Worthing & Hance 1991; Montgomery 1993)

8.4×10^{-3} ($20^{\circ}C$, 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·m³/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, $t_{1/2}$:

Volatilization:

Photolysis:

Oxidation:

Hydrolysis: $t_{1/2} = 223$ d at pH 4, $t_{1/2} = 200$ d at pH 7, and $t_{1/2} = 151$ d at pH 9 at 22°C (Tomlin 1994).

Biodegradation: rate constants $k = -0.00745 \text{ h}^{-1}$ in nonsterile sediment and $k = -0.00199 \text{ h}^{-1}$ in sterile sediment by shake-tests at Range Point and $k = -0.00129 \text{ h}^{-1}$ in nonsterile water by shake-tests at Range Point (Walker et al. 1988).

Biotransformation:

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

$k_1 = (8.81 \pm 0.72) \times 10^{-3} \text{ mL g}^{-1} \text{ d}^{-1}$ (guppy, De Bruijn & Hermens 1991)

$k_2 = (0.60 \pm 0.02) \text{ d}^{-1}$ (guppy, De Bruijn & Hermens 1991)

$k_2 = 0.42 \text{ d}^{-1}$ (guppy, calculated- K_{OW} , De Bruijn & Hermens 1991)

$k_2 = 0.07 \text{ h}^{-1}$ (whole body willow shiner, Tsuda et al. 1992)

$k_2 = 0.34 \text{ h}^{-1}$ (carp, Tsuda et al. 1992)

$k_2 = (0.64 \pm 0.09) \times 10^{-3} \text{ (NADPH) min}^{-1} \cdot \text{mg protein}^{-1}$ (rainbow trout, De Bruijn et al. 1993)

$k_2 = (0.12 \pm 0.02) \times 10^{-3} \text{ (GSH) min}^{-1} \cdot \text{mg protein}^{-1}$ (rainbow trout, De Bruijn et al. 1993)

$k_2 = 0.14 \text{ h}^{-1}$ (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);

$t_{1/2} = 189 \text{ d}$ at 6°C , 71 d at 2°C in darkness for Mill-Q water at pH 6.1; $t_{1/2} = 149 \text{ d}$ at 6°C , $t_{1/2} = 42 \text{ d}$ at 22°C in darkness, $t_{1/2} = 2 \text{ d}$ under sunlight conditions for river water at pH 7.3; $t_{1/2} = 104 \text{ d}$ at 6°C , $t_{1/2} = 33 \text{ d}$ at 22°C in darkness for filtered river water, pH 7.3; $t_{1/2} = 227 \text{ d}$ at 6°C , $t_{1/2} = 26 \text{ d}$ at 22°C in darkness, $t_{1/2} = 5 \text{ d}$ under sunlight conditions for seawater at pH 8.1 (Lartiges & Garrigues 1995).

Ground water:

Sediment:

Soil: selected field $t_{1/2} = 34 \text{ d}$ (Wauchope et al. 1992; Hornsby et al. 1996);

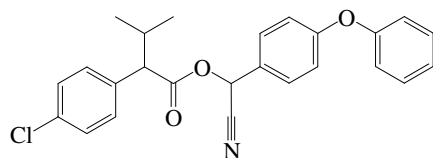
$t_{1/2} \sim 1 \text{ d}$ in soil and water (Tomlin 1994).

Biota: excretion rate constant $k = 0.07 \text{ h}^{-1}$ from whole body willow shiner (Tsuda et al. 1992);

elimination rate constants $k = (0.64 \pm 0.09) \times 10^{-3} \text{ (NADPH)}$ and $k = (0.12 \pm 0.02) \times 10^{-3} \text{ (GSH) min}^{-1} \cdot \text{mg protein}^{-1}$ (rainbow trout, De Bruijn et al. 1993);

excretion rate constant $k = 0.34 \text{ h}^{-1}$ with $t_{1/2} = 2.0 \text{ d}$ 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, Somicidin, 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 ($^{\circ}C$): liquid

Boiling Point ($^{\circ}C$):

decomposes on distillation (Hartley & Kidd 1987; Tomlin 1994)

Density (g/cm^3 at $20^{\circ}C$):

1.26 (22 $^{\circ}C$, Spencer 1982)

1.17 (23 $^{\circ}C$, Hartley & Kidd 1987; Milne 1995)

1.175 (tech. grade at 25 $^{\circ}C$, 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 $^{\circ}C$ (assuming $\Delta S_{fus} = 56$ J/mol K), F: 1.0

Water Solubility (g/m^3 or mg/L at 25 $^{\circ}C$ or as indicated):

0.085 (shake flask-GC, Coats & O'Donnell-Jafferey 1979)

0.085 (Verschuereen 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 $^{\circ}C$, Worthing 1979, 1987; Spencer 1982)

<1.0 (20 $^{\circ}C$, Hartley & Kidd 1987; Montgomery 1993; Milne 1995)

<0.02 (Davies & Lee 1987; quoted, Kawamoto & Urano 1989)

<1.0 (tech. grade at 20 $^{\circ}C$, Worthing & Walker 1991)

0.002 (20–25 $^{\circ}C$, selected, Wauchope 1989; Wauchope et al. 1992; Hornsby et al. 1996)

Vapor Pressure (Pa at 25 $^{\circ}C$ or as indicated):

4.90×10^{-7} (Barlow 1978)

3.07×10^{-5} (Worthing 1979)

1.33×10^{-5} (22 $^{\circ}C$, 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 $^{\circ}C$, selected, Wauchope et al. 1992; Hornsby et al. 1996)

1.92×10^{-7} (20 $^{\circ}C$, Tomlin 1994)

1.78×10^{-6} (solid P^S , converted from P_L determined by GC-RT correlation, Tsuzuki 2001)

Henry's Law Constant ($\text{Pa}\cdot\text{m}^3/\text{mol}$ 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, $\log K_{\text{OW}}$ 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, $\log \text{BCF}$:

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	(<i>Oncorhynchus mykiss</i> , Muir et al. 1994; quoted, Devillers et al. 1996)
2.70	(calculated, Pait et al. 1992)

Sorption Partition Coefficient, $\log K_{\text{OC}}$:

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 $k(\text{aerobic}) = 0.055 \text{ d}^{-1}$ with $t_{1/2} = 13 \text{ d}$ at 20°C by aerobic activated sludge, and $k(\text{anaerobic}) = 0.055 \text{ d}^{-1}$ with $t_{1/2} = 13 \text{ d}$ at 20°C by anaerobic microorganisms (batch contacting method, Kawamoto & Urano 1990).

Half-Lives in the Environment:

Air:

Surface water: $t_{1/2} = 14 \text{ d}$ in 100 mL of a pesticide-seawater solution under outdoor light, $t_{1/2} > 14 \text{ d}$ under outdoor dark condition and $t_{1/2} > 28 \text{ d}$ under indoor condition (Schimmel et al. 1983);

$t_{1/2} = 27\text{--}42$ 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:

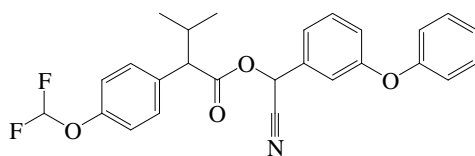
Sediment: $t_{1/2} = 34$ d in 10 g of sediment/100 mL of a pesticide-seawater solution in untreated condition and $t_{1/2} > 28$ d in sterile condition (Schimmel et al. 1983).

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-phenoxyphenyl)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 ($^{\circ}C$):

<25 (dark amber liquid, Montgomery 1993)

Boiling Point ($^{\circ}C$):

108.0 (at 0.35 mmHg, Hartley & Kidd 1987; Worthing & Hance 1991; Montgomery 1993; Tomlin 1994; Milne 1995)

Density (g/cm^3 at $20^{\circ}C$):

1.189 ($22^{\circ}C$, Hartley & Kidd 1987; Montgomery 1993; Tomlin 1994; Milne 1995)

1.190 ($22^{\circ}C$, Worthing & Hance 1991)

Molar Volume (cm^3/mol):

499.9 (calculated-Le Bas method at normal boiling point)

379.4 ($22^{\circ}C$, calculated-density)

Dissociation Constant, pK_a :

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

Entropy of Fusion, ΔS_{fus} (J/mol K):

Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S_{fus} = 56$ J/mol K), F: 1.0

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$ or as indicated):

0.049 (in seawater, Schimmel et al. 1983)

0.50 ($21^{\circ}C$, Hartley & Kidd 1987; Worthing & Walker 1987, 1991; Tomlin 1994; Milne 1995)

0.06 (20 – $25^{\circ}C$, selected, Wauchope 1989; Hornsby et al. 1996)

0.50 ($21^{\circ}C$, Montgomery 1993)

Vapor Pressure (Pa at $25^{\circ}C$ 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 – $25^{\circ}C$, 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 ($Pa \cdot m^3/mol$ at $25^{\circ}C$ or as indicated):

8187 (21 – $25^{\circ}C$, 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)
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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, $t_{1/2}$:

Volatilization:

Photolysis: $t_{1/2} \sim 21$ d for degradation on soil plates by simulated sunlight and $t_{1/2} = 4.0$ d in aqueous solutions (Tomlin 1994).

Oxidation:

Hydrolysis: $t_{1/2} = 40, 52,$ 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: $t_{1/2} = 34$ d in an estuarine environment (Schimmel et al. 1983; quoted, Montgomery 1993).

Ground water:

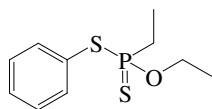
Sediment:

Soil: $t_{1/2} \sim 2$ months in soil (Tomlin 1994);

field $t_{1/2} = 21$ 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/cm³ at 20°C):

1.160 (25°C, Hartley & Kidd 1987; Tomlin 1994; Milne 1995)

1.154 (Worthing & Hance 1991; Montgomery 1993)

Molar Volume (cm³/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 $\Delta S_{fus} = 56$ J/mol K), F: 1.0

Water Solubility (g/m³ 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·m³/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, $t_{1/2}$:

Volatilization:

Photolysis: $t_{1/2} = 12$ d in water at pH 5 and 25°C (Worthing & Hance 1991; Tomlin 1994).

Oxidation:

Hydrolysis: alkaline chemical hydrolysis rate constant $k = 1 \times 10^{-4} \text{ M}^{-1} \text{ s}^{-1}$ with $t_{1/2} > 365$ d (selected, sediment/water, Schnoor & McAvoy 1981; quoted, Schnoor 1992);

hydrolysis $t_{1/2} = 74$ –127 d in water at 40°C and pH 7, $t_{1/2} = 101$ 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);

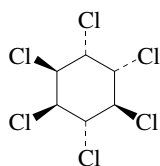
$t_{1/2} > 24$ wk in sterile sandy loam and $t_{1/2} = 3.0$ wk in nonsterile sandy loam; $t_{1/2} > 24$ wk in sterile organic soil and $t_{1/2} = 4.0$ wk in nonsterile organic soil (Miles et al. 1979);

$t_{1/2} = 60$ d from screening model calculations (Jury 1987b);

$t_{1/2} = 16.5$ –28 d at 24°C (Worthing & Hance 1991);

selected field $t_{1/2} = 40$ d (Wauchope et al. 1992; quoted, Richards & Baker 1993; Hornsby et al. 1996).

Biota: biochemical $t_{1/2} = 60$ 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, (1 α , 2 α , 3 α , 4 α , 5 β , 6 β -1, 2, 3, 4, 5, 6-hexachloro-cyclohexane

CAS Registry No: 319-84-6

Molecular Formula: C₆H₆Cl₆

Molecular Weight: 290.830

Melting Point (°C):

158 (Lide 2003)

Boiling Point (°C): 288

Density (g/cm³ at 20°C):

Molar Volume (cm³/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 $\Delta S_{\text{fus}} = 56$ J/mol K), F: 0.0496 (mp at 158°C)

Water Solubility (g/m³ 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 ($Pa \cdot m^3/mol$ or at $25^\circ C$ 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* ($23^\circ C$, gas stripping-GC/ECD, distilled water, measured range 0.5 – $45^\circ C$, Kucklick et al. 1991)

$\log [H/(Pa \cdot m^3 \cdot mol^{-1})] = -2810/(T/K) + 9.31$, temp range 0.5 – $45^\circ C$ (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 , $45^\circ C$, gas stripping-GC/ECD, artificial seawater, Kucklick et al. 1991)

$\log [H/(Pa \cdot m^3 \cdot mol^{-1})] = -2969/(T/K) + 9.88$, temp range 0.5 – $45^\circ C$ (gas stripping-GC measurements, artificial seawater, Kucklick et al. 1991)

0.87 ($20^\circ C$), 2.40, 1.10, 0.677, 0.710 ($23^\circ C$) (quoted, Iwata et al. 1993)

0.215, 0.491, 0.373, 0.630, 0.630 ($8.5^\circ C$ in Green Bay, $18.9^\circ C$ in Lake Michigan, $18.5^\circ C$ in Lake Huron, $22.3^\circ C$ in Lake Erie, $22.3^\circ C$ 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)

$\log [H/(Pa \cdot m^3/mol)] = 8.98 - 1714/(T/K)$ (Passivirta et al. 1999)

0.43* ($20^\circ C$, gas stripping-GC, measured range 10 – $40^\circ C$, Jantunen et al. 2000)

$\log [H/(Pa \cdot m^3/mol)] = 10.88 - 3298/(T/K)$; temp range 10 – $40^\circ C$ (gas stripping-GC, Jantunen et al. 2000)

0.53 ($20^\circ C$, 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* ($20^\circ C$, dynamic headspace-GC, DHS method, measured range 5 – $35^\circ C$, Sahsuvar et al. 2003)

0.42* ($20^\circ C$, gas stripping-GC, BS method, measured range 5 – $35^\circ C$, Sahsuvar et al. 2003)

0.39* ($20^\circ C$, mean value of DHS and BS methods, temp range 5 – $35^\circ C$, Sahsuvar et al. 2003)

$\log [H/(Pa \cdot m^3/mol)] = 10.13 - 3088/(T/K)$; temp range 5 – $35^\circ C$ (Sahsuvar et al. 2003)

0.646, 0.741 (LDV literature-derived value, FAV final adjusted value, Xiao et al. 2004)

$\log [H/(Pa \cdot m^3/mol)] = -3171/(T/K) + 10.45$ (LDV linear regression of literature data, Xiao et al. 2004)

$\log [H/(Pa \cdot m^3/mol)] = -3099/(T/K) + 10.26$ (FAV final adjusted eq., Xiao et al. 2004)

Octanol/Water Partition Coefficient, $\log K_{OW}$ at $25^\circ C$ 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)

$3.79^* \pm 0.001$ (shake flask-slow stirring-GC, measured range 5 – $45^\circ C$, 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, Sugiura 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 $t_{1/2} \sim 6$ 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);

$t_{1/2} \sim 500$ 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 $t_{1/2} \sim 2.3$ d based on reaction with OH radical at 25°C (Atkinson 1987);

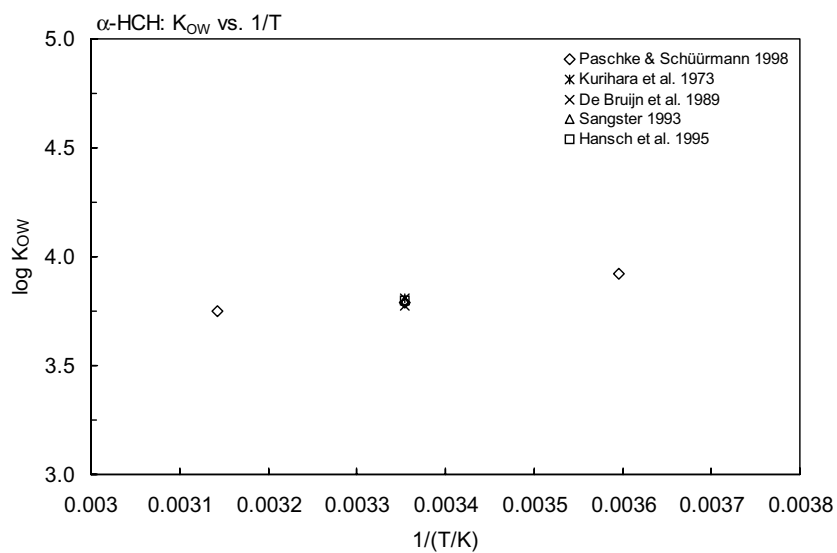


FIGURE 18.1.1.47.2 Logarithm of K_{OW} versus reciprocal temperature for α -HCH.

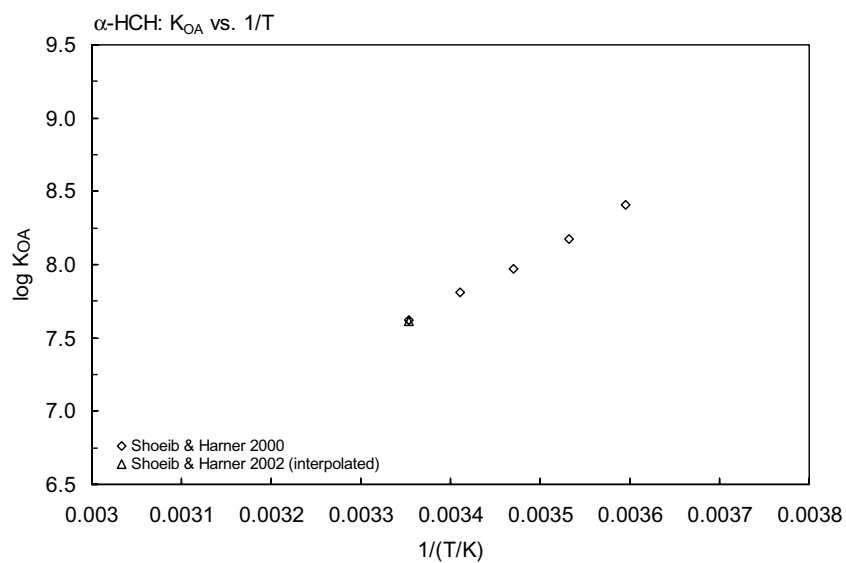


FIGURE 18.1.1.47.3 Logarithm of K_{OA} versus reciprocal temperature for α -HCH.

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)		
$\ln (k_H/\text{atm}) = A - B/(T/K)$		(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)
			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 m³/mol)	22.3	0.630	eq. 4a	H/(Pa m³/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 m³/mol)					20	0.39
A	9.88					30	0.85
B	2969					35	1.30
						eq. 4a	H/(Pa m³/mol)
						A	10.13 ± 0.29
						B	3088 ± 84
							enthalpy of transfer air-water
							$\Delta H_{wA}/(\text{kJ mol}^{-1}) = 59.3$

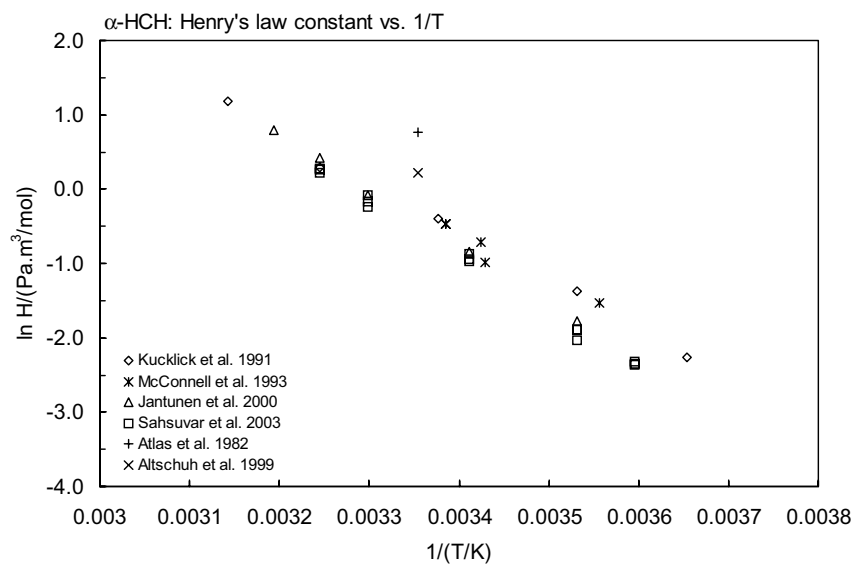
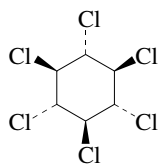


FIGURE 18.1.1.47.4 Logarithm of Henry's law constant versus reciprocal temperature for α -HCH.

18.1.1.48 β -HCH

Common Name: β -HCH

Synonym: β -BHC, β -Hexachlorocyclohexane, $1\alpha,2\beta,3\alpha,4\beta,5\alpha,6\beta$ -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 ($^{\circ}C$):

309 (Slade 1945; Ballschmiter & Wittlinger 1991)

Boiling Point ($^{\circ}C$):

Density (g/cm^3 at $20^{\circ}C$):

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 $25^{\circ}C$ (assuming $\Delta S_{fus} = 56 J/mol K$, F: 0.00164 (mp at $309^{\circ}C$))

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$ or as indicated and reported temperature dependence equations):

- 5.0 ($20^{\circ}C$, Slade 1945; Gunther et al. 1968; Horvath 1982)
- 0.70 ($20^{\circ}C$, shake flask-GC, Kanazawa et al. 1971)
- 0.20, 0.13 ($28^{\circ}C$, shake flask-centrifuge, membrane filter-GC, max. $0.1 \mu m$ particle size, Kurihara et al. 1973)
- 0.70 ($20^{\circ}C$, Brooks 1974)
- 0.24 (generator column-GC/ECD, Weil et al. 1974)
- 0.13–0.70 (Callahan et al. 1979)
- 2.04 ($20^{\circ}C$, 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)
- $\log [S_L/(mol m^{-3})] = -110.1/(T/K) - 0.211$ (supercooled liquid, final adjusted eq., Xiao et al. 2004)

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

- 0.67* ($20^{\circ}C$, static method, measured range 20 – $60^{\circ}C$, Slade 1945)
- 3.73×10^{-5} * ($20^{\circ}C$, effusion-manometer, measured range 0 – $110^{\circ}C$, Balson 1947)
- 4.90×10^{-5} ($20^{\circ}C$, 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 $25^{\circ}C$ 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 – $25^{\circ}C$, 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)
 $\log [H/(\text{Pa m}^3/\text{mol})] = 9.96 - 3400/(T/K)$; 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)
 $\log [H/(\text{Pa m}^3/\text{mol})] = -3454/(T/K) + 10.16$ (LDV linear regression of literature data, Xiao et al. 2004)
 $\log [H/(\text{Pa m}^3/\text{mol})] = -3673/(T/K) + 10.89$ (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)
 $3.88^* \pm 0.01$ (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 χ , 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, $t_{1/2}$:

Volatilization:

Photolysis:

Hydrolysis:

Oxidation:

Biodegradation: calculated $t_{1/2} = 178$ h in sewage sludge from experiments S1–S3 (Buser & Müller 1995).

Biotransformation:

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

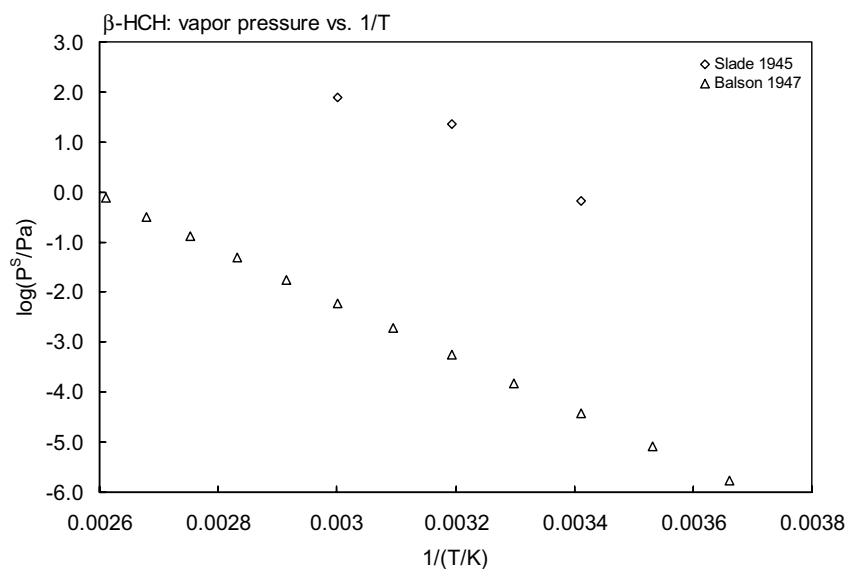
$k_1 = 0.46 \text{ d}^{-1}$, 0.33 d^{-1} , 0.53 d^{-1} , and 0.18 d^{-1} (golden orfe, carp, brown trout, and guppy at steady state, Sugiura et al. 1979)

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	$\ln H = A - B/(t/K)$ H/(Pa m ³ /mol)	
		80	0.04933		
		90	0.1293	A	9.96 ± 0.23
		100	0.3200	B	3400 ± 68
		110	0.7653		
		$\log P = A - B/(T/K)$ P/mmHg		enthalpy of transfer air-water $\Delta H_{WA}/(\text{kJ mol}^{-1}) = 65.1$	
		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.

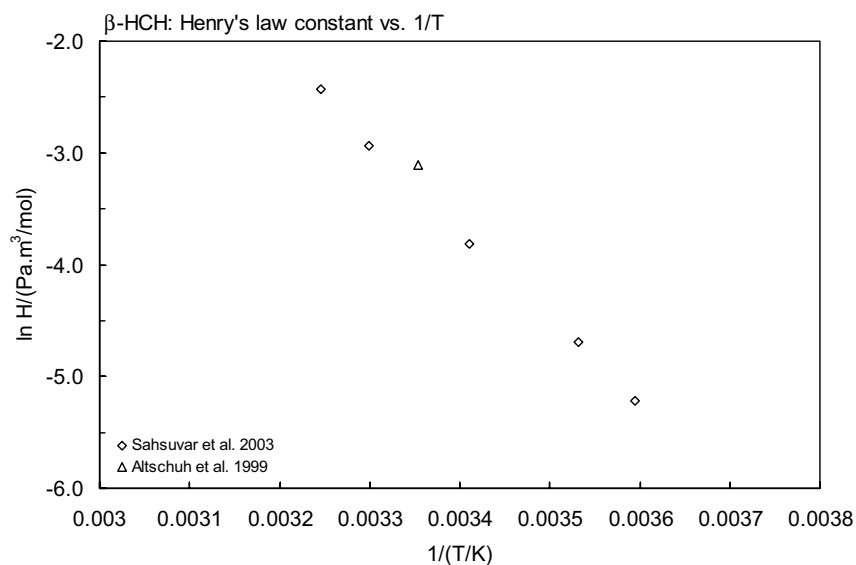


FIGURE 18.1.1.48.2 Logarithm of Henry's law constant versus reciprocal temperature for β-HCH.

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
		35	8.3682
		25	8.875
enthalpy of phase transfer: ΔH _{OW} /(kJ mol ⁻¹) = - 8.20		log K _{OA} = A + B/(T/K)	
entropy of phase transfer: ΔS _{OW} /(J K ⁻¹ mol ⁻¹) = 62.7		A	-7.692
		B	4937
		enthalpy of phase change ΔH _{OA} /(kJ mol ⁻¹) = 94.5	

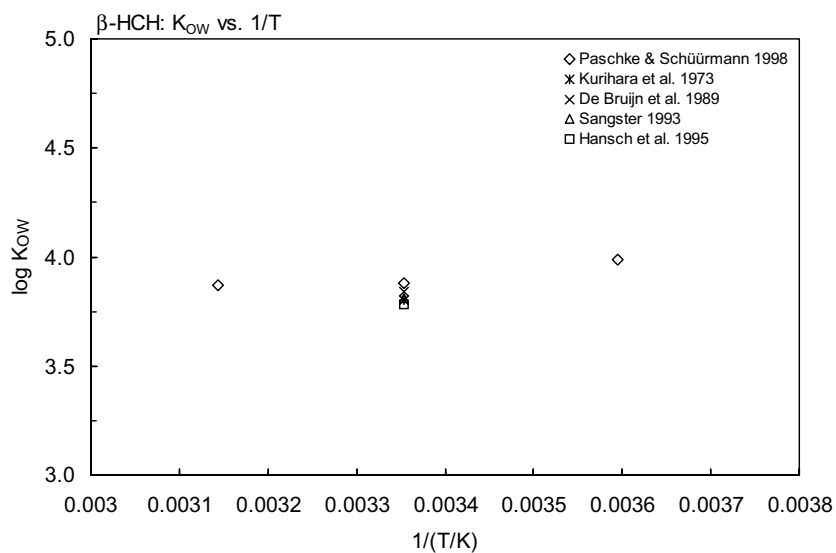


FIGURE 18.1.1.48.3 Logarithm of K_{OW} versus reciprocal temperature for β -HCH.

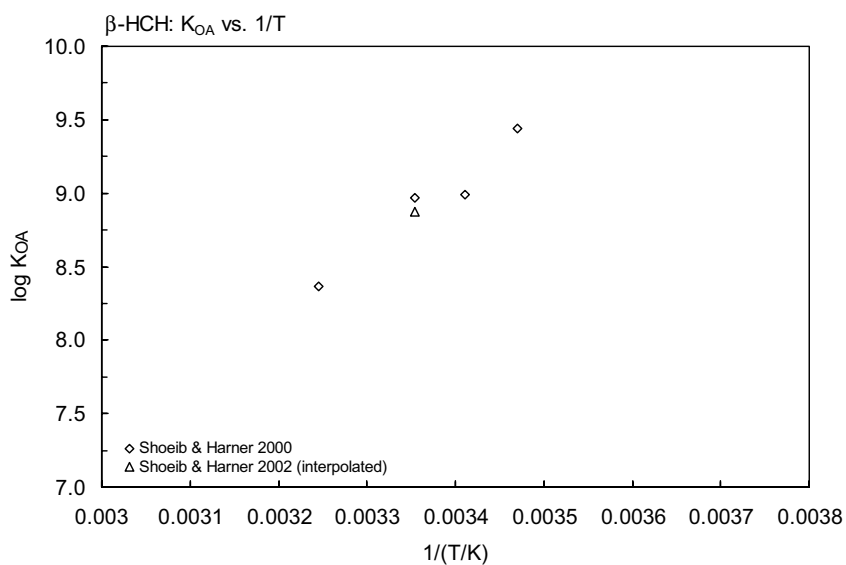
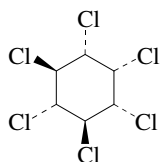


FIGURE 18.1.1.48.4 Logarithm of K_{OA} versus reciprocal temperature for β -HCH.

18.1.1.49 δ -HCH

Common Name: δ -HCH

Synonym: δ -BHC, δ -Hexachlorocyclohexane, $1\alpha,2\alpha,3\alpha,4\beta,5\alpha,6\beta$ -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 ($^{\circ}C$):

141.5 (Lide 2003)

Boiling Point ($^{\circ}C$):

Density (g/cm^3 at $20^{\circ}C$):

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 $25^{\circ}C$ (assuming $\Delta S_{fus} = 56$ J/mol K), F: 0.0719 (mp at $141.5^{\circ}C$)

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$ or as indicated):

10 ($20^{\circ}C$, Slade 1945)

15.7, 10.7 ($28^{\circ}C$, shake flask-centrifuge, membrane filter-GC, max. $0.1 \mu m$ particle size, Kurihara et al. 1973)

11.6, 8.64 ($28^{\circ}C$, shake flask-centrifuge, sonic and centrifuge-GC, max. $0.05 \mu m$ particle size, Kurihara et al. 1973)

8.64–31.4 (shake flask-GC, Kurihara et al. 1973)

10 ($20^{\circ}C$, quoted, Günther et al. 1968)

21.3 ($20^{\circ}C$, shake flask-GC, Kanazawa et al. 1971)

31.4 (generator column-GC/ECD, Weil et al. 1974)

9.01 ($20^{\circ}C$, Deutsche Forschungsgemeinschaft 1983; Ballschmiter & Wittlinger 1991; Fischer et al. 1991)

Vapor Pressure (Pa at $25^{\circ}C$ or as indicated. Additional data at other temperatures designated * are compiled at the end of this section):

2.67* ($20^{\circ}C$, static method, measured range 20 – $60^{\circ}C$, Slade 1945)

2.27×10^{-3} * ($20^{\circ}C$, effusion manometer, Balson 1947)

0.150 (GC-RT correlation, Watanabe & Tatsukawa 1989)

0.0309 (supercooled liquid value, Majewski & Capel 1995)

Henry's Law Constant ($Pa \cdot m^3/mol$ at $25^{\circ}C$ or as indicated):

0.018 (20 – $25^{\circ}C$, 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 $25^{\circ}C$ 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, $t_{1/2}$:

Biodegradation: calculated $t_{1/2} = 126$ 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	ΔH _{OW} /(kJ mol ⁻¹) = − 7.60		25	8.848
		60	0.2780	entropy of phase transfer:			
		70	0.7866	ΔS _{OW} /(J K ⁻¹ mol ⁻¹) = 69.9		log K _{OA} = A + B/(T/K)	
						A	−7.447
						B	4856
		log P = A − B/(T/K)					
		eq. 1	P/mmHg				
		A	12.635			enthalpy of phase change	
		B	5100			ΔH _{OA} /(kJ mol ⁻¹) = 93.0	
		temp range: 55–75°C					

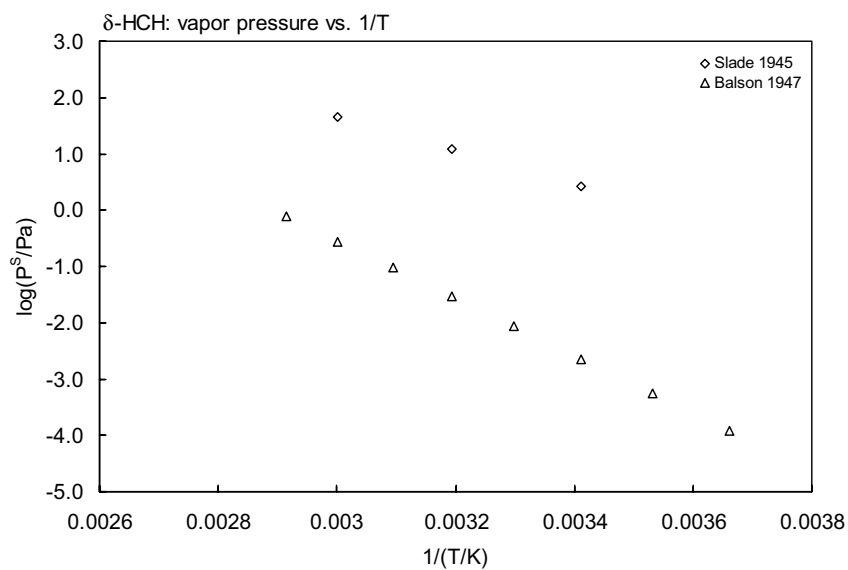


FIGURE 18.1.1.49.1 Logarithm of vapor pressure versus reciprocal temperature for δ-HCH.

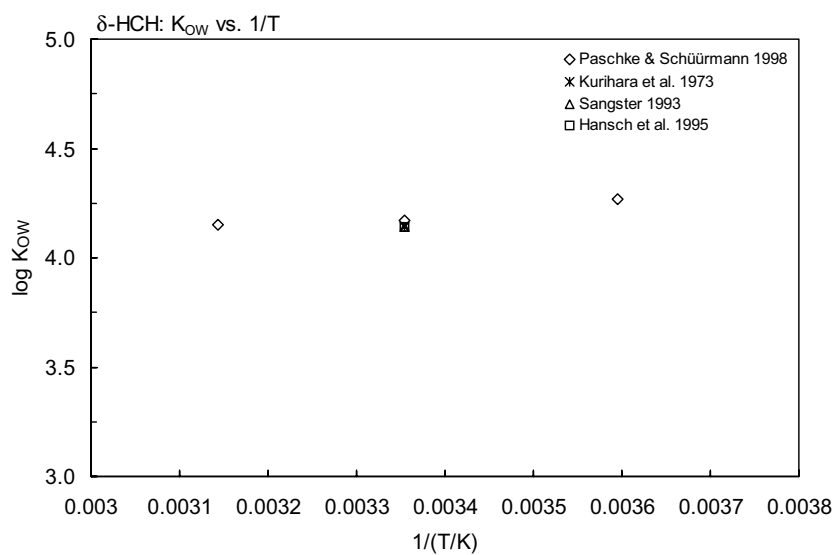


FIGURE 18.1.1.49.2 Logarithm of K_{OW} versus reciprocal temperature for δ-HCH.

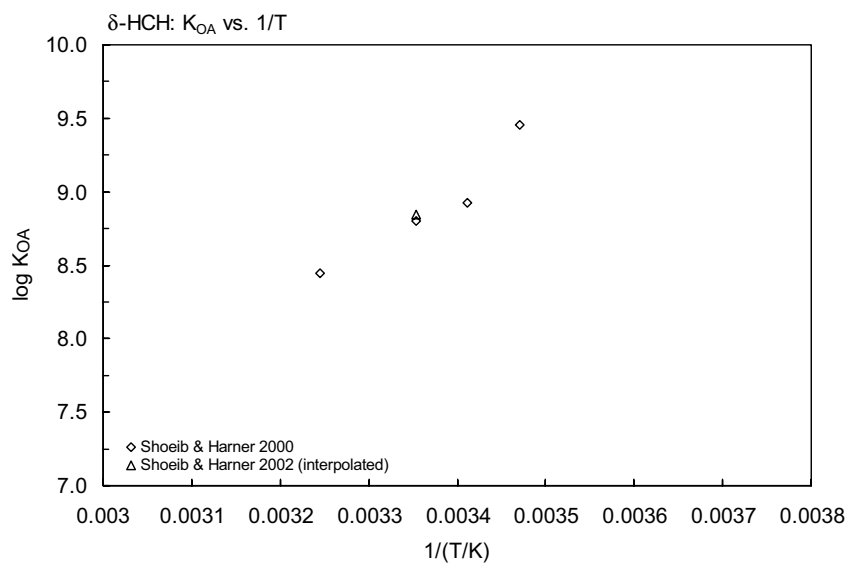
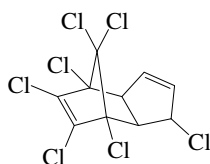


FIGURE 18.1.1.49.3 Logarithm of K_{OA} versus reciprocal temperature for δ -HCH.

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-heptachloro-dicyclopentadiene

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 ($^{\circ}C$):

95.5 (Lide 2003)

Boiling Point ($^{\circ}C$):

135–145 (at 1–1.5 mmHg, Montgomery 1993; Tomlin 1994)

Density (g/cm^3 at $20^{\circ}C$):

1.65–1.67 ($25^{\circ}C$, 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 $25^{\circ}C$ (assuming $\Delta S_{fus} = 56 J/mol K$), F: 0.203 (mp at $95.5^{\circ}C$)

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$ or as indicated. Additional data at other temperatures designated * are compiled at the end of this section):

0.056 ($25-29^{\circ}C$, 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 $15-45^{\circ}C$, 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 ($25-29^{\circ}C$, Worthing & Hance 1991; Tomlin 1994)

0.18 (Montgomery 1993)

0.056 ($20-25^{\circ}C$, 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)

$\log [C_L/(mol m^{-3})] = -770/(T/K) + 0.13$ (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)
- $\log (P_s/\text{Pa}) = 14.977 - 4966.6/(T/K)$; measured range 36.4–95.6°C (solid, gas saturation-GC, Rordorf 1989)
- $\log (P_L/\text{Pa}) = 11.811 - 3816.5/(T/K)$; 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)
- $\log (P_L/\text{Pa}) = 11.88 - 3995/(T/K)$ (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)
- $\log (P_L/\text{Pa}) = -3870/(T/K) + 12.11$ (supercooled liquid, linear regression of literature data, Shen & Wania 2005)

Henry's Law Constant ($\text{Pa}\cdot\text{m}^3/\text{mol}$ 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 $k = 3.0 \text{ d}^{-1}$ (Glotfelty et al. 1984; quoted, Glotfelty et al. 1989);
 calculated rate constant $k = 5.0 \text{ d}^{-1}$ (Glotfelty et al. 1989).

Photolysis:

Oxidation: $t_{1/2} = 5.2\text{--}51.7 \text{ h}$ 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 $t_{1/2} = 23.1 \text{ h}$, based on rate constant $k = 2.97 \times 10^{-2} \text{ h}^{-1}$ at pH 7.0 and 25°C (Demayo 1972; quoted, Callahan et al. 1979; Kollig et al. 1987; Howard et al. 1991);

rate constant $k = 61 \text{ yr}^{-1}$ at pH 7.0 and 25°C (Kollig 1993)

$t_{1/2} = 5.4 \text{ d}$ at pH 2, $t_{1/2} = 0.96 \text{ d}$ at pH 7 in natural waters (Capel & Larson 1995)

Biodegradation: aqueous aerobic $t_{1/2} = 360\text{--}1567 \text{ h}$, based on unacclimated aerobic soil grab sample test data (Castro & Yoshida 1971; quoted, Howard et al. 1991);

rate constant $k = 0.011 \text{ d}^{-1}$ by die-away test in soil (Rao & Davidson 1980; quoted, Scow 1982);

estimated $t_{1/2} = 220 \text{ d}$ in soil (Jury et al. 1990);

aqueous anaerobic $t_{1/2} = 1440\text{--}6268 \text{ h}$, based on unacclimated aerobic biodegradation half-life (Howard et al. 1991)

$t_{1/2}(\text{aerobic}) = 15 \text{ d}$, $t_{1/2}(\text{anaerobic}) = 60 \text{ d}$ in natural waters (Capel & Larson 1995)

Biotransformation:

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

Half-Lives in the Environment:

Air: $t_{1/2} = 9.8\text{--}59.0 \text{ h}$, based on estimated photooxidation half-life in air (Atkinson 1987; quoted, Howard et al. 1991);

atmospheric transformation lifetime was estimated to be $<1 \text{ d}$ (Kelly et al. 1994).

Surface water: persistence up to 2 wk in river water (Eichelberger & Lichtenberg 1971);

$t_{1/2} = 38$ d in surface waters in the Netherlands in case a first order reduction process may be assumed (Zoeteman et al. 1980)

$t_{1/2} = 23.1$ – 129.4 h, based on hydrolysis half-lives (Kollig et al. 1987 and Chapman & Cole 1982; quoted, Howard et al. 1991)

Biodegradation $t_{1/2}$ (aerobic) = 15 d, $t_{1/2}$ (anaerobic) = 60 d, hydrolysis $t_{1/2} = 5.4$ d at pH 2, $t_{1/2} = 0.96$ d at pH 7 in natural waters (Capel & Larson 1995).

Ground water: $t_{1/2} = 23.1$ – 129.4 h, based on hydrolysis half-lives (Kollig et al. 1987 and Chapman & Cole 1982; quoted, Howard et al. 1991).

Sediment:

Soil: $t_{1/2} \sim 2$ – 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 $t_{1/2} = 0.91$ 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);

$t_{1/2} < 10$ d and subject to plant uptake via volatilization (Callahan et al. 1979; quoted, Ryan et al. 1988);

first-order $t_{1/2} = 63$ d from biodegradation rate constant $k = 0.011$ d⁻¹ by die-away test in soil (Rao & Davidson 1980; quoted, Scow 1982);

field $t_{1/2} = 0.3$ d in moist fallow soil (Glottfelty 1981; quoted, Nash 1983);

microagroecosystem $t_{1/2} = 3$ 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 $t_{1/2} = 9$ – 10 months in soil (Hartley & Kidd 1987; quoted, Montgomery 1993);

$t_{1/2} = 23.1$ – 129.4 h, based on hydrolysis half-lives (Kollig et al. 1987 and Chapman & Cole 1982; quoted, Howard et al. 1991);

estimated biodegradation $t_{1/2} = 220$ d in soil (Jury et al. 1990);

selected field $t_{1/2} = 250$ d (Augustijn-Beckers et al. 1994; Hornsby et al. 1996);

$t_{1/2} = 9$ – 10 months when used at agricultural rates (Tomlin 1994)

$t_{1/2} = 7$ – 14 yr in soil (Geyer et al. 2000)

Biota: biochemical $t_{1/2} = 2000$ 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					
$\Delta H_{OA}/(kJ\ mol^{-1}) = 66.2$					

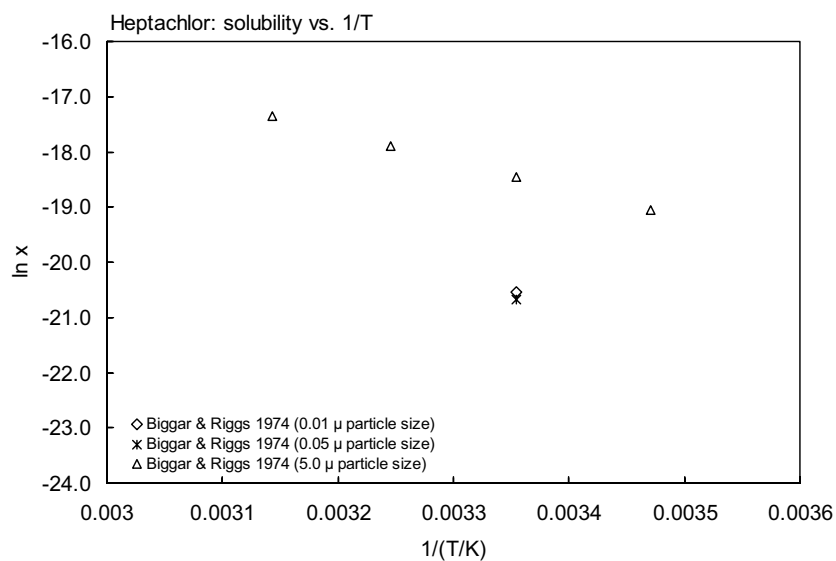


FIGURE 18.1.1.50.1 Logarithm of mole fraction solubility ($\ln x$) versus reciprocal temperature for heptachlor.

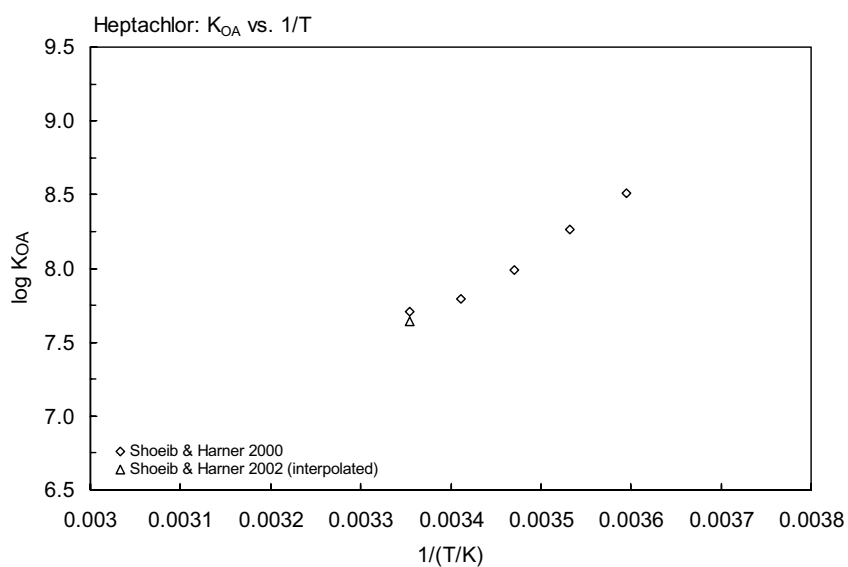
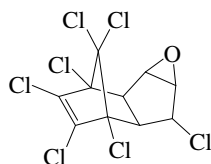


FIGURE 18.1.1.50.2 Logarithm of K_{OA} versus reciprocal temperature for heptachlor.

18.1.1.51 Heptachlor epoxide



Common Name: Heptachlor epoxide

Synonym: β -Heptachlorepoxyde, Epoxyheptachlor, HCE, Velsicol 53-CS-17

Chemical Name: 1,4,5,6,7,8,8-heptachloro-2,3-epoxy-3a,4,7,7a-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 ($^{\circ}C$):

160 (Lide 2003)

Boiling Point ($^{\circ}C$):

Density (g/cm^3 at $20^{\circ}C$):

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 $25^{\circ}C$ (assuming $\Delta S_{fus} = 56 J/mol K$), F : 0.0474 (mp at $160^{\circ}C$)

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$ or as indicated. Additional data at other temperatures designated * are compiled at the end of this section):

0.035 ($25-29^{\circ}C$, 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 $15-45^{\circ}C$, 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, $20-25^{\circ}C$, 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 $25^{\circ}C$ or as indicated):

0.045 (estimated, Mabey et al. 1982)

0.00256 (estimated, Howard 1991)

3.47×10^{-4} ($20^{\circ}C$, Montgomery 1993)

0.0997 (supercooled liquid value, $20-25^{\circ}C$, 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 $25^{\circ}C$ 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 ($20-25^{\circ}C$, 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 \pm 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, $k < 3600 \text{ M}^{-1} \text{ h}^{-1}$ for reaction with singlet oxygen, and $k = 20 \text{ M}^{-1} \text{ h}^{-1}$ 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 $k = 3 \times 10^{-12} \text{ mL cell}^{-1} \text{ h}^{-1}$ (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)

$t_{1/2} = 792\text{--}13248$ h, based on estimated unacclimated aqueous aerobic biodegradation half-life (Howard et al. 1991)

biodegradation $t_{1/2}(\text{aerobic}) = 33$ d, $t_{1/2}(\text{anaerobic}) = 1$ d in natural waters (Capel & Larson 1995)

Ground water: $t_{1/2} = 24\text{--}26496$ h, based on estimated unacclimated aqueous aerobic and anaerobic biodegradation half-lives (Howard et al. 1991)

Sediment:

Soil: $t_{1/2} = 792\text{--}13248$ h, based on aerobic soil grab sample data (Howard et al. 1991)

$t_{1/2} \sim 3$ 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			
$t/^{\circ}\text{C}$	$S/\text{g}\cdot\text{m}^{-3}$	$S/\text{g}\cdot\text{m}^{-3}$	$S/\text{g}\cdot\text{m}^{-3}$
particle size	0.01 μ	0.05 μ	5.0 μ
15			0.110
25	0.025	0.120	0.200
35			0.350
45			0.600

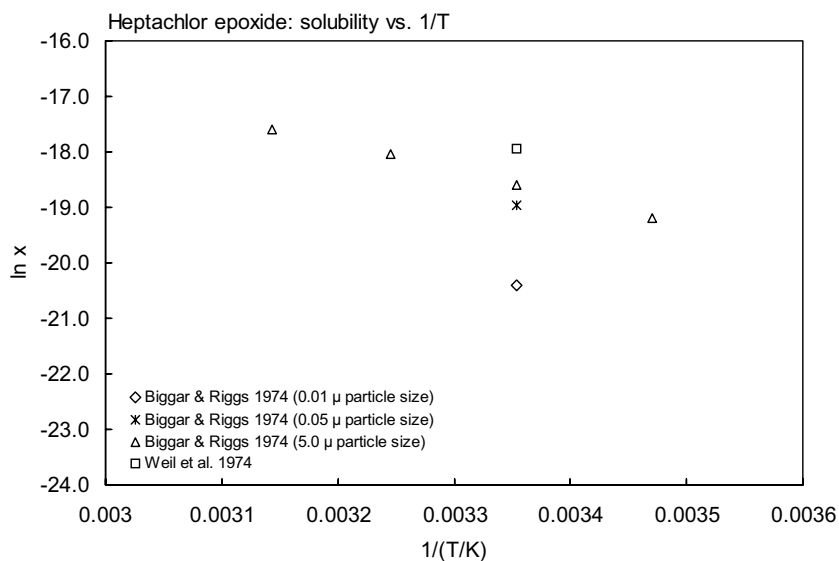
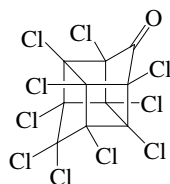


FIGURE 18.1.1.51.1 Logarithm of mole fraction solubility ($\ln x$) versus reciprocal temperature for heptachlor epoxide.

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 ($^{\circ}C$):

350 (dec. Howard 1991; Montgomery 1993; Lide 2003)

Boiling Point ($^{\circ}C$):

Density (g/cm^3 at $20^{\circ}C$):

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 $25^{\circ}C$ (assuming $\Delta S_{fus} = 56 J/mol K$), F : 6.5×10^{-4} (mp at $350^{\circ}C$)

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$ or as indicated):

4.0 ($100^{\circ}C$, Günther et al. 1968)

2.7 (quoted Weil 1978 unpublished result, Kilzer et al. 1979)

3.0 ($20^{\circ}C$, Kenaga & Goring 1978, Kenaga 1980)

7.6 ($24^{\circ}C$, shake flask-nephelometry/fluor., Hollifield 1979; quoted, Howard 1991; Montgomery 1993)

Vapor Pressure (Pa at $25^{\circ}C$):

3.0×10^{-5} (Kilzer et al. 1979; quoted, Howard 1991; Montgomery 1993)

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

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 xanthurus*, *Palaemonetes pugio*, *Callinectes 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, $t_{1/2}$:

Volatilization: $t_{1/2} = 3.8\text{--}46$ 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 $t_{1/2} = 7488$ to 17,280 h (312 d to 2 yr), based on aerobic aquatic microcosm study, anaerobic $t_{1/2} = 29,952\text{--}69,120$ 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)

- $k_1 = 0.273\text{ d}^{-1}$; $k_2 = 0.037\text{ d}^{-1}$ with $t_{1/2} = 18.7$ d, uncontaminated water + 4% ration contaminated food,
 $k_1 = 217.3\text{ d}^{-1}$; $k_2 = 0.03\text{ d}^{-1}$ with $t_{1/2} = 23.5$ d, contaminated water + 4% ration uncontaminated food,
 $k_1 = 0.265\text{ d}^{-1}$; $k_2 = 0.037\text{ d}^{-1}$ with $t_{1/2} = 18.7$ d, uncontaminated water + 8% ration contaminated food,
 $k_1 = 185.5\text{ d}^{-1}$; $k_2 = 0.027\text{ d}^{-1}$ with $t_{1/2} = 25.5$ d, contaminated water + 8% ration uncontaminated food,
 $k_1 = 0.262\text{ d}^{-1}$; $k_2 = 0.032\text{ d}^{-1}$ with $t_{1/2} = 21.5$ d, contaminated food (4% ration) then water,
 $k_1 = 214\text{ d}^{-1}$; $k_2 = 0.023\text{ d}^{-1}$ with $t_{1/2} = 29.9$ d, contaminated water then food (a 4% ration)
 $k_1 = 0.292\text{ d}^{-1}$; $k_2 = 0.043\text{ d}^{-1}$ with $t_{1/2} = 16.2$ d, contaminated food (a 8% ration) then water,
 $k_1 = 154\text{ d}^{-1}$; $k_2 = 0.020\text{ d}^{-1}$ with $t_{1/2} = 35.4$ 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)

- $k_1 = 0.475\text{ d}^{-1}$; $k_2 = 0.017\text{ d}^{-1}$ with $t_{1/2} = 28$ d, uncontaminated water + 4% ration contaminated food,
 $k_1 = 175\text{ d}^{-1}$; $k_2 = 0.014\text{ d}^{-1}$ with $t_{1/2} = 47.8$ d, contaminated water + 4% ration uncontaminated food,
 $k_1 = 0.499\text{ d}^{-1}$; $k_2 = 0.019\text{ d}^{-1}$ with $t_{1/2} = 36.3$ d, contaminated food (4% ration) then water,
 $k_1 = 182\text{ d}^{-1}$; $k_2 = 0.013\text{ d}^{-1}$ with $t_{1/2} = 51.5$ d, contaminated water then food (a 4% ration)
 $k_1 = 0.399\text{ d}^{-1}$; $k_2 = 0.021\text{ d}^{-1}$ with $t_{1/2} = 32.3$ d, contaminated food (a 8% ration) then water,
 $k_1 = 170\text{ d}^{-1}$; $k_2 = 0.011\text{ d}^{-1}$ with $t_{1/2} = 63.7$ d, contaminated water then food (a 4% ration)

Half-Lives in the Environment:

Air: estimated $t_{1/2} = 438,000$ to 4.2×10^7 h or 50–200 yr (Howard et al. 1991).

Surface water: $t_{1/2} = 7488$ 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 $t_{1/2} = 14,976$ to 34,560 h (624 d to 4 yr) based on aqueous aerobic biodegradation (Howard et al. 1991).

Sediment:

Soil: estimated $t_{1/2} = 7488$ to 17,280 h (312 d to 2 yr) based on aerobic aquatic microcosm study (Howard et al. 1991).

Biota: clearance $t_{1/2} = 28$ d (shrimp, 10–20 d exposure, Bahner 1977)

Clearance $t_{1/2} = 16.2\text{--}35.4$ d for spot *Leiostomus xanthurus* (Fisher et al. 1986):

$t_{1/2}(4W) = 18.7$ d for kepone contaminated water + uncontaminated food at 4% ration

$t_{1/2}(4F) = 23.5$ d for uncontaminated water + kepone contaminated food at 4% ration

$t_{1/2}(8W) = 18.7$ d for kepone contaminated water + uncontaminated food at 8% ration,

$t_{1/2}(8F) = 25.5$ d for uncontaminated water + kepone contaminated food at 8% ration

$t_{1/2}(4FW\text{-}food) = 21.5$ d for dietary accumulation in combined exposure (food-water) at 4% ration

$t_{1/2}(4FW\text{-}water) = 29.9$ d for dietary accumulation in combined exposure (water-food) at 4% ration

$t_{1/2}(8FW\text{-}food) = 16.2$ d for dietary accumulation in combined exposure (food-water) at 8% ration

$t_{1/2}(8FW\text{-}water) = 35.4$ d for dietary accumulation in combined exposure (water-food) at 8% ration

Clearance $t_{1/2} = 32.3\text{--}63.7$ d for grass shrimps *Palaemonetes pugio* (Fisher & Clark 1990):

$t_{1/2}(4W) = 47.8$ d for kepone contaminated water + uncontaminated food at 4% ration

$t_{1/2}(4F) = 40.6$ d for uncontaminated water + kepone contaminated food at 4% ration

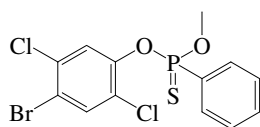
$t_{1/2}(4FW\text{-}food) = 36.3$ d for dietary accumulation in combined exposure (food-water) at 4% ration

$t_{1/2}(4FW\text{-}water) = 51.5$ d for dietary accumulation in combined exposure (water-food) at 4% ration

$t_{1/2}(8FW\text{-}food) = 32.3$ d for dietary accumulation in combined exposure (food-water) at 8% ration

$t_{1/2}(8FW\text{-}water) = 63.7$ 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: C₁₃H₁₀BrCl₂O₂PS

Molecular Weight: 412.066

Melting Point (°C):

71 (Lide 2003)

Boiling Point (°C):

Density (g/cm³ at 20°C):

1.53 (25°C, Merck Index 1989)

Molar Volume (cm³/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/m³ 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·m³/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:

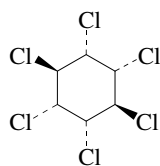
- 2.81 (*Daphnia magna*, wet wt. basis, Macek et al. 1979)
 2.88, 3.16 (fish: flowing water, static water; Kenaga 1980; Kenaga & Goring 1980)
 2.58, 2.86 (calculated-S, calculated- K_{OC} , Kenaga 1980)
 3.78 (*Pseudorasbora parva*, Kanazawa 1981)
 3.16 (mosquito fish, wet wt. basis, De Bruijn & Hermens 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 χ , 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-scabidol, 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; $1\alpha,2\alpha,3\beta,4\alpha,5\alpha,6\beta$ -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 ($^{\circ}C$):

112.5 (Slade 1945; Howard 1991; Montgomery 1993; Milne 1995; Lide 2003)

Boiling Point ($^{\circ}C$):

323.4 (Howard 1991; Montgomery 1993; Lide 2003)

Density (g/cm^3 at $20^{\circ}C$):

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 $25^{\circ}C$ (assuming $\Delta S_{fus} = 56 J/mol K$), F:

0.12 ($20^{\circ}C$, Suntio et al. 1988)

0.138 (Mackay et al. 1986)

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

10 ($20^{\circ}C$, Slade 1945; Günther et al. 1968; Spencer 1973, 1982)

7.3* (shake flask-UV spectrophotometry, measured range $25-45^{\circ}C$, Richardson & Miller 1960)

0.50–6.60 (particle size of $0.04-5\mu$, 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)

$\log (P_s/\text{Pa}) = 16.99 - 5566/(T/K)$, 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. $\ln (P/\text{Pa}) = (34.53 \pm 0.21) - (11754 \pm 72)/(T/K)$, 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)

$\log (P/\text{kPa}) = (11.23 \pm 0.50) - (4832 \pm 150)/(T/K)$; 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)

$\log (P_L/\text{Pa}) = 13.80 - 4330/(T/K)$, (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)

$\log (P_L/\text{Pa}) = -3890/(T/K) + 11.94$ (supercooled liquid, linear regression of literature data, Xiao et al. 2004)

$\log (P_L/\text{Pa}) = -3905/(T/K) + 11.98$ (supercooled liquid, final adjusted eq., Xiao et al. 2004)

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

$\log [H/(\text{Pa}\cdot\text{m}^3 \text{ mol}^{-1})] = -2382/(T/K) + 7.54$, 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)

$\log [H/(\text{Pa}\cdot\text{m}^3 \text{ mol}^{-1})] = -2703/(T/K) + 8.68$; 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)

$\log [H/(\text{Pa}\cdot\text{m}^3/\text{mol})] = 11.58 - 3049/(T/K)$ (Passivirta et al. 1999)

0.18* (20°C, air stripping-GC, measured range 10–40°C, Jantunen et al. 2000)

$\log [H/(\text{Pa m}^3/\text{mol})] = 9.51 - 3005/(T/K)$; 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)
 $\log [H/(\text{Pa m}^3/\text{mol})] = 10.14 - 3208/(T/K)$; 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)
 $\log [H/(\text{Pa m}^3/\text{mol})] = -2940/(T/K) + 9.29$ (LDV linear regression of literature data, Xiao et al. 2004)
 $\log [H/(\text{Pa m}^3/\text{mol})] = -3117/(T/K) + 9.94$ (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, Gorge & 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 χ , 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: $t_{1/2} = 191 \text{ d}$ was estimated from water (Mackay & Leinonen 1975, quoted, Howard 1991)
 estimated $t_{1/2} > 200 \text{ d}$ (Callahan et al. 1979);
 $t_{1/2}(\text{exptl.}) = 3.2 \text{ d}$ in nonstirred water and $t_{1/2}(\text{exptl.}) = 1.5 \text{ d}$ 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);
 $t_{1/2} = 22 \text{ d}$, 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 $k = 4.4 \times 10^{-2} \text{ h}^{-1}$ and predicted $k = 1.4 \times 10^{-2} \text{ h}^{-1}$ from soil with $t_{1/2} = 49.5 \text{ h}$ (Thomas 1982);
 $t_{1/2}(\text{calc}) = 2760 \text{ h}$ from water (Thomas 1982);
 measured rate constant $k(\text{exptl.}) = 3.0 \text{ d}^{-1}$ (Glottfelty et al. 1984; quoted, Glottfelty et al. 1989);
 calculated rate constant $k = 0.01 \text{ d}^{-1}$ (Glottfelty et al. 1989);
 $t_{1/2} = 266 \text{ d}$ from lab. and field experiments (Jury et al. 1984; quoted, Spencer & Cliath 1990);
 half-lives in soil surfaces at $20 \pm 1^\circ\text{C}$: $t_{1/2} = 5.5$ 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 $20 \pm 1^\circ\text{C}$: $t_{1/2} = 0.56 \text{ d}$ in bean, $t_{1/2} = 0.40 \text{ d}$ in turnips and $t_{1/2} = 0.31 \text{ d}$ in oats (Dörfler et al. 1991).
- Photolysis: $k_p(\text{aq.}) = 1.429 \times 10^{-2} \text{ d}^{-1}$ for photolysis in natural waters (Malaiyandi et al. 1982)
 $k_p(\text{aq.}) = 8.9 \times 10^{-4} \text{ h}^{-1}$ for Milli-Q water, $k_p = 4.1 \times 10^{-3} \text{ h}^{-1}$ for natural surface water samples from eutrophic pond, $k_p = 3.9 \times 10^{-4} \text{ h}^{-1}$ from eutrophic pond, $k_p = 4.5 \times 10^{-4} \text{ h}^{-1}$ 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_{NO_3} with NO_3 radical and k_{O_3} with O_3 or as indicated, *data at other temperatures see reference:
 $k_{OH} = 6.94 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ with a $t_{1/2} \sim 2.3 \text{ d}$ (Atkinson 1987; quoted, Howard 1991)
 $k(\text{aq.}) = 4.2 \times 10^8 \text{ M}^{-1} \text{ s}^{-1}$ for the reaction (Fenton with reference to DBCP) with hydroxyl radical in aqueous solutions at pH 2.9 and at $24 \pm 1^\circ\text{C}$ (Buxton et al. 1988; quoted, Faust & Hoigné 1990; Haag & Yao 1992)
 $k(\text{aq.}) \leq 0.04 \text{ M}^{-1} \text{ s}^{-1}$ for direct reaction with ozone in water at pH 2.7–6.3 and 23°C , with a $t_{1/2} \geq 10 \text{ d}$ 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)

$k_{\text{OH}}(\text{aq.}) = (5.8 \pm 1.9) \times 10^8 \text{ M}^{-1} \text{ s}^{-1}$ (Fenton with reference to DBCP); and $k = (5.2 \pm 0.9) \times 10^8 \text{ M}^{-1} \text{ s}^{-1}$ (photo-Fenton with reference to DBCP) for the reaction with hydroxyl radicals in aqueous solutions at pH 2.9 and at $24 \pm 1^\circ\text{C}$ (Haag & Yao 1992)

Hydrolysis: $k(\text{neutral}) = 1.6 \times 10^{-4} \text{ h}^{-1}$ indicating that neutral hydrolysis is unimportant, rate constants of 7.5×10^{-3} , 8.99×10^{-4} , and $1.07 \times 10^{-3} \text{ h}^{-1}$ 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)

$k(\text{neutral}) = (1.2 \pm 0.2) \times 10^{-4} \text{ h}^{-1}$ with a calculated $t_{1/2} = 206 \text{ d}$ at pH 7 (Ellington et al. 1987, 1988; quoted, Montgomery 1993)

$t_{1/2} = 42 \text{ yr}$ at pH 8 and 5°C (Ngabe et al. 1993)

$t_{1/2} = 191 \text{ d}$ at pH 7, and $t_{1/2} = 11 \text{ h}$ at pH 9 at 22°C (Tomlin 1994)

$t_{1/2} = 240 \text{ d}$ at pH 2, $t_{1/2} = 210 \text{ d}$ at pH 7 and $t_{1/2} = 0.015 \text{ d}$ at pH 12 in natural waters (Capel & Larson 1995)

Biodegradation: $k = 0.0026 \text{ d}^{-1}$ 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 $>300 \text{ d}$ for river, lake and ground water, respectively (Zoeteman et al. 1980; quoted, Howard 1991);

$t_{1/2} = 266 \text{ d}$ for 100-d leaching screening test in 0–10 cm depth of soil (Jury et al. 1984, 1987a, b; Jury & Ghodrati 1989)

$t_{1/2}(\text{aerobic}) = 31 \text{ d}$, $t_{1/2}(\text{anaerobic}) = 5.9 \text{ d}$ in natural waters (Capel & Larson 1995)

$t_{1/2}(\text{calc}) = (20.4 \pm 0.1) \text{ h}$ in sewage sludge from experiments S1–S3 (Buser & Müller 1995)

Biotransformation:

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

$k_1 = 3.13 \text{ h}^{-1}$; $k_2 = 0.0313 \text{ h}^{-1}$ (mussels, Ernst 1977)

$k_1 = 130 \text{ d}^{-1}$; $k_2 = 0.063 \text{ d}^{-1}$ (rainbow trout, Oliver & Niimi 1985)

$k_1 = 14, 179, 196 \text{ h}^{-1}$ (zebrafish: egg, yolk sac fry, juvenile, Gorge & Nagel 1990)

$k_2 = 0.06 \text{ h}^{-1}$ (*Chironomus riparius*-water only system, Lydy et al. 1992)

$k_2 = 0.0661 \text{ h}^{-1}$ (*Chironomus riparius*-screened system, Lydy et al. 1992)

$k_2 = 0.08 \text{ h}^{-1}$ (*Chironomus riparius*-3% organic carbon system, Lydy et al. 1992)

$k_2 = 0.0661 \text{ h}^{-1}$ (*Chironomus riparius*-15% organic carbon system, Lydy et al. 1992)

$k_1 = 9.0\text{--}26.4 \text{ h}^{-1}$; $k_2 = 0.04\text{--}0.18 \text{ h}^{-1}$ (rainbow trout in early life stages on wet wt. basis, Vigano et al. 1992)

$k_1 = 180\text{--}939 \text{ h}^{-1}$; $k_2 = 0.031\text{--}0.13 \text{ h}^{-1}$ (rainbow trout in early life stages on lipid basis, Vigano et al. 1992)

Half-Lives in the Environment:

Air: $t_{1/2} \sim 2.3 \text{ d}$ was estimated, based on rate constant $6.94 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \cdot \text{s}^{-1}$ 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 $<1 \text{ d}$ (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. $t_{1/2} = 7.9 \pm 1.2 \text{ yr}$ at Eagle Harbor, $t_{1/2} = 4.3 \pm 0.5 \text{ yr}$ at Sleeping Bear Dunes and $t_{1/2} = 4.9 \pm 0.5 \text{ yr}$ at Sturgeon Point, when accounting the agricultural application effects, half-lives are, $t_{1/2} = 9.1 \pm 1.3 \text{ yr}$ at Eagle Harbor, $t_{1/2} = 4.6 \pm 0.4 \text{ yr}$ at Sleeping Bear Dunes and $t_{1/2} = 5.4 \pm 0.4 \text{ yr}$ at Sturgeon Point (Buehler et al. 2004)

Surface water: $t_{1/2} = 10\text{--}138 \text{ d}$ in various locations in the Netherlands in case a first order reduction process may be assumed; and $t_{1/2} = 3\text{--}30 \text{ d}$ in rivers and $t_{1/2} = 30\text{--}300 \text{ d}$ in lakes (Zoeteman et al. 1980);

hydrolysis $t_{1/2}(\text{exptl}) = 92 \text{ h}$, $t_{1/2}(\text{calc}) = 89 \text{ h}$ for Roselawn Cemetery Pond at pH 9.3; $t_{1/2}(\text{exptl}) = 771 \text{ h}$,

$t_{1/2}(\text{calc}) = 578 \text{ h}$ for Cross Lake at pH 7.3; $t_{1/2}(\text{exptl}) = 648 \text{ h}$, $t_{1/2}(\text{calc}) = 231 \text{ h}$ for Indiana Quarry at pH 7.8;

photolysis half-lives for direct sunlight during July and adjusted for mid-winter: $t_{1/2} = 779 \text{ h}$, 1560 h for Milli-Q water at pH 6.98, $t_{1/2} = 169 \text{ h}$, 339 h for Roselawn Pond at pH 9.3, $t_{1/2} = 1791 \text{ h}$, 3590 h for Cross Lake and $t_{1/2} = 1540 \text{ h}$, 3090 h for Indiana Quarry (Saleh et al. 1982);

$t_{1/2} > 10 \text{ d}$ 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 (Glottfelty 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		

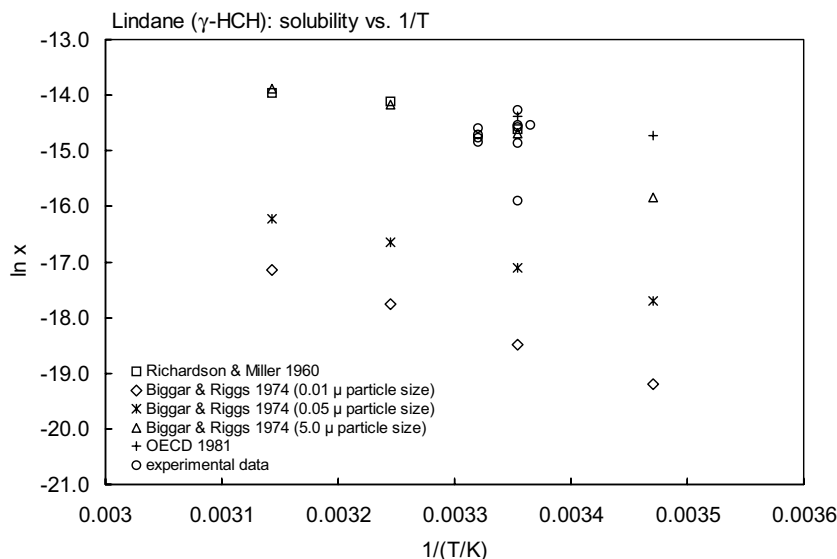


FIGURE 18.1.1.54.1 Logarithm of mole fraction solubility ($\ln x$) versus reciprocal temperature for lindane (γ -HCH).

TABLE 18.1.1.54.2

Reported vapor pressures of lindane at various temperatures and the coefficients for the vapor pressure equations

$$\begin{array}{ll} \log P = A - B/(T/K) & (1) \\ \log P = A - B/(C + t/^{\circ}\text{C}) & (2) \\ \log P = A - B/(C + T/K) & (3) \\ \log P = A - B/(T/K) - C \cdot \log(T/K) & (4) \end{array} \quad \begin{array}{ll} \ln P = A - B/(T/K) & (1a) \\ P = A - B/(C + t/^{\circ}\text{C}) & (2a) \end{array}$$

1.

Balson 1947		Spencer & Cliath 1970		Wania et al. 1994		Boehncke et al. 1996	
effusion manometer		gas saturation-GC		gas saturation-GC		Knudsen effusion	
$t/^{\circ}\text{C}$	P/Pa	$t/^{\circ}\text{C}$	P/Pa	$t/^{\circ}\text{C}$	P/Pa	$t/^{\circ}\text{C}$	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}
		$\Delta H_v = 101.13 \text{ kJ/mol}$		A	16.99		
eq. 1	P/mmHg			B	5566	eq. 1a	P/Pa
A	15.515					A	34.53
B	6020					B	11754
temp range: 60–92 $^{\circ}\text{C}$				enthalpy of sublimation:		temp range: 293–323 K	
$\Delta H_v = 115.06 \text{ kJ/mol}$		Rordorf 1989		$\Delta H_{\text{sub}} = 106.6 \text{ kJ/mol}$		enthalpy of sublimation:	
		gas saturation-GC				$\Delta H_{\text{sub}} = 97.7 \text{ kJ/mol}$	
		25	0.067				
		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	Combining the above 4 equations, the final equation			
98	13.183	104	30.903	$\log (P/\text{kPa}) = 11.23 \pm 0.5 - (4832 \pm 150)/(T/\text{K})$			
66	0.8128	80	4.3652	for temperature range 310 to 384 K			
71	1.2303	83	5.6234	$\Delta H_{\text{sub}} = 92.5$ kJ/mol at 350 K			
76	2.0417	88	9.1201	at 25°C P = 0.0104 Pa			
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				

(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	eq. 1	kPa				
A	10.78	A	11.79				
B	4709	B	5025				
for temp 323–370 K		for temp 339–384 K					

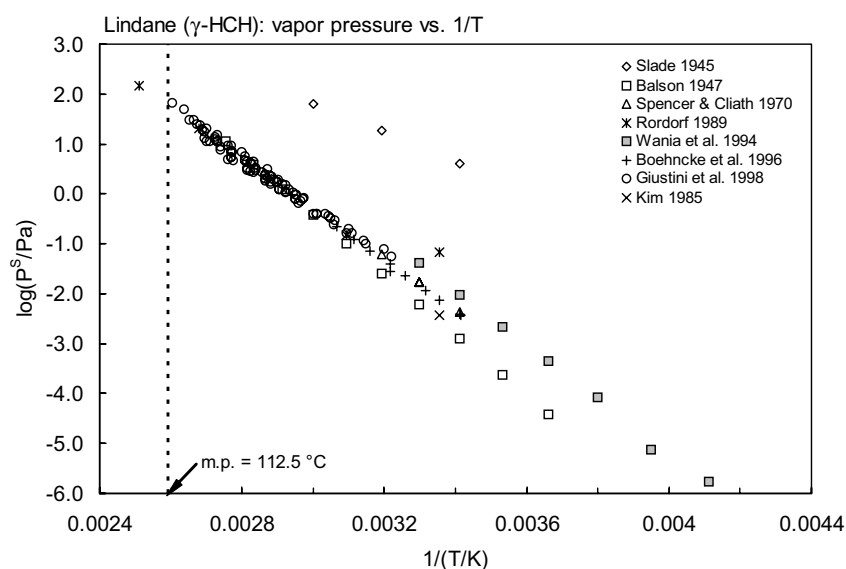
FIGURE 18.1.1.54.2 Logarithm of vapor pressure versus reciprocal temperature for lindane (γ -HCH).

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)
$\ln (k_H/\text{atm}) = A - B/(T/K)$	(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)
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 m ³ /mol)	t/°C	H/(Pa m ³ /mol)	t/°C	H/(Pa m ³ /mol)	t/°C	H/(Pa m ³ /mol)
25	0.353	Lake Erie					
35	0.624	22.3	0.310	eq. 4a	H/(Pa m ³ /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 m ³ /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 m ³ /mol)					eq. 4a	H/(Pa m ³ /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							
$\Delta H_{WA}/(\text{kJ mol}^{-1}) = 61.4$							

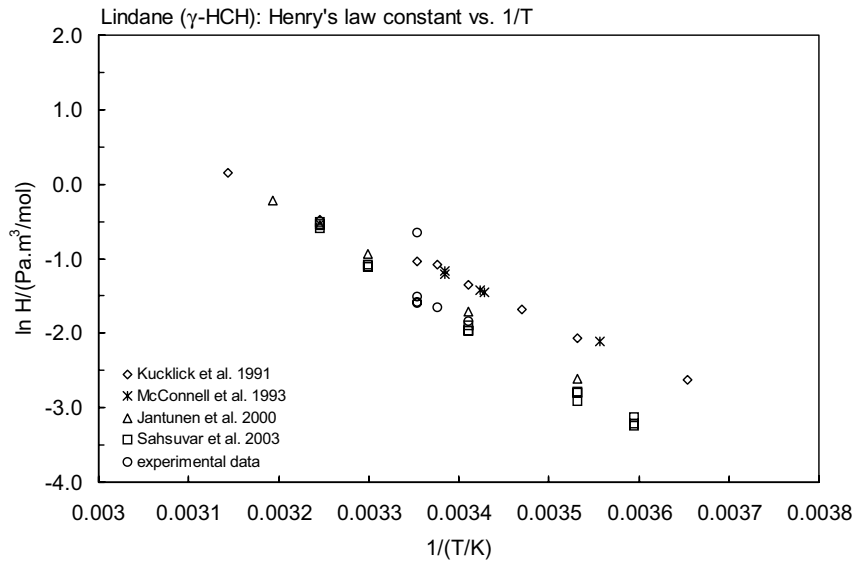


FIGURE 18.1.1.54.3 Logarithm of Henry's law constant versus reciprocal temperature for lindane (γ-HCH).

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
		25	7.8473
		25	7.849
enthalpy of phase transfer: $\Delta H_{OW}/(\text{kJ mol}^{-1}) = -10.40$		$\log K_{OA} = A + B/(T/K)$	
entropy of phase transfer: $\Delta S_{OW}/(\text{J K}^{-1} \text{mol}^{-1}) = 52.2$		A	-3.611
		B	3415
		enthalpy of phase change $\Delta H_{OA}/(\text{kJ mol}^{-1}) = 65.4$	

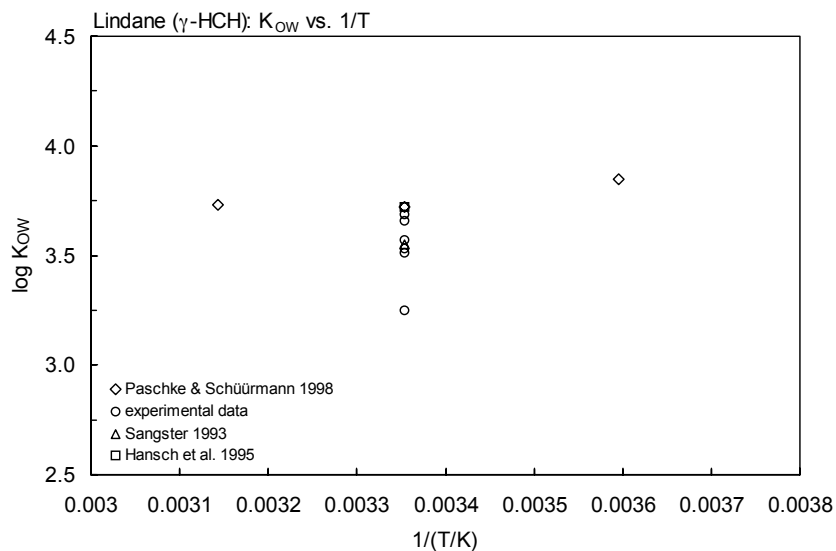


FIGURE 18.1.1.54.4 Logarithm of K_{OW} versus reciprocal temperature for lindane (γ -HCH).

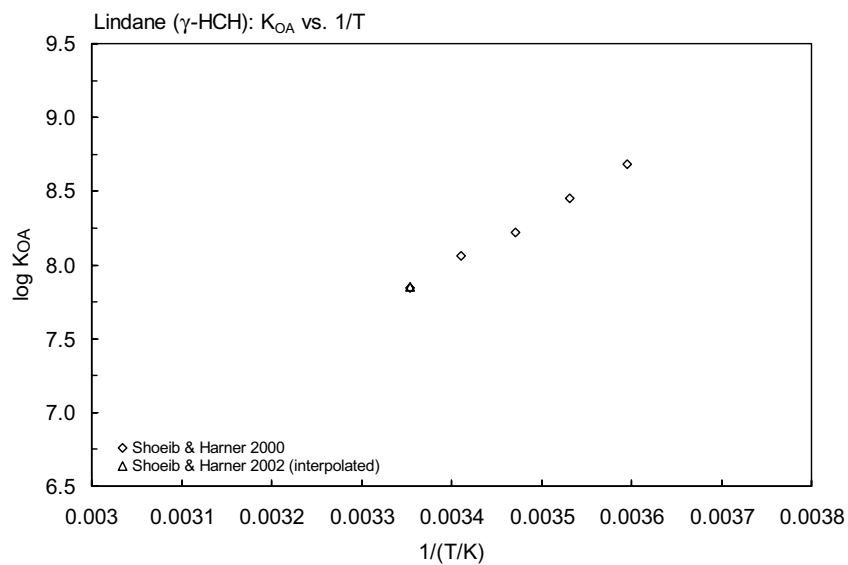
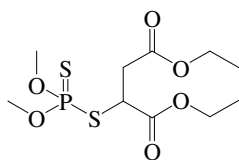


FIGURE 18.1.1.54.5 Logarithm of K_{OA} versus reciprocal temperature for lindane (γ -HCH).

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: C₁₀H₁₉O₆PS₂

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/cm³ at 20°C):

1.23 (25°C, Spencer 1982; Hartley & Kidd 1987; Worthing & Hance 1991; Montgomery 1993)

Molar Volume (cm³/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/m³ 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 ($\text{Pa}\cdot\text{m}^3/\text{mol}$ 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 $\log B_b$, 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 $\geq 0.1\%$, OC $\geq 0.5\%$, 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, $t_{1/2}$:

- Volatilization: $t_{1/2} = 131$ d, based on volatilization rate from water with a wind speed of 0–2.5 m/s (Sanders & Seiber 1984; quoted, Howard 1991).
- Photolysis: $t_{1/2} = 15$ h for direct sunlight photolysis in aqueous media (Wolfe et al. 1976)
 $t_{1/2} = 900$ h in distilled water at pH 6 with wavelength $\lambda > 290$ nm; $t_{1/2} = 16$ h by sunlight in a natural water from Suwannee River (Wolfe et al. 1977)
 $t_{1/2} = 990$ –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_{NO_3} with NO_3 radical and k_{O_3} with O_3 or as indicated, *data at other temperatures see reference:
 photooxidation $t_{1/2} = 1.0$ –9.8 h, based on an estimated rate constant for the vapor-phase reaction with hydroxyl radical in air (Howard et al. 1991)
 $k_{OH}(\text{calc}) = 64 \times 10^{-12}$ cm³ molecule⁻¹ s⁻¹ at room temp. (Winer & Atkinson 1990)
 calculated lifetime $\tau = 3$ h for reaction with OH radical in the troposphere (Atkinson et al. 1992)
- Hydrolysis: $t_{1/2} = 10.5$ d at pH 7.4 and 20°C (Freed et al. 1977, 1979; Montgomery 1993)
 $t_{1/2} = 120$ d at pH 6.1 and $t_{1/2} = 11$ 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)
 $k(\text{acid}) = (4.8 \pm 0.2) \times 10^{-5}$ M⁻¹ s⁻¹ with $t_{1/2} > 4$ yr for acid degradation at pH 4 at 27°C; $k(\text{alkaline}) = (5.5 \pm 0.3) \text{ M}^{-1} \text{ s}^{-1}$ with a $t_{1/2} = 36$ h for alkaline degradation at pH 8 at 27°C, $t_{1/2} = 1$ h at 40°C and $t_{1/2} = 40$ h at 0°C and pH 8; all for 10^{-4} M in 1% acetonitrile and water at 27°C; $t_{1/2} = 20$ h for distilled water and $t_{1/2} = 22$ h for natural river water from Withlacoochee River, pH 8.2 (Wolfe et al. 1977)
 $k(\text{acid}) = 4.8 \times 10^{-5} \text{ M}^{-1} \text{ s}^{-1}$; $k(\text{neutral}) = 7.7 \times 10^{-9} \text{ s}^{-1}$ and $k(\text{alkaline}) = 5.5 \text{ M}^{-1} \text{ s}^{-1}$ all for 10^{-4} M in 1% acetonitrile and water at 27°C (Wolfe et al. 1977; quoted, Harris 1982)
 $t_{1/2} = 8.8$ yr, based on reported $k = 2.5 \times 10^{-2} \text{ M}^{-1} \text{ s}^{-1}$ at pH 7 and 0°C; $t_{1/2}(\text{base}) = 14$ h at pH 9 and 27°C (Howard et al. 1991)
 $t_{1/2} = 9$ d at pH 6 (Montgomery 1993)
 $t_{1/2} = 3200$ d at pH 7, $t_{1/2} = 0.0006$ d at pH 12 in natural waters (Capel & Larson 1995)
- Biodegradation: $k = 6.2 \times 10^{-8} \text{ mL cell}^{-1} \text{ d}^{-1}$ (Paris et al. 1975; quoted, Scow 1982)
 $k = 5.0 \times 10^{-8} \text{ mL cell}^{-1} \text{ d}^{-1}$ (Baughman & Lassiter 1978; quoted, Scow 1982)
 $k = 2.6$ – $16.1 \times 10^{-7} \text{ mL cell}^{-1} \text{ d}^{-1}$ (Paris et al. 1978; quoted, Scow 1982);
 $k = 1.4 \text{ d}^{-1}$ in soil (Rao & Davidson 1980; quoted, Scow 1982)
 $k = (4.5 \pm 0.74) \times 10^{-11} \text{ L cell}^{-1} \text{ h}^{-1}$ in North American waters (Paris et al. 1981)
 $t_{1/2}(\text{aq. aerobic}) = 100$ –1236 h, based on estimated aqueous aerobic biodegradation half-life; $t_{1/2}(\text{aq. anaerobic}) = 400$ –4944 h based on unacclimated aerobic biodegradation (Howard et al. 1991).
 $t_{1/2}(\text{aerobic}) = 4.2$ d, $t_{1/2}(\text{anaerobic}) = 17$ d in natural waters (Capel & Larson 1995)
- Biotransformation: transformation rate $k = 7.8 \times 10^{-3} \text{ mg (mg fungi)}^{-1} \text{ h}^{-1}$ by a fungi *Aspergillus orgzae* at 28°C in aqueous solution (Lewis et al. 1975)
 $k = 1.9 \times 10^{-1} \text{ mg (mg fungi)}^{-1} \text{ d}^{-1}$ in aquatic systems (Lewis et al. 1975; quoted, Scow 1982)
- Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants:
 $k_1 = 1.07 \text{ d}^{-1}$ (carp, Bender 1969; quoted, McLeese et al. 1976)
 $k_2 = 0.08 \text{ d}^{-1}$ (carp, calculated, from k_1 of Bender 1969, McLeese et al. 1976)
 $k_2 = 0.49 \text{ h}^{-1}$ (willow shiner, Tsuda et al. 1989)

Half-Lives in the Environment:

Air: $t_{1/2} = 1.0\text{--}9.8$ 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);

$t_{1/2} = 100\text{--}1236$ 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 $t_{1/2}(\text{aerobic}) = 4.2$ d, $t_{1/2}(\text{anaerobic}) = 17$ 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: $t_{1/2} = 200\text{--}2472$ 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 $k = 0.902\text{ d}^{-1}$ with $t_{1/2} = 0.8$ d under aerobic conditions, $k = 0.302\text{ d}^{-1}$ with $t_{1/2} = 2.3$ d under anaerobic conditions in sediment from San Diego Creek, Orange County, CA; first-order degradation $k = 0.506\text{ d}^{-1}$ with $t_{1/2} = 1.4$ d under aerobic conditions, $k = 0.431\text{ d}^{-1}$ 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);

$t_{1/2} = 72\text{--}168$ 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);

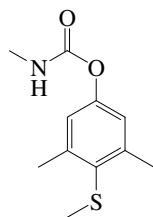
$t_{1/2} = 1$ d for soil depth < 5 cm, $t_{1/2} = 7$ d for soil depth 5–20 cm and $t_{1/2} = 14$ d for soil depth > 20 cm (Dowd et al. 1993).

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, Ensulol, Mercaptodimethur, Mesulol, Mesulol 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 ($^{\circ}C$):

120 (Lide 2003)

Boiling Point ($^{\circ}C$):

Density (g/cm^3 at $20^{\circ}C$):

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 $25^{\circ}C$ (assuming $\Delta S_{fus} = 56 J/mol K$), F: 0.117 (mp at $120^{\circ}C$)

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$ or as indicated):

30 ($20^{\circ}C$, Hartley & Kidd 1987; Worthing & Walker 1987; Milne 1995)

27 ($20^{\circ}C$, Tomlin 1994)

24 ($20-25^{\circ}C$, selected, Hornsby et al. 1996)

Vapor Pressure (Pa at $25^{\circ}C$ or as indicated):

0.015 ($60^{\circ}C$, Hartley & Kidd 1987)

1.5×10^{-5} ($20^{\circ}C$, Tomlin 1994)

3.6×10^{-5} (Tomlin 1994)

0.016 ($20-25^{\circ}C$, selected, Hornsby et al. 1996)

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

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)

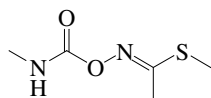
Environmental Fate Rate Constants, k , or Half-Lives, $t_{1/2}$:

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: C₅H₁₀N₂O₂S

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/cm³ at 20°C):

1.2946 (25°C, Spencer 1982; Worthing & Hance 1991; Tomlin 1994)

1.2946 (24°C, Milne 1995; Montgomery 1993)

Molar Volume (cm³/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/m³ 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·m³/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 $t_{1/2} \sim .14$ 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 $k = 8.9 \times 10^{-5} \text{ h}^{-1}$ 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 $k = -0.000215 \text{ h}^{-1}$ in nonsterile sediment, $k = -0.000747 \text{ h}^{-1}$ in sterile sediment by shake-tests at Range Point and $k = -0.000175 \text{ h}^{-1}$ in nonsterile water and $k = -0.000383 \text{ h}^{-1}$ 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: $t_{1/2} \sim 1.14$ months, based on rate constant $k = 2.919 \times 10^{-13} \text{ cm}^3/\text{molecules}$ for the vapor-phase reaction with $8 \times 10^5/\text{cm}^3$ 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).

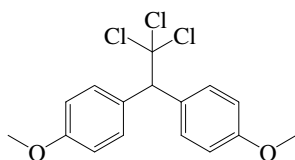
Sediment:

Soil: field $t_{1/2} = 30$ d (20–25°C, selected, Hornsby et al. 1996).

Biota: $t_{1/2} \sim 3\text{--}5$ d in plants following leaf application (Harvey & Reiser 1973; quoted, Tomlin 1994);

$t_{1/2} = 0.4\text{--}8.5$ d on cotton plants, $t_{1/2} = 0.8\text{--}1.2$ d on mint plants and $t_{1/2} \sim 2.5$ 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, Methoricide, 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 ($^{\circ}C$):

87 (Lide 2003)

Boiling Point ($^{\circ}C$):

Density (g/cm^3 at $20^{\circ}C$):

1.41 ($25^{\circ}C$, 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 $25^{\circ}C$ (assuming $\Delta S_{fus} = 56 J/mol K$), F: 0.246 (mp at $87^{\circ}C$)

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$ 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 $25-45^{\circ}C$, 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 $15-45^{\circ}C$, 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 ($20-25^{\circ}C$, selected, Wauchope et al. 1992; Hornsby et al. 1996)

0.04 ($24^{\circ}C$, Montgomery 1993)

Vapor Pressure (Pa at $25^{\circ}C$ or as indicated):

$< 1.33 \times 10^{-4}$ ($20-25^{\circ}C$, Weber et al. 1980)

1.910×10^{-4} (estimated, Howard 1991)

Henry's Law Constant ($Pa \cdot m^3/mol$ at $25^{\circ}C$ 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 (*Triaenodes 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, $t_{1/2}$:

Volatilization: $t_{1/2} = 4.5$ 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 $t_{1/2} = 690$ h in water, $t_{1/2} = 4100$ h in hydrocarbon media; 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)

photodecomposition $t_{1/2} > 300$ h in distilled water, $t_{1/2} = 2.2$ h in Suwannee River water, $t_{1/2} = 5.4$ h in Tombigbee River water, $t_{1/2} = 2.9$ h in Alabama River water with methoxychlor at 40 ppb under sunlight (Zepp et al. 1976)
 $t_{1/2} = 300\text{--}2070$ 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 $t_{1/2} = 2.2\text{--}5.4$ 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 $t_{1/2} \sim 1.12\text{--}11.2$ h in air, based on rate constant for the vapor-phase reaction with hydroxyl radical in air (Atkinson 1987; quoted, Howard et al. 1991)

$k(\text{aq.}) = (270 \pm 80) \text{ M}^{-1} \text{ s}^{-1}$ for direct reaction with ozone in water at pH 2 and $24 \pm 1^\circ\text{C}$, with $t_{1/2} = 21$ min at pH 7 (Yao & Haag 1991).

$k_{\text{OH}}(\text{aq.}) = 2 \times 10^{10} \text{ M}^{-1} \text{ s}^{-1}$ for the reaction with hydroxyl radicals in aqueous solutions at $24 \pm 1^\circ\text{C}$ (Haag & Yao 1992).

Hydrolysis: $k(\text{alkaline}) = 3.8 \times 10^{-4} \text{ M}^{-1} \text{ s}^{-1}$ with $t_{1/2} = 2100$ d at 27°C , $k(\text{neutral}) = 2.2 \times 10^{-8} \text{ s}^{-1}$ at pH 3–7 corresponds to a $t_{1/2} = 367$ d at pH 9 and 27°C (Wolf et al. 1977)

Overall rate constant $k = 5.5 \times 10^{-8} \text{ s}^{-1}$ with $t_{1/2} = 147$ d; $k = 3.0 \times 10^{-8} \text{ s}^{-1}$ with $t_{1/2} = 270$ d at 25°C and pH 7 (Mabey & Mill 1978)

$k(\text{alkaline}) = 3.8 \times 10^{-4} \text{ M}^{-1} \text{ s}^{-1}$, $k(\text{neutral}) = 2.2 \times 10^{-8} \text{ s}^{-1}$, $1 \times 10^{-8} \text{ M}$ in water at 27°C (Harris 1982)

$t_{1/2} = 1.05$ yr, based on neutral and base catalyzed hydrolysis rate constants Howard et al. 1991)

$k = 0.60 \text{ yr}^{-1}$ at pH 7 and 25°C (Kollig 1993)

$t_{1/2} = 370$ 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)

Biodegradation: $t_{1/2}(\text{aq. aerobic}) = 4320\text{--}8760$ 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)

$t_{1/2}(\text{aq. anaerobic}) = 1200\text{--}4320$ h (50 d to 6 months), based on anaerobic soil die-away test study data (Fogel et al. 1982; quoted, Howard et al. 1991)

$k = -0.00236 \text{ h}^{-1}$ in nonsterile sediment and $k = -0.000639 \text{ h}^{-1}$ in sterile sediment by shake-tests at Range Point and $k = -0.000139 \text{ h}^{-1}$ in nonsterile water and $k = -0.00000327 \text{ h}^{-1}$ in sterile water by shake-tests at Range Point (Walker et al. 1988)

$t_{1/2}(\text{aerobic}) = 180$ d, $t_{1/2}(\text{anaerobic}) = 50$ d in natural waters (Capel & Larson 1995).

Biotransformation:

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

$k_1 = 14.4\text{--}37.5 \text{ h}^{-1}$ (*Chironomus tentans* larvae in pond sediment-water system, 96-h exposure, calculated by using first-order kinetic and concn factors, Muir et al. 1983)

$k_1 = 11.4\text{--}82.0 \text{ h}^{-1}$ (*Chironomus tentans* larvae in river sediment-water system, 96-h exposure, calculated by using first-order kinetic and concn factors, Muir et al. 1983)

$k_1 = 35.8\text{--}54.9 \text{ h}^{-1}$ (*Chironomus tentans* larvae in sediment (sand)-water system, 96-h exposure, calculated by using first-order kinetic and concn factors, Muir et al. 1983)

$k_1 = 35.8\text{--}54.9 \text{ h}^{-1}$ (*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)

$k_2 = 45.4\text{--}38.6 \text{ h}^{-1}$ (*Chironomus tentans* larvae in pond sediment-water system, calculated by concentration decay curve, Muir et al. 1983)

$k_2 = 0.030 \text{ h}^{-1}$ (*Chironomus tentans* larvae in sediment (sand)-water system, calculated by concentration decay curve, Muir et al. 1983)

Half-Lives in the Environment:

Air: $t_{1/2} \sim 1.12\text{--}11.2$ 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)

$t_{1/2} = 2.2\text{--}5.4$ h, based on measured photooxidation in river water exposed to midday May sunlight (Zepp et al. 1976; quoted, Howard et al. 1991);

measured $k = (270 \pm 80) \text{ M}^{-1} \text{ s}^{-1}$ for direct reaction with ozone in water at pH 2.7–6.4 and $24 \pm 1^\circ\text{C}$, with a $t_{1/2} = 2.1$ min at pH 7 (Yao & Haag 1991)

biodegradation $t_{1/2}(\text{aerobic}) = 180$ d, $t_{1/2}(\text{anaerobic}) = 50$ 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: $t_{1/2} = 1200\text{--}8760$ 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);

$t_{1/2} = 4320\text{--}8760$ 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);

$t_{1/2} = 0.4\text{--}8.5$ d on cotton plants, $t_{1/2} = 0.8\text{--}1.2$ d on mint plants and $t_{1/2} \sim 2.5$ 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			
$t/^\circ\text{C}$	$\text{S/g}\cdot\text{m}^{-3}$	$t/^\circ\text{C}$	$\text{S/g}\cdot\text{m}^{-3}$	$\text{S/g}\cdot\text{m}^{-3}$	$\text{S/g}\cdot\text{m}^{-3}$
		particle size	0.01 μ	0.05 μ	5.0 μ
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

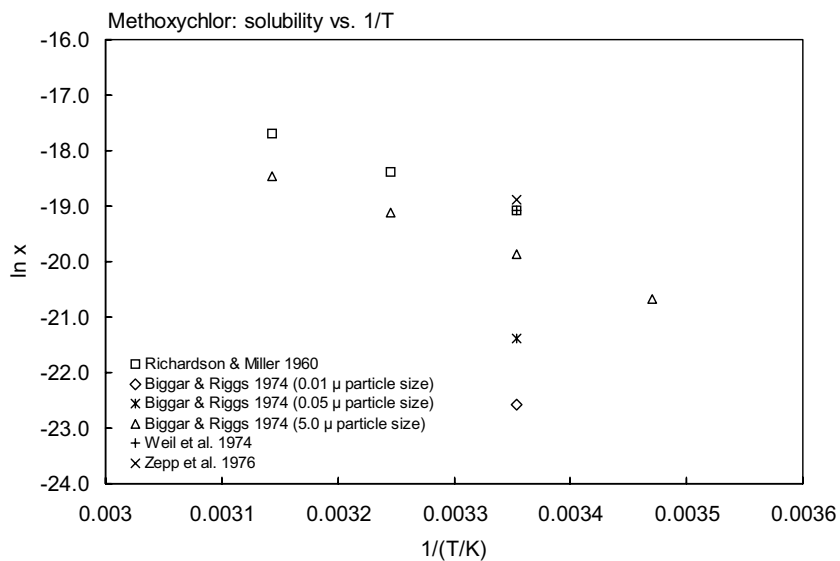
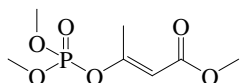


FIGURE 18.1.1.58.1 Logarithm of mole fraction solubility ($\ln x$) versus reciprocal temperature for methoxychlor.

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: C₇H₁₃O₆P

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/cm³ 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 (cm³/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/m³ 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·m³/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 χ , Sabljic et al. 1995)
2.12, 1.56	(soil, <i>cis</i> -mevinphos, estimated-class-specific model, estimated-general model, Gramatica et al. 2000)
2.28, 1.67	(soil, <i>trans</i> -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:

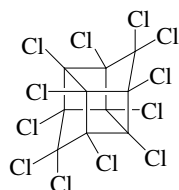
Ground water:

Sediment:

Soil: selected field $t_{1/2} = 3$ d (Wauchope et al. 1992; Hornsby et al. 1996).

Biota: estimated $t_{1/2} = 19 \pm 2$ and 24 ± 7 h in lettuce in the summer and $t_{1/2} = 20 \pm 11$ h in the fall, $t_{1/2} = 50$ h in cauliflower in the summer and $t_{1/2} = 18 \pm 1$ h in the fall, $t_{1/2} = 25 \pm 2$ 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 ($^{\circ}C$):

485 (dec., Smith et al. 1978; Spencer 1982; Kühne et al. 1995; Milne 1995; Lide 2003)

Boiling Point ($^{\circ}C$):

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 $25^{\circ}C$ (assuming $\Delta S_{fus} = 56$ J/mol K), F: 3.1×10^{-5} (mp at $485^{\circ}C$)

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$ 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} ($22^{\circ}C$, shake flask-GC, Smith et al. 1978)

0.02 ($24^{\circ}C$, Verschueren 1983)

7.0×10^{-5} (20 – $25^{\circ}C$, estimated, Augustijn-Beckers et al. 1994; Hornsby et al. 1996)

Vapor Pressure (Pa at $25^{\circ}C$ or indicated and reported temperature dependence equations):

8.0×10^{-4} ($50^{\circ}C$, Smith, et al. 1978)

1.3×10^{-4} ($20^{\circ}C$, Smith et al. 1978)

1.0×10^{-4} ($20^{\circ}C$, selected, Suntio et al. 1988)

9.0×10^{-7} ($10^{\circ}C$, 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} ($12^{\circ}C$, extrapolated supercooled liquid value, Hinckley et al. 1990)

1.1×10^{-4} (20 – $25^{\circ}C$, selected, Augustijn-Beckers et al. 1994; Hornsby et al. 1996)

Henry's Law Constant ($Pa \cdot m^3/mol$ and reported temperature dependence equations):

1013 ($20^{\circ}C$, calculated, Smith et al. 1978)

53.2 ($22^{\circ}C$, gas stripping-GC/ECD, Yin & Hassett 1986)

$\log [H/(atm \cdot m^3/mol)] = 12.709 - 4711/(T/K)$, temp range: 8 – $24^{\circ}C$ (gas stripping-GC, Yin & Hassett 1986)

840 ($20^{\circ}C$, calculated-P/C, Suntio et al. 1988)

44.1 ($20^{\circ}C$, 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} , Dorrough & 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*; *Thalassidsira 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 \pm 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, $t_{1/2}$:

Volatilization: $k = 5.37 \times 10^{-2} \text{ h}^{-1}$ (Hill et al. 1976) with $t_{1/2} = 500 \text{ h}$ from river, $t_{1/2} = 700 \text{ h}$ from pond, $t_{1/2} = 1980 \text{ h}$ from eutrophic lake, and 1 $t_{1/2} = 980 \text{ h}$ from oligotrophic lake (Smith et al. 1978).

Photolysis: rate constants $k < 5.0 \times 10^{-8} \text{ s}^{-1}$ (laboratory data, Smith et al. 1978);

$k = 4.2 \times 10^{-3} \text{ d}^{-1}$ (field data, Smith et al. 1978);

$t_{1/2} = 3.9 \times 10^3 \text{ h}$ (aquatic half-life, Haque et al. 1980);

$k = 0.123 \text{ d}^{-1}$ (sunlight, distilled water containing 2.0 mg DOC/L humic acid, Mudambi & Hassett 1988);

$k = 0.033 \text{ d}^{-1}$ (sunlight, distilled water, summer, Mudambi & Hassett 1988);

$k = 0.102 \text{ d}^{-1}$ (sunlight, Lake Ontario water, Mudambi & Hassett 1988);

$k = 0.019 \text{ d}^{-1}$ (sunlight, distilled water, fall, Mudambi & Hassett 1988).

Oxidation: laboratory data $k < 30 \text{ M}^{-1} \text{ s}^{-1}$ (Smith et al. 1978); $t_{1/2} \gg 0.7 \text{ yr}$ (Smith et al. 1978; quoted, Cheung 1984).

Hydrolysis: laboratory data rate constant $k = 1 \times 10^{-10} \text{ s}^{-1}$ (Smith et al. 1978); $k = 2 \times 10^{-10} \text{ s}^{-1}$ with $t_{1/2} = 250 \text{ yr}$ (Cheung 1984);

degradation rate constant $k = 1.93 \times 10^{-4} \text{ h}^{-1}$ (Mackay et al. 1985; quoted, Mackay & Paterson 1991).

Biodegradation: slow process (Cheung 1984).

Biotransformation:

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

$k_1 > 8.50 \text{ d}^{-1}$ (rainbow trout, Oliver & Niimi 1985)

$k_2 < 0.0007 \text{ d}^{-1}$ (rainbow trout, Oliver & Niimi 1985)

$k_2 = 0.017 \text{ d}^{-1}$ with $t_{1/2} = 42 \text{ d}$ and $k_2 = 0.009 \text{ d}^{-1}$ with $t_{1/2} = 78 \text{ d}$ 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 $t_{1/2} = 0.83 \text{ h}$ in river or stream, $t_{1/2} = 420 \text{ h}$ in pond, and $t_{1/2} = 1480 \text{ h}$ by sorption in both eutrophic lake and oligotrophic lake; with photolysis $t_{1/2} > 8000 \text{ h}$ and oxidation $t_{1/2} > 1000 \text{ h}$ in pond, river, eutrophic lake and oligotrophic lake (Smith et al. 1978);

degradation rate constant $k = 1.93 \times 10^{-4} \text{ h}^{-1}$ (Mackay et al. 1985; quoted, Mackay & Paterson 1991);

$t_{1/2} = 7 \text{ d}$ in sunlit, air-equilibrated humic acid solution, or natural water (Mudambi & Hassett 1988; Burns et al. 1996).

Ground water:

Soil: estimated field $t_{1/2} = 3000 \text{ d}$ (Augustijn-Beckers et al. 1994; Hornsby et al. 1996)

$t_{1/2} = 8.2 \text{ yr}$, extremely persistent in soil (Geyer et al. 2000)

Biota: $t_{1/2} > 1000 \text{ d}$ (Skea et al. 1981; Oliver & Niimi 1985);

$t_{1/2} > 28 \text{ d}$ in fathead minnow to ^{14}C mirex (Huckins et al. 1982);

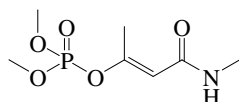
$t_{1/2} > 500 \text{ d}$ (4°C , rainbow trout, Niimi & Palazzo 1985);

$t_{1/2} = 114 \text{ d}$ as observed and $t_{1/2} = 495 \text{ d}$ as adjusted (12°C , rainbow trout, Niimi & Palazzo 1985);

$t_{1/2} = 103 \text{ d}$ as observed and $t_{1/2} > 1000 \text{ d}$ as adjusted (18°C , rainbow trout, Niimi & Palazzo 1985).

Depuration $t_{1/2} = 42\text{--}78 \text{ d}$ 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: C₇H₁₄NO₅P

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/cm³ at 20°C):

1.33 (Hartley & Kidd 1987; Worthing & Hance 1991; Montgomery 1993; Milne 1995)

1.22 (Tomlin 1994)

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: 0.508 (mp at 55°C)

Water Solubility (g/m³ 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·m³/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, $t_{1/2}$:

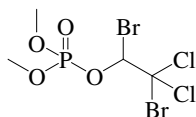
Hydrolysis: calculated $t_{1/2} = 96$ d at pH 5, $t_{1/2} = 66$ d at pH 7 and $t_{1/2} = 17$ d at pH 9 and 20°C (Worthing & Hance 1991; Montgomery 1993; Tomlin 1994).

Half-Lives in the Environment:

Soil: selected field $t_{1/2} = 30$ d (Wauchope et al. 1992; Hornsby et al. 1996);

$t_{1/2} = 1$ –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 ($^{\circ}C$):

27 (Lide 2003)

Boiling Point ($^{\circ}C$):

110/0.5 mmHg (Spencer 1982; Hartley & Kidd 1987; Worthing & Walker 1987; Montgomery 1993; Tomlin 1994)

Density (g/cm^3 at $20^{\circ}C$):

1.96 ($20^{\circ}C$, Hartley & Kidd 1987; Montgomery 1993; Tomlin 1994)

1.97 ($20^{\circ}C$, 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 $25^{\circ}C$ (assuming $\Delta S_{fus} = 56 J/mol K$), F: 0.956 (mp at $27^{\circ}C$)

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$):

practically insoluble in water (Hartley & Kidd 1987; Worthing & Walker 1987)

0.3, 2000 (quoted, Wauchope et al. 1992)

2000 (20 – $25^{\circ}C$, selected, Wauchope et al. 1992; Hornsby et al. 1996)

10 (Montgomery 1993)

Vapor Pressure (Pa at $25^{\circ}C$ or as indicated and reported temperature dependence equations):

0.266 ($20^{\circ}C$, Hartley & Kidd 1987; Worthing & Walker 1987; Tomlin 1994)

6.0×10^{-2} , 0.67, 5.20, 31.0, 150 (25 , 50 , 70 , 100 , $125^{\circ}C$, gas saturation-GC, Rordorf 1989)

$\log(P_L/Pa) = 12.307 - 4034.2/(T/K)$; measured range 50.5 – $120^{\circ}C$ (liquid, gas saturation-GC, Rordorf 1989)

0.267, 0.00267 (Wauchope et al. 1992)

0.0267 (20 – $25^{\circ}C$, selected, Wauchope et al. 1992; Hornsby et al. 1996)

0.267 ($20^{\circ}C$, Montgomery 1993)

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

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, $t_{1/2}$:

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).

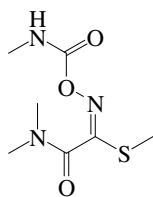
Ground water:

Sediment:

Soil: field $t_{1/2} = 1$ 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 ($^{\circ}C$):

109 (Lide 2003)

Boiling Point ($^{\circ}C$):

dec (Lide 2003)

Density (g/cm^3 at $20^{\circ}C$):

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 $25^{\circ}C$ (assuming $\Delta S_{fus} = 56$ J/mol K), F: 0.150 (mp at $109^{\circ}C$)

0.15 ($20^{\circ}C$, Suntio et al. 1988)

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$ 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 – $25^{\circ}C$, selected, Wauchope et al. 1992; Hornsby et al. 1996)

Vapor Pressure (Pa at $25^{\circ}C$ or as indicated):

0.0306 (Khan 1980; Spencer 1982)

0.0306 (20 – $25^{\circ}C$, selected, Wauchope et al. 1992; Hornsby et al. 1996)

0.0311 (Montgomery 1993)

0.0310 (Tomlin 1994)

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

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 – $25^{\circ}C$, 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 from 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 χ , 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 \geq 0.1%, OC \geq 0.5%, average, Delle Site 2001)
1.08	(sediment: organic carbon OC \geq 0.5%, average, Delle Site 2001)

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

Volatilization:

Photolysis: $t_{1/2} = 55.4$ h (absorbance wavelength 223 nm) (Montgomery 1993).

Oxidation:

$k(aq.) = (620 \pm 150) \text{ M}^{-1} \text{ s}^{-1}$ for direct reaction with ozone in water at pH 2–7 and $24 \pm 1^\circ\text{C}$, with a $t_{1/2} = 54$ s at pH 7 (Yao & Haag 1991).

Hydrolysis: hydrolysis $t_{1/2} > 31$ d at pH 5, 8 d at pH 7 and $t_{1/2} = 3$ h at pH 9 (Tomlin 1994).

Biodegradation: decomposition rate constants range from $k = 0.182 \text{ d}^{-1}$ 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 $t_{1/2} = 3.1$ to 6.5 d in five Israeli soils (Gerstl 1984);
 $t_{1/2} = 6$ 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 $k = (620 \pm 150) \text{ M}^{-1} \text{ s}^{-1}$ for direct reaction with ozone in water at pH 2.0–7.0 and $24 \pm 1^\circ\text{C}$, with $t_{1/2} = 54$ s at pH 7 (Yao & Haag 1991).

Ground water:

Sediment:

Soil: $t_{1/2} = 9$ –15 d (Harvey & Han 1978);

$t_{1/2} = 12$ –68 d for soils from Holland depending on the moisture content (Smelt et al. 1979);

$t_{1/2} = 15$ 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 $t_{1/2} = 4$ –13 d at 25°C and, $t_{1/2} = 32.7$ d at 15°C , $t_{1/2} = 3.8$ d at 35° in Bet Dagan soil; rate constants between $k = 0.11$ – 0.23 d^{-1} and with $t_{1/2} \sim 4$ d in 5 Israeli soils (Gerstl 1984);

$t_{1/2} = 6$ d in screening model calculations (Jury et al. 1987b);

$t_{1/2} = 7$ d (Worthing & Hance 1991);

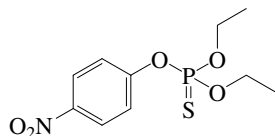
$t_{1/2} = 8$ –50 d (Ou & Rao 1986) and

$t_{1/2} = 10.2$ –13.1, 6.2, 7.1 and 17.8 d in Pitstone, Devizes, Sutton, Veany soils, respectively (Montgomery 1993);

field $t_{1/2} = 4$ 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, Aphonite, 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 rodiax, T-47, Thiofos, Tiophos, Tox 47, Vapophos, Vitrex

Chemical Name: *O,O*-diethyl *O*-4-(nitrophenyl) phosphorothioate; diethyl 4-nitrophenyl phosphorothioate; phosphorothioic 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 ($^{\circ}C$):

6.1 (Melnikov 1971; Freed et al. 1977; Montgomery 1993; Tomlin 1994; Milne 1995; Lide 2003)

Boiling Point ($^{\circ}C$):

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 $20^{\circ}C$):

1.265 ($25^{\circ}C$, Spencer 1982; Hartley & Kidd 1987; Milne 1995)

1.26 ($25^{\circ}C$, Merck Index 1989; Montgomery 1993)

1.2694 ($25^{\circ}C$, 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 $25^{\circ}C$ (assuming $\Delta S_{fus} = 56 J/mol K$), F: 1.0

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$ or as indicated):

24 (Macy 1948; Günther et al. 1968; Melnikov 1971; Spencer 1973)

18–31 (rm temp., > 95% purity with max. particle size 0.07–5.0 μ , shake flask-GC, Robeck et al. 1965)

11.9 ($20^{\circ}C$, NIEHS 1975; quoted, Freed et al. 1977)

11.9 ($20^{\circ}C$, 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 ($20^{\circ}C$, 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 m³/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 $t_{1/2} \sim 13$ d in nonstirred aqueous solutions and $t_{1/2} \sim 8.7$ 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 $t_{1/2} < 1$ 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 $t_{1/2} = 88$ h (Hazardous Substances Data Bank 1989; quoted, Montgomery 1993)

$t_{1/2} = 55$ d without addition of humic substances; $t_{1/2} = 18$ d and $t_{1/2} = 9$ 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_{NO_3} with NO_3 radical and k_{O_3} with O_3 or as indicated, *data at other temperatures see reference:

$k_{OH}(\text{calc}) = 92 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ (Winer & Atkinson 1990).

Hydrolysis:

$k(\text{second-order alkaline}) = 1.2 \times 10^{-3} \text{ M}^{-1} \text{ s}^{-1}$ at 27°C (Ketelaar 1950; quoted, Wolfe 1980)

$t_{1/2} = 130$ d at pH 7.4 and 20°C (NIEHS 1975; quoted, Freed et al. 1977, 1979; Montgomery 1993)

$t_{1/2} = 5240$ 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 $t_{1/2}$ 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)

$t_{1/2} = 24$ wk at pH 6, $t_{1/2} = 19$ wk at pH 7.4 and 20°C (Freed et al. 1979; quoted, Howard 1991; Montgomery 1993)

$t_{1/2} = 43$ wk at pH 5, $t_{1/2} = 24$ wk at pH 6, and $t_{1/2} = 15$ wk at pH 8 and 20°C (Chapman & Cole 1982; quoted, Howard 1991; Montgomery 1993)

$k(\text{alkaline}) = 2.3 \times 10^{-2} \text{ M}^{-1} \text{ s}^{-1}$, $k(\text{neutral}) = 4.5 \times 10^{-8} \text{ s}^{-1}$ in aqueous buffer at 20°C (Harris 1982)

$k = 2.4 \text{ yr}^{-1}$ at pH 7.0 and 25°C (Kollig 1993); $t_{1/2} = 3.5$ wk at pH 6 (Montgomery 1993)

$t_{1/2} = 272$ d at pH 4, $t_{1/2} = 260$ d at pH 7, and $t_{1/2} = 130$ 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)

$t_{1/2} > 4250$ d from biodegradation rate constant in aquatic systems from river water samples (Williams 1977; quoted, Scow 1982);

$k = 0.029 \text{ d}^{-1}$ in soil by die-away tests from soil incubation studies (Rao & Davidson 1980; quoted, Scow 1982)

$t_{1/2} = 18$ 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)

$k < 0.00016 \text{ d}^{-1}$ 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)

$t_{1/2} = 3670$ h at pH 5 and $t_{1/2} = 523$ h at pH 9 in water at 20°C (Gomaa & Faust 1972)

estimated $t_{1/2} > 4250$ d from biodegradation rate constant in aquatic systems from river water samples (Williams 1977; quoted, Scow 1982);

$t_{1/2} = 5240$ 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 $t_{1/2}$ 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)

$t_{1/2} = 7.84$ d in the Indian River water at 24 ppt salinity; pH 8.16 (Wang & Hoffman 1991);

photolysis $t_{1/2} = 55$ d without addition of humic substances; $t_{1/2} = 18$ d and 9 d with concn of humic acid 20 mg/L and 50 mg/L, respectively, under light intensity $\lambda > 290$ nm (Mansour & Feicht 1994);

$t_{1/2} = 120$ d at 6°C , $t_{1/2} = 84$ d at 22°C in darkness for Milli-Q water at pH 6.1; $t_{1/2} = 120$ d at 6°C , $t_{1/2} = 86$ d at 22°C in darkness, 8 d under sunlight conditions for river water at pH 7.3; $t_{1/2} = 122$ d at 6°C , $t_{1/2} = 33$ d at 22°C in darkness for filtered river water at pH 7.3; $t_{1/2} = 542$ d at 6°C , $t_{1/2} = 44$ d at 22°C in darkness, $t_{1/2} = 18$ 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);

$t_{1/2} > 24$ wk in sterile sandy loam and $t_{1/2} < 1.0$ wk in nonsterile sandy loam; $t_{1/2} > 24$ wk in sterile organic soil and $t_{1/2} = 1.5$ wk in nonsterile organic soil (Miles et al. 1979);

estimated first-order $t_{1/2} = 23.9$ 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 $t_{1/2} = 20$ –100 d (Willis & McDowell 1982);

reported $t_{1/2} = 18$ 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 $t_{1/2} = 23$ d and av. degradation rate constant $k = 0.0315$ d⁻¹ in sandy clay with $t_{1/2} = 22$ d (Sattar 1990);

$t_{1/2} = 14$ d (selected, Halfon et al. 1996);

field $t_{1/2} = 14$ d (20–25°C, selected, Hornsby et al. 1996);

soil $t_{1/2} = 6$ 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 18.1.1.64.1

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)
$\log P = A - B/(C + t/^{\circ}\text{C})$	(2)	$P = A - B/(C + t/^{\circ}\text{C})$	(2a)
$\log P = A - B/(C + T/K)$	(3)		
$\log P = A - B/(T/K) - C \cdot \log (T/K)$	(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

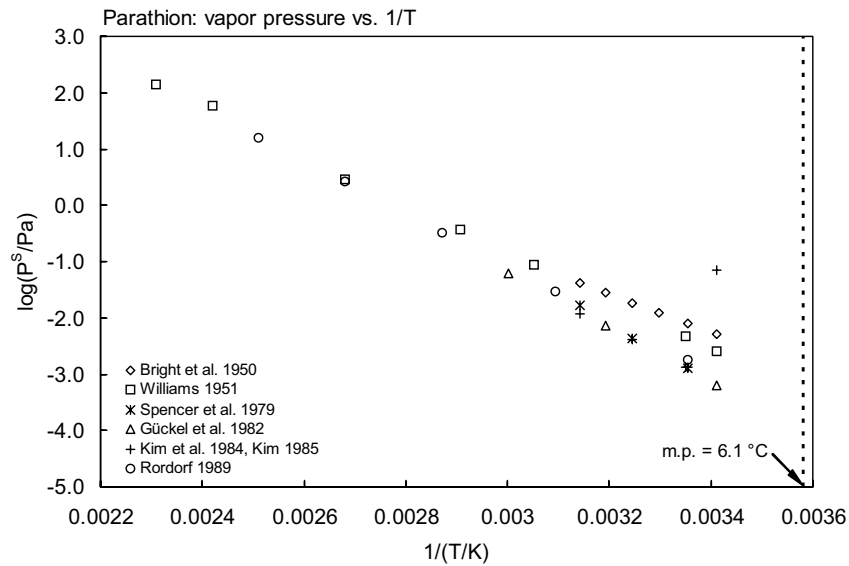
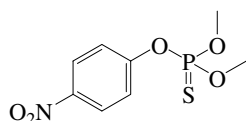


FIGURE 18.1.1.64.1 Logarithm of vapor pressure versus reciprocal temperature for parathion.

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 ($^{\circ}C$):

38 (Lide 2003)

Boiling Point ($^{\circ}C$):

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 $20^{\circ}C$):

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 $25^{\circ}C$ (assuming $\Delta S_{fus} = 56$ J/mol K), F: 0.746 (mp at $38^{\circ}C$)

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$ 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 ($19.5^{\circ}C$, shake flask-GC, Bowman & Sans 1979, 1983b)

55 ($20^{\circ}C$, Freed et al. 1979)

55–60 (Worthing 1979, 1983; Hartley & Kidd 1987)

60 (Khan 1980)

53 (Weber et al. 1980)

55 ($20^{\circ}C$, Worthing & Hance 1991; Tomlin 1994)

60 (20 – $25^{\circ}C$, selected, Wauchope et al. 1992; Hornsby et al. 1996)

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

0.00133 ($20^{\circ}C$, Wolfdietrich 1965; von Rümker & Horay 1972)

0.00129 ($20^{\circ}C$, Gückel et al. 1973)

0.0023 (Grover et al. 1976)

0.00229* ($24.9^{\circ}C$, gas saturation-GC, measured range 24.9 – $45.1^{\circ}C$, Spencer et al. 1979)

$\log(P/mmHg) = 14.37 - 3700/(T/K)$; temp range 24.9 – $34.9^{\circ}C$ (gas saturation, Spencer et al. 1979)

$\log(P/mmHg) = 10.61 - 4543/(T/K)$; above mp 35.2 – $35.4^{\circ}C$ (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)
 $\log (P/\text{mmHg}) = 9.0935 - 4063.65/(T/K)$; 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)
 $\log (P/\text{mmHg}) = 17.0502 - 6520.21/(T/K)$; 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 ($\text{Pa}\cdot\text{m}^3/\text{mol}$ 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 $k < 0.01 \text{ kg ha}^{-1} \text{ d}^{-1}$ in a flooded rice field (Seiber et al. 1986; Seiber & McChesney 1987; quoted, Seiber et al. 1989)

Photolysis: lab. rate constant $k = 2.7 \times 10^{-7} \text{ s}^{-1}$ in early January with photolysis $t_{1/2} = 240 \text{ h}$, 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);

$t_{1/2} = 8 \text{ d}$ in summer and $t_{1/2} = 38 \text{ d}$ in winter for direct sunlight photolysis in natural water (Smith et al. 1978; quoted, Howard 1991; Howard et al. 1991);

photolytic $t_{1/2} = 200 \text{ h}$ 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_{NO_3} with NO_3 radical and k_{O_3} with O_3 or as indicated, *data at other temperatures see reference:

$k = 3.0 \text{ M}^{-1} \text{ s}^{-1}$ (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:

$k = .4 \times 10^{-2} \text{ mol min}^{-1}$ with $t_{1/2} = 125 \text{ h}$ for pH <11.0 at 15°C (Ketelaar & Gersmann 1958; quoted, Freed 1976)

$k = 1.1 \times 10^{-7} \text{ s}^{-1}$ 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)

$t_{1/2} = 1.7 \text{ wk}$ at pH about 6 and room temp. (Cowart et al. 1971; quoted, Smith et al. 1978)

$k = 1.1 \times 10^{-7} \text{ s}^{-1}$ with $t_{1/2} = 72 \text{ d}$ at pH 7 and 25°C (Mabey & Mill 1978; quoted, Howard et al. 1991)

$k = 9 \times 10^{-7} \text{ s}^{-1}$ (Smith et al. 1978)

$k(\text{alkaline}) = 5.3 \times 10^{-3} \text{ M}^{-1} \text{ s}^{-1}$ at 27°C and pH 10 (Smith et al. 1978; quoted, Wolfe 1980)

$t_{1/2} = 68 \text{ d}$ at pH 5, $t_{1/2} = 40 \text{ d}$ at pH 7, $t_{1/2} = 33 \text{ d}$ at pH 9 at 25°C (Tomlin 1994).

Biodegradation:

$k = 1.7 \times 10^{-7} \text{ -g cell}^{-1} \text{ h}^{-1}$ (Smith et al. 1978);

$t_{1/2}(\text{aq. aerobic}) = 360\text{--}1680 \text{ h}$, based on an unacclimated aerobic river die-away test data (Bourquin et al. 1979; Spain et al. 1980; quoted, Howard et al. 1991);

$t_{1/2}(\text{aq. anaerobic}) = 24\text{--}168 \text{ h}$, based on unacclimated anaerobic soil and sediment grab sample data (Adhya et al. 1981; Wolfe et al. 1986; quoted, Howard et al. 1991);

$t_{1/2} = 15 \text{ d}$ 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);

$k = (0.003 \pm 0.0003) \text{ h}^{-1}$ with half-life of 220.9 h in surface aerobic soils at Williamsburg,

$k = (0.0017 \pm 0.00009) \text{ h}^{-1}$ with half-life of 410 h in subsurface aerobic soils at Sault Ste. Marie (Ward 1985)

$k = 0.30 \text{ d}^{-1}$ in river sediment, $k = 0.02 \text{ d}^{-1}$ in river water (Cripe et al. 1987; quoted, Battersby 1990)

Biotransformation:

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

$$k_1 = (2.59 \pm 0.88) \times 10^{-3} \text{ mL g}^{-1} \text{ d}^{-1} \text{ (guppy, De Bruijn \& Hermens 1991)}$$

$$k_2 = (2.38 \pm 0.14) \text{ d}^{-1} \text{ (guppy, De Bruijn \& Hermens 1991)}$$

$$k_2 = 1.71 \text{ d}^{-1} \text{ (guppy, calculated-} K_{OW} \text{, De Bruijn \& Hermens 1991)}$$

$$k_2 = (0.12 \pm 0.02) \times 10^{-3} \text{ (NADPH) min}^{-1} \text{ mg protein}^{-1} \text{ (rainbow trout, De Bruijn et al. 1993)}$$

$$k_2 = (0.11 \pm 0.03) \times 10^{-3} \text{ (GSH) min}^{-1} \text{ mg protein}^{-1} \text{ (rainbow trout, De Bruijn et al. 1993)}$$

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 $k = 4.77 \times 10^{-4} \text{ min}^{-1}$ 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 $k = 0.30 \text{ d}^{-1}$ in river sediment and $k = 0.02 \text{ d}^{-1}$ 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 $k = 3.80 \times 10^{-4} \text{ min}^{-1}$ 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: $k = (3.5 \pm 0.6) \times 10^{-3} \text{ min}^{-1}$ in Beaver Dam sediments samples at pH 6.7, $k = (2.9 \pm 1.2) \times 10^{-3} \text{ min}^{-1}$ in Memorial Park sediments samples at pH 6.5 and $k = (2.8 \pm 2.4) \times 10^{-3} \text{ min}^{-1}$ in Hickory Hills sediments samples at pH 6.9 near Athens, Georgia (Wolfe et al. 1986);

reaction rate $k = 2.85 \times 10^{-5} \text{ min}^{-1}$ 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 $k = 0.029, 0.042 \text{ d}^{-1}$ (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 $k = 0.16 \text{ d}^{-1}$ with $t_{1/2} = 4$ d under laboratory conditions and rate constant $k = 0.046 \text{ d}^{-1}$ 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

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

$$\log P = A - B/(C + t/^{\circ}\text{C}) \quad (2) \qquad \ln P = A - B/(C + t/^{\circ}\text{C}) \quad (2a)$$

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

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

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

$$\Delta H_v = 109.2 \text{ kJ/mol}$$

above the melting point

eq. 1	P/mmHg
A	10.61
B	4543

$$\Delta H_v = 87.03 \text{ kJ/mol}$$

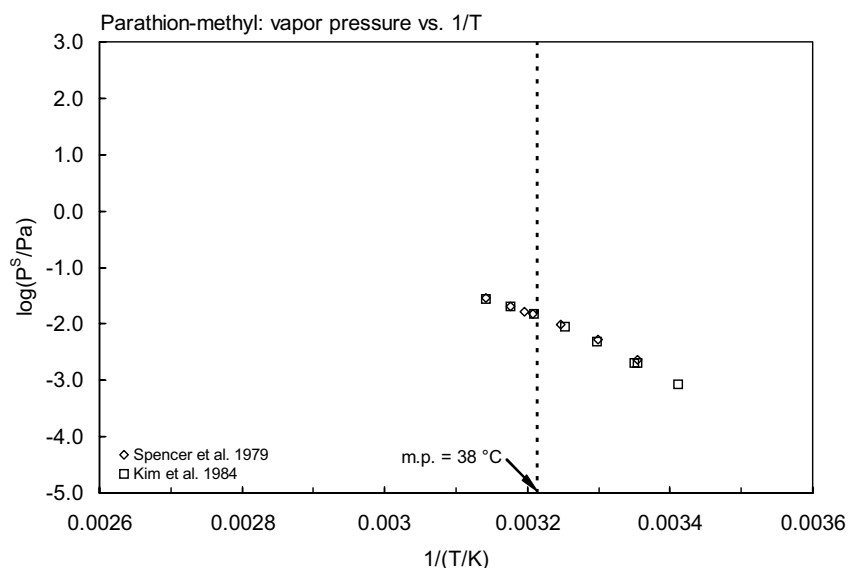
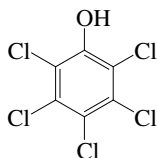


FIGURE 18.1.1.65.1 Logarithm of vapor pressure versus reciprocal temperature for parathion-methyl.

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 ($^{\circ}C$):

191 (Firestone 1977; Weast 1982–83; Hartley & Kidd 1987)

187 (Schmidt-Bleek et al. 1982)

174 (Lide 2003)

Boiling Point ($^{\circ}C$):

310 (Verschueren 1977, 1983; Callahan et al. 1979)

309–310 (Hartley & Kidd 1987)

310 (dec, Lide 2003)

Density ($20^{\circ}C$, g/cm^3):

1.987 (Firestone 1977)

1.978 (Schmidt-Bleek et al. 1982; Verschueren 1983)

1.980 ($22^{\circ}C$, 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 $25^{\circ}C$ (assuming $\Delta S_{fus} = 56 J/mol K$) F: 0.0345 (mp at $174^{\circ}C$)

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$ or as indicated):

15.4 (gravimetric, Carswell & Nason 1938)

18 ($27^{\circ}C$, 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 \pm 2	(shake flask-UV at pH 2.5, Valsaraj et al. 1991)
32 \pm 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 m³/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 (Verschuereen 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. relictus*, 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} m²/s and in water 7×10^{-10} m²/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 $k = 5 \times 10^{-4}$ 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 $k = 3.4 \times 10^{-4}$ s⁻¹ for a depth of 300 cm at pH 7 with light intensity of 0.04 watts/cm² 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 $k = 0.07 \text{ h}^{-1}$ with $t_{1/2} = 10 \text{ d}$ in winter; $k = 0.25 \text{ h}^{-1}$ with $t_{1/2} = 10 \text{ d}$ 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 $t_{1/2} = 0.75 \text{ h}$ in Xenotest 1200 (Svenson & Björndal 1988);

aqueous photolysis $t_{1/2} = 1\text{--}110 \text{ h}$ (Hwang et al. 1986; Sugiura et al. 1984; selected, Howard et al. 1991);

$t_{1/2} = 7.43 \text{ d}$ assuming a linear rate of photolysis during 96-h period (Smith et al. 1987);

photodegradation rate constant $k = 0.60 \text{ h}^{-1}$ corresponding to $t_{1/2} = 1.0 \text{ h}$ (summer), $k = 0.37 \text{ h}^{-1}$ corresponding to $t_{1/2} = 2 \text{ h}$ (winter) in distilled water; and $k = 0.37 \text{ h}^{-1}$ corresponding to $t_{1/2} = 2 \text{ h}$ (summer), $k = 0.27 \text{ h}^{-1}$ corresponding to $t_{1/2} = 3.0 \text{ h}$ (winter) in estuarine water under irradiation by natural sunlight (quoted from Hwang et al. 1987, Sanders et al. 1993).

Oxidation: rate constant $k \gg 3.0 \times 10^5 \text{ M}^{-1}\cdot\text{s}^{-1}$ for the reaction with ozone in water at pH 2.0 (Hoigné & Bader 1983);

photooxidation $t_{1/2} = 66\text{--}3480 \text{ h}$ 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 $t_{1/2} = 139.2\text{--}1392 \text{ h}$, 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 $k = (0.2 \pm 5.5) \times 10^6 \text{ M}^{-1}\cdot\text{s}^{-1}$ for the reaction with singlet oxygen in aqueous phosphate buffer at $(27 \pm 1)^\circ\text{C}$ (Tratnyek & Hoigné 1991);

atmospheric $t_{1/2} < 24 \text{ h}$ at noon in mid-summer to $t_{1/2} = 216 \text{ h}$ 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: $t_{1/2} = 1800\text{--}2160 \text{ h}$ and $480\text{--}\infty \text{ h}$ to obtain 75% degradation in mineral medium and seawater, respectively (De Kreuk & Hanstveit 1981);

aqueous aerobic $t_{1/2} = 552\text{--}4272 \text{ h}$, based on unacclimated and acclimated aerobic sediment grab sample data (Delaune et al. 1983; Baker & Mayfield 1980; quoted, Howard et al. 1991);

aqueous anaerobic $t_{1/2} = 1008\text{--}36480 \text{ h}$, 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 $k = 0.0017 \text{ L } \mu\text{g}^{-1}\cdot\text{d}^{-1}$ (Moos et al. 1983);

microbial degradation negligible in darkness (Hwang et al. 1986);

degradation rate constant $k = 0.12 \pm 0.01 \text{ h}^{-1}$ in the absence of light (Minero et al. 1993).

Biotransformation: degradation rate $k = 3 \times 10^{-14} \text{ mol}\cdot\text{cell}^{-1}\cdot\text{h}^{-1}$ with microorganisms in Seneca River waters (Banerjee et al. 1984).

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

$k_1 = 18.3 \text{ h}^{-1}$, 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)

$k_1 = 222 \text{ d}^{-1}$, 1677 d^{-1} (flagfish: whole fish; fish lipid, Smith et al. 1990)

$k_2 = 1.03 \text{ d}^{-1}$, 1.03 d^{-1} (flagfish: whole fish; fish lipid, Smith et al. 1990)

$k_2 = 1.03 \text{ d}^{-1}$, 0.95 d^{-1} (flagfish: BCF based, toxicity based, Smith et al. 1990)

$k_2 = 0.00195 \pm 0.00063 \text{ h}^{-1}$ (*M. relictus*, Landrum & Dupuis 1990)

$k_2 = 0.00330 \pm 0.00140 \text{ h}^{-1}$ (*P. hoyi*, Landrum & Dupuis 1990)

Half-Lives in the Environment:

Air: $t_{1/2} = 139.2\text{--}1392 \text{ h}$, based on an estimated rate constant for the vapor-phase reaction with hydroxyl radicals in air (Howard et al. 1991);

photolysis $t_{1/2} = 6.5 \text{ h}$ in noonday summer sunshine (Howard 1991);

$t_{1/2} = 216 \text{ h}$ at latitude of 43.70°N at noon in January to $t_{1/2} < 24 \text{ h}$ in mid-summer for reaction with hydroxyl radicals (Bunce et al. 1991).

Surface water: calculated photolysis $t_{1/2} = 4.75 \text{ h}$ from a determined rate $k = 3.4 \times 10^{-4} \text{ s}^{-1}$ 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 $t_{1/2} = 1.5 \text{ d}$ was estimated from photolytic destruction by sunlight in an aqueous solution at Davis, California (Wong & Crosby 1978; quoted, Callahan et al. 1979);

photolytic $t_{1/2} = 10\text{--}15 \text{ d}$ (Brockway et al. 1984);

rate constant $k \gg 3.0 \times 10^5 \text{ M}^{-1} \text{ s}^{-1}$ 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 al. 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).

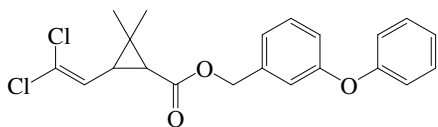
Biota: biological $t_{1/2}$ ~ 30 d in guppy *Lebistes reticulatus* (Landner et al. 1977);

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: C₂₁H₂₀Cl₂O₃

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/cm³ 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 (cm³/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/m³ 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}	(<i>cis</i> isomer, GC-RT correlation, supercooled liquid P_L , Hinckley et al. 1990)
8.1×10^{-6}	(<i>trans</i> 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 <i>cis</i> isomer at 20°C, Worthing & Hance 1991; Montgomery 1993; Tomlin 1994)
1.5×10^{-6}	(pre <i>trans</i> 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)
$1.4 \times 10^{-5*}$	(<i>cis</i> 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	(<i>cis</i> -form, HPLC-RT correlation, Muir et al. 1985)
5.7 ± 0.7	(<i>trans</i> -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	(<i>Pimephales promelas</i> , Spehar et al. 1983;)
1.49–1.84	(<i>trans</i> -form on sediment, 24 h BCF for chironomid larvae in water, Muir et al. 1985)
1.08–2.13	(<i>trans</i> -form on sediment, 24 h BCF for chironomid larvae in sediment, Muir et al. 1985)
0.95–1.70	(<i>trans</i> -form on sediment, 24 h BCF for chironomid larvae in sediment/pore water, Muir et al. 1985)
0.90–2.22	(<i>cis</i> -form on sediment, 24 h BCF for chironomid larvae in water, Muir et al. 1985)
1.46–2.62	(<i>cis</i> -form on sediment, 24 h BCF for chironomid larvae in sediment, Muir et al. 1985)
1.32–2.47	(<i>cis</i> -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	(<i>Oncorhynchus mykiss</i> , 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	(<i>cis</i> -form, silt, K_p on 34% DOC, Muir et al. 1985)
2.64	(<i>cis</i> -form, clay, K_p on 77% DOC, Muir et al. 1985)
2.64	(<i>trans</i> -form, silt, K_p on 23% DOC, Muir et al. 1985)
2.64	(<i>trans</i> -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 $\geq 0.1\%$, OC $\geq 0.5\%$, average, Delle Site 2001)

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

Volatilization:

Photolysis: photodegradation rate constant $k = 1.73 \times 10^{-3} \text{ min}^{-1}$ and $t_{1/2} = 400 \text{ min}$ with TiO_2 as catalyst after 20 h irradiation at 222 nm (Hidaka et al. 1992).

Oxidation:

Hydrolysis:

Biodegradation:

$k = 1.24 \times 10^{-2} \text{ h}^{-1}$ by bacteria strain *A. sobria* with $t_{1/2} = 56 \text{ h}$, $k = 1.13 \times 10^{-2} \text{ h}^{-1}$ by *E. carotovora* with $t_{1/2} = 61 \text{ h}$, $k = 8.66 \times 10^{-3} \text{ h}^{-1}$ by *Y. frederiksenii* with $t_{1/2} = 80 \text{ h}$ and $k = 1.43 \times 10^{-3} \text{ h}^{-1}$ for the control, uninoculated solution with $t_{1/2} = 485 \text{ d}$ in aqueous soil-free phase (*cis*-permethrin, Lee et al. 2004)

$k = 1.50 \times 10^{-2} \text{ h}^{-1}$ by *A. sobria* with $t_{1/2} = 45 \text{ h}$, $k = 1.51 \times 10^{-2} \text{ h}^{-1}$ by *E. carotovora* with $t_{1/2} = 46 \text{ h}$, $k = 1.85 \times 10^{-2} \text{ h}^{-1}$ by *Y. frederiksenii* with $t_{1/2} = 37 \text{ h}$ and $k = 2.85 \times 10^{-3} \text{ h}^{-1}$ for the control, uninoculated solution with $t_{1/2} = 259 \text{ d}$ in aqueous soil-free phase (*trans*-permethrin, Lee et al. 2004)

Biotransformation:

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

$k_1 = 1.5\text{--}2.3 \text{ h}^{-1}$ (*Chironomus tentans* larvae in pond sediment-water system for *trans*-permethrin, 96-h exposure, Muir et al. 1983)

$k_1 = 1.50 \text{ h}^{-1}$ (*Chironomus tentans* larvae in river sediment-water system for *trans*-permethrin, 96-h exposure, Muir et al. 1983)

$k_1 = 3.3\text{--}12.1 \text{ h}^{-1}$ (*Chironomus tentans* larvae in sediment (sand)-water system for *trans*-permethrin, 96-h exposure, Muir et al. 1983)

$k_1 = 4.9\text{--}14.7 \text{ h}^{-1}$ (*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)

$k_2 = 0.041 \text{ h}^{-1}$ (*Chironomus tentans* larvae in pond sediment-water system for *trans*-permethrin, calculated by concentration decay curve, Muir et al. 1983)

$k_2 = 0.021 \text{ h}^{-1}$ (*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: $t_{1/2} > 21 \text{ d}$ in 100 mL pesticide-seawater solution under indoor conditions, $t_{1/2} = 14 \text{ d}$ under outdoor light conditions and $t_{1/2} > 14 \text{ d}$ under outdoor dark conditions (Schimmel et al. 1983);

biodegradation half-lives by bacteria strains: $t_{1/2} = 56 \text{ h}$ by *A. sobria*, $t_{1/2} = 61 \text{ h}$ by *E. carotovora*, $t_{1/2} = 80 \text{ h}$ by *Y. frederiksenii* and $t_{1/2} = 485 \text{ d}$ for the control, uninoculated solution for *cis*-permethrin; $t_{1/2} = 45 \text{ h}$ by *A. sobria*, $t_{1/2} = 46 \text{ h}$ by *E. carotovora*, $t_{1/2} = 37 \text{ h}$ by *Y. frederiksenii* and $t_{1/2} = 259 \text{ d}$ 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: $t_{1/2} < 2.5 \text{ d}$ for untreated sediment and $t_{1/2} > 28 \text{ d}$ for sterile sediment (Schimmel et al. 1983).

Soil: reported $t_{1/2} < 38 \text{ d}$ 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 $t_{1/2} = 30 \text{ d}$ (Wauchope et al. 1992; Hornsby et al. 1996);

soil $t_{1/2} = 30 \text{ d}$ (Pait et al. 1992);

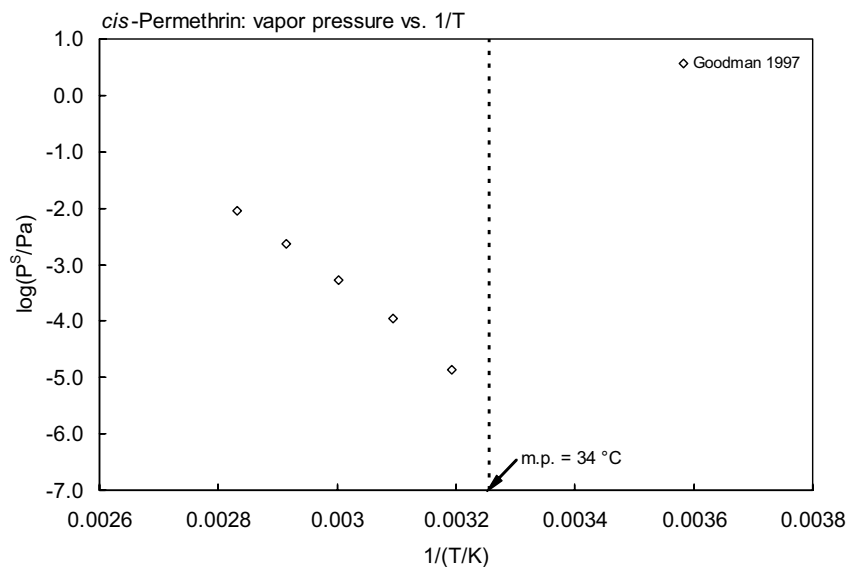
$t_{1/2} = 32 \text{ d}$ for forest soil (Dowd et al. 1993).

Biota: elimination $t_{1/2} \sim 16.7 \text{ h}$ in pond sediment-water, $t_{1/2} = 32.9 \text{ h}$ in sand-water systems (*Chironomus tentans* larvae, Muir et al. 1983)

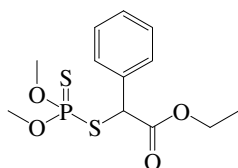
TABLE 18.1.1.67.1

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 ($^{\circ}C$):

17.5 (Khan 1980; Spencer 1982)

17–18 (Worthing & Hance 1991; Tomlin 1994)

Boiling Point ($^{\circ}C$): 78–80 (Spencer 1982)

Density (g/cm^3 at $20^{\circ}C$):

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 $25^{\circ}C$ (assuming $\Delta S_{fus} = 56$ K/ml K), F: 1.0

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$ or as indicated):

200 (Martin & Worthing 1977)

11 (20 – $25^{\circ}C$, shake flask-GC, Kanazawa 1981)

11 ($20^{\circ}C$, Khan 1980; Hartley & Kidd 1987)

11 ($24^{\circ}C$, Worthing & Walker 1987, 1991; Tomlin 1994)

11 (20 – $25^{\circ}C$, selected, Augustijn-Beckers et al. 1994; Hornsby et al. 1996)

Vapor Pressure (Pa at $25^{\circ}C$ or as indicated):

0.005 ($40^{\circ}C$, Hartley & Kidd 1987)

0.0053 ($40^{\circ}C$, Worthing & Hance 1991; Tomlin 1994)

3.5×10^{-4} (20 – $25^{\circ}C$, 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 ($Pa \cdot m^3/mol$):

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, $t_{1/2}$:Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants:

- excretion rate constant $k = 0.05 \text{ h}^{-1}$ from whole body willow shiner (Tsuda et al. 1992);
- excretion rate constant $k = 0.52 \text{ h}^{-1}$ with $t_{1/2} = 1.3 \text{ h}$ (Tsuda et al. 1993).

Half-Lives in the Environment:

Air:

Surface water:

Ground water:

Sediment:

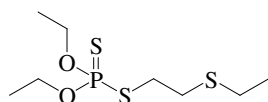
Soil: selected field $t_{1/2} = 11 \text{ d}$ (Augustijn-Beckers et al. 1994; Hornsby et al. 1996);

$t_{1/2} = 10 \text{ d}$ in silty clay loam and other soils (Tomlin 1994).

Biota: excretion rate constant $k = 0.05 \text{ h}^{-1}$ from whole body willow shiner (Tsuda et al. 1992);

excretion rate constant $k = 0.52 \text{ h}^{-1}$ with $t_{1/2} = 1.3 \text{ h}$ (Tsuda et al. 1993).

18.1.1.69 Phorate



Common Name: Phorate

Synonym: AC 3911, American Cyanamid 3911, ENT 24042, Foraate, 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 ($^{\circ}C$):

−42.9 (Spencer 1982)

<−15 (Montgomery 1993; Lide 2003)

Boiling Point ($^{\circ}C$):

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 $20^{\circ}C$):

1.156 ($25^{\circ}C$, Merck Index 1989; Montgomery 1993; Milne 1995)

1.167 (tech. grade at $25^{\circ}C$, 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 $25^{\circ}C$ (assuming $\Delta S_{fus} = 56$ J/mol K), F: 1.0

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$ or as indicated):

19 ($26^{\circ}C$, 95% pure, shake flask-GC, Lord & Burt 1964)

14 ($15^{\circ}C$, 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 ($20^{\circ}C$, 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 – $25^{\circ}C$, selected, Wauchope 1989; Wauchope et al. 1992; Hornsby et al. 1996)

20 ($24^{\circ}C$, Montgomery 1993)

Vapor Pressure (Pa at $25^{\circ}C$ or as indicated):

0.112 ($20^{\circ}C$, 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 ($20^{\circ}C$, 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 ($\text{Pa}\cdot\text{m}^3/\text{mol}$ 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, $\log K_{\text{OW}}$:

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, $\log \text{BCF}$:

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, $\log K_{\text{OC}}$:

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 $\log K_{\text{OM}}$ of 2.82, Briggs 1981)
2.32–3.60	(reported as $\log K_{\text{OM}}$, Mingelgrin & Gerstl 1983)
2.82	(screening model calculations, Jury et al. 1987a, b; Jury & Ghodrati 1989)
2.58, 2.88	(reported as $\log K_{\text{OM}}$, estimated as $\log K_{\text{OM}}$, 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 $k = 7.2 \times 10^{-3} \text{ h}^{-1}$ with a calculated $t_{1/2} = 96 \text{ h}$ at pH 7 (Ellington et al. 1987, 1988; quoted, Montgomery 1993);
calculated rate constant $k = 100 \times 10^{-12} \text{ cm}^3/\text{molecule}\cdot\text{s}$ for the vapor-phase reaction with hydroxyl radical in air (Winer & Atkinson 1990);

$t_{1/2} = 3.2 \text{ d}$ at pH 7 and $t_{1/2} = 3.9 \text{ d}$ at pH 9 (Worthing & Hance 1991);

rate constant $k = 62 \text{ yr}^{-1}$ at pH 7.0 and 25°C (Kollig 1993).

Biodegradation: $t_{1/2} = 82 \text{ d}$ for a 100 d leaching and screening test in 0–10 cm depth of soil (Rao & Davidson 1980; quoted, Jury et al. 1983);

$t_{1/2} = 82 \text{ d}$ in soil (Jury et al. 1984, 1987a, b, 1990; Jury & Ghorati 1989);

first-order rate constant $k = -0.0403 \text{ h}^{-1}$ in nonsterile sediment and $k = -0.0209 \text{ h}^{-1}$ in sterile sediment by shake-tests at Range Point and first-order rate constant $k = -0.0206 \text{ h}^{-1}$ in nonsterile water and $k = -0.0186 \text{ h}^{-1}$ in sterile water by shake-tests at Range Point (Walker et al. 1988);

first-order rate constants $k = -0.0241 \text{ h}^{-1}$ in nonsterile sediment and $k = -0.0185 \text{ h}^{-1}$ in sterile sediment by shake-tests at Davis Bayou and first-order rate constants $k = -0.0262 \text{ h}^{-1}$ in nonsterile water and $k = -0.0185 \text{ h}^{-1}$ 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: $t_{1/2} = 68 \text{ d}$ 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 $t_{1/2} = 82 \text{ d}$ in soil (Jury et al. 1984, 1987a, b, 1990; Jury & Ghodrati 1989; quoted, Montgomery 1993);

$t_{1/2} = 2\text{--}14 \text{ d}$ (Worthing & Hance 1991);

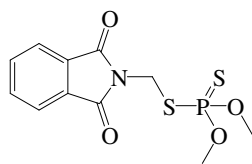
estimated field $t_{1/2} = 60 \text{ d}$ (Wauchope et al. 1992; quoted, Richards & Baker 1993; selected, Halfon et al. 1996; Hornsby et al. 1996);

soil $t_{1/2} = 25 \text{ d}$ (Pait et al. 1992).

Biota: $t_{1/2} = 1.4 \text{ d}$ half-lives in coastal Bermuda grass and alfalfa (Leuck & Bowman 1970; quoted, Montgomery 1993) and $t_{1/2} = 3.6 \text{ d}$ (Dobson et al. 1960; quoted, Montgomery 1993);

biochemical $t_{1/2} = 82 \text{ d}$ 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-thioylthiome-thylphthalimide; *S*-[(1,3-dihydro-1,3-dioxo-2*H*-isoindol-2-yl)methyl] *O,O*-dimethyl phosphorodithioate; phospho-rodithioic 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 ($^{\circ}C$):

72.0–72.7, 66.5–69.5 (pure, technical grade, Montgomery 1993; Tomlin 1994)

72 (Lide 2003)

Boiling Point ($^{\circ}C$):

decompose rapidly $>100^{\circ}C$ (Montgomery 1993)

Density (g/cm^3 at $20^{\circ}C$):

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 $25^{\circ}C$ (assuming $\Delta S_{fus} = 56$ J/mol K), F: 0.346 (mp at $72^{\circ}C$)

0.3 ($20^{\circ}C$, Suntio et al. 1988)

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$ or as indicated):

25 (Bright et al. 1950, Melnikov 1971; Spencer 1982)

25 (Hartley & Kidd 1987; Tomlin 1994; Milne 1995)

20 (20 – $25^{\circ}C$, selected, Wauchope et al. 1992; Hornsby et al. 1996)

22–25 (Montgomery 1993)

Vapor Pressure (Pa at $25^{\circ}C$ or as indicated):

6.03×10^{-4} ($20^{\circ}C$, Freed et al. 1977)

0.133 ($50^{\circ}C$, Spencer 1982; Hartley & Kidd 1987)

6.53×10^{-5} (20 – $25^{\circ}C$, selected, Wauchope et al. 1992; Hornsby et al. 1996)

6.03×10^{-5} , 0.133 (30, $50^{\circ}C$, 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 ($Pa \cdot m^3/mol$):

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 ($20^{\circ}C$, 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).

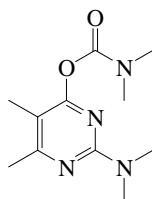
Ground water:

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 ($^{\circ}C$):

90.5 (Spencer 1982; Hartley & Kidd 1987; Worthing 1987; Tomlin 1994; Lide 2003)

Boiling Point ($^{\circ}C$):

Density (g/cm^3 at $20^{\circ}C$):

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 $25^{\circ}C$ (assuming $\Delta S_{fus} = 56 J/mol K$), F: 0.228 (mp at $90.5^{\circ}C$)

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$):

2700 (Kenaga 1980b; Spencer 1982; Hartley & Kidd 1987; Worthing & Walker 1987)

2000 (pH 4, $20^{\circ}C$, Tomlin 1994)

2700 (selected, Augustijn-Beckers et al. 1994; Hornsby et al. 1996)

Vapor Pressure (Pa at $25^{\circ}C$):

0.004 ($30^{\circ}C$, 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 ($Pa \cdot m^3/mol$ at $25^{\circ}C$):

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, $t_{1/2}$:

Volatilization:

Photolysis: aqueous solutions are unstable to UV light with $t_{1/2} < 1$ d at pH 5.7 or 9 (Tomlin 1994).

Oxidation:

Hydrolysis:

Biodegradation: $t_{1/2} = 7\text{--}234$ 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 $t_{1/2} < 1$ d at pH 5.7 or 9 (Tomlin 1994).

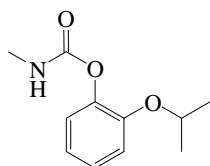
Ground water:

Sediment:

Soil: $t_{1/2} = 7\text{--}234$ d depending on soil type, organic matter ranging from 1.7–51.9% at pH 5.5–8.1 (Tomlin 1994);
field $t_{1/2} \sim 10$ 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 ($^{\circ}C$)

91.50 (Spencer 1982; Howard 1991; Kühne et al. 1995)

84–87 (Montgomery 1993)

87 (Lide 2003)

Boiling Point ($^{\circ}C$):

Density (g/cm^3 at $20^{\circ}C$):

Molar Volume (cm^3/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 $25^{\circ}C$ (assuming $\Delta S_{fus} = 56$ J/mol K), F: 0.246 (mp at $87^{\circ}C$)

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$ or as indicated):

2000 ($20^{\circ}C$, Spencer 1973; 1982)

2000 (Kenaga 1980; Kanazawa 1981)

2000 ($20^{\circ}C$, Worthing & Walker 1983, 1987, Worthing & Hance 1991)

1860 ($20^{\circ}C$, shake flask-GC, Bowman & Sans 1983)

1800 (20 – $25^{\circ}C$, selected, Wauchope et al. 1992; Hornsby et al. 1996)

1740, 1930, 2440 (10, 20, $30^{\circ}C$, Montgomery 1993)

Vapor Pressure (Pa at $25^{\circ}C$ or as indicated):

1.333 ($120^{\circ}C$, Melnikov 1971; Spencer 1973, 1982)

4.13×10^{-4} ($20^{\circ}C$, Hartley & Graham-Bryce 1980)

4.13×10^{-5} ($20^{\circ}C$, selected exptl. value from literature, Kim 1985)

0.0593, 0.0113 ($20^{\circ}C$, GC-RT correlation, GC-RT correlation with mp correction, Kim 1985)

4.00×10^{-4} ($20^{\circ}C$, Howard 1991)

1.69×10^{-3} (20 – $25^{\circ}C$, selected, Wauchope et al. 1992, Hornsby et al. 1996)

1.30×10^{-3} ($20^{\circ}C$, Montgomery 1993; Siebers et al. 1994)

Henry's Law Constant ($Pa \cdot m^3/mol$ at $25^{\circ}C$ or as indicated):

0.1308 ($20^{\circ}C$, 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)
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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 χ , 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 $k = 3.70 \times 10^{-3} \text{ h}^{-1}$ 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);

$t_{1/2} \sim 4$ h reacting with photochemically produced hydroxyl radical in air (Howard 1991).

Surface water: $t_{1/2} = 38\text{--}672$ 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: $t_{1/2} = 38\text{--}1344$ 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:

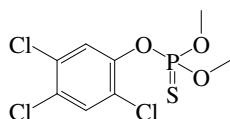
Soil: $t_{1/2} = 38\text{--}672$ h, based on estimated hydrolysis half-life at pH 9 (Aly & El-Dib 1971; quoted, Howard et al. 1991) and estimated unacclimated aqueous aerobic biodegradation half-life (Howard et al. 1991)

Field $t_{1/2} = 14\text{--}50$ d (Wauchope et al. 1992)

On sandy loam soil: first-order rate constants for photolytic decline, $k = 1.65 \times 10^{-3} \text{ h}^{-1}$ irradiated in moisture-maintained soil, $k = 0.91 \times 10^{-3} \text{ h}^{-1}$ irradiated in air-dried soil, $k = 0.91 \times 10^{-3} \text{ h}^{-1}$ in dark control moist soil and $k = 0.23 \times 10^{-3} \text{ h}^{-1}$ in dark control air-dried sandy loam soil from Madia, CA. The initial metabolism rate $k = 3.70 \times 10^{-3} \text{ h}^{-1}$ 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, Rovon, 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 ($^{\circ}C$):

40–42 (Spencer 1982)

41 (Montgomery 1993; Milne 1995; Lide 2003)

Boiling Point ($^{\circ}C$):

Density (g/cm^3 at $20^{\circ}C$):

1.48 ($25^{\circ}C$, 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 $25^{\circ}C$ (assuming $\Delta S_{fus} = 56$ J/mol K), F: 0.697 (mp at $41^{\circ}C$)

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$ or as indicated):

44 (Günther et al. 1968; Melnikov 1971)

1.08 ($20^{\circ}C$, shake flask-GC, Chiou et al. 1977)

1.08 (20 – $25^{\circ}C$, shake flask-GC/ECD, Freed et al. 1979)

2.5 ($20^{\circ}C$, Spencer 1982)

0.60 ($20^{\circ}C$, shake flask-GC, Bowman & Sans 1979, 1983)

0.98 ($20^{\circ}C$, corrected supercooled liq. value, shake flask-GC, Bowman & Sans 1979,83)

6.0 (Dow Chemical unpublished data, Kenaga 1980a, b; Kenaga & Goring 1980)

40 ($22^{\circ}C$, Khan 1980)

1.0 ($20^{\circ}C$, shake flask-HPLC, Ellgehausen et al. 1981)

1.61 ($20^{\circ}C$, selected, Suntio et al. 1988)

40 (Montgomery 1993; Milne 1995)

Vapor Pressure (Pa at $25^{\circ}C$ or as indicated):

0.0533 ($20^{\circ}C$, Eichler 1965; Melnikov 1971)

0.0071 (20 – $25^{\circ}C$, Freed et al. 1979)

1.067 (Spencer 1982)

0.0017 ($20^{\circ}C$, GC-RT correlation without mp correlation, Kim et al. 1984; Kim 1985)

0.0011 ($20^{\circ}C$, GC-RT correlation with mp correction, Kim et al. 1984; Kim 1985)

0.016 ($20^{\circ}C$, selected, Suntio et al. 1988)

0.0045 ($20^{\circ}C$, Montgomery 1993)

Henry's Law Constant (Pa· m^3/mol at $25^{\circ}C$ or as indicated):

3.22 ($20^{\circ}C$, calculated-P/C, Suntio et al. 1988)

0.857 (20 – $25^{\circ}C$, 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 <i>Poecilia reticulata</i> , 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 $t_{1/2} \sim 3$ d at pH 6 (Montgomery 1993).

Biodegradation:

Biotransformation:

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

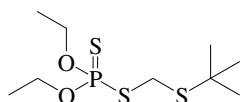
$k_1 = 0.01337 \text{ mL g}^{-1} \text{ d}^{-1}$ (guppy, 0.5–420 h exposure, De Bruijn & Hermens 1991)

$k_2 = 0.38 \text{ d}^{-1}$ (guppy, De Bruijn & Hermens 1991)

$k_2 = 0.14 \text{ d}^{-1}$ (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: C₉H₂₁O₂PS₃

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/cm³ at 20°C):

1.105 (24°C, Worthing & Hance 1991; Montgomery 1993; Tomlin 1994; Milne 1995)

Molar Volume (cm³/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/m³ 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·m³/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	(<i>Triaenodes tardus</i> , Belluck & Felsot 1981)

Sorption Partition Coefficient, log K_{OC} at 25°C or as indicated:

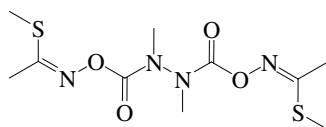
3.04	(soil, calculated-S per Kenaga & Goring 1978, Kenaga 1980)
2.76, 3.29	(quoted, calculated-MCI χ , Gerstl & Helling 1987)
2.70	(soil, 20–25°C, selected, Wauchope et al. 1992; Hornsby et al. 1996)
2.46–3.03	(Montgomery 1993)
2.82	(soil, calculated-MCI χ , Sabljic et al. 1995)
2.80, 3.30	(soil, estimated-class-specific 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 ($^{\circ}C$):

168–172 (Hartley & Kidd 1987; Montgomery 1993; Tomlin 1994)

173–174 (Tomlin 1994)

173 (Lide 2003)

Boiling Point ($^{\circ}C$):

Density (g/cm^3 at $20^{\circ}C$): 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 $25^{\circ}C$ (assuming $\Delta S_{fus} = 56\ J/mol\ K$), F : 0.0353 (mp at $173^{\circ}C$)

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$):

35 (Hartley & Kidd 1987; Montgomery 1993; Tomlin 1994)

19.1 (20 – $25^{\circ}C$, selected, Wauchope et al. 1992; Hornsby et al. 1996)

Vapor Pressure (Pa at $25^{\circ}C$):

0.0043 ($20^{\circ}C$, Hartley & Kidd 1987; Montgomery 1993)

1.33×10^{-5} (20 – $25^{\circ}C$, Wauchope et al. 1992; Hornsby et al. 1996)

0.0054 ($20^{\circ}C$, Tomlin 1994)

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

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, $t_{1/2}$:

Hydrolysis: $t_{1/2} \sim 9$ d at pH 3 (Montgomery 1993);

stable at pH 6, rapidly hydrolyzed at pH 9 and slowly at pH 3, $t_{1/2} \sim 9$ d (Tomlin 1994).

Half-Lives in the Environment:

Air:

Surface water: hydrolysis $t_{1/2} \sim 9$ d at pH 3 (Montgomery 1993);

stable at pH 6, rapidly hydrolyzed at pH 9 and slowly at pH 3, $t_{1/2} \sim 9$ d (Tomlin 1994).

Ground water:

Sediment:

Soil: $t_{1/2} = 3$ –8 d in various soils (Hartley & Kidd 1987)

field $t_{1/2} = 7$ 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/cm³ at 20°C):

1.65 (25°C, Spencer 1982; Montgomery 1993)

Molar Volume (cm³/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 $\Delta S_{\text{fus}} = 56$ J/mol K), F:

0.30 (Mackay et al. 1986)

Water Solubility (g/m³ 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)
 $\log [C/(\text{mol/m}^3)] = 0.77 - 1071/(T/K)$ (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)
 $\log(P/\text{Pa}) = 12.25 - 4487/(T/K)$ (Wania & Mackay 1993)
 5.3×10^{-4} (20–25°C, selected, Hornsby et al. 1996)
 $(2.3\text{--}7.10) \times 10^{-4}$ (supercooled P_L , capillary GC-RT correlation, for 21 toxaphene components-chlorinated bornane and camphene congeners, Bidleman et al. 2003)

Henry's Law Constant ($\text{Pa}\cdot\text{m}^3/\text{mol}$ 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)
 $\log[H/(\text{Pa}\cdot\text{m}^3/\text{mol})] = 11.48 - 3416/(T/K)$ (Wania & Mackay 1993)
 0.36* (technical toxaphene, gas stripping-GC, measured range 10–40°C, Jantunen & Bidleman 2000)
 $\log[H/(\text{Pa}\cdot\text{m}^3/\text{mol})] = 10.42 - 3209/(T/K)$; 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 prenioidosa*, 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)

$k = (8.0 \pm 2.2) \times 10^{-6} \text{ h}^{-1}$ at pH 7 with a calculated $t_{1/2} = 10$ yr (Ellington et al. 1987, 1988)

$k = 7.0 \times 10^{-2} \text{ yr}^{-1}$ 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_{NO_3} with NO_3 radical and k_{O_3} with O_3 or as indicated, *data at other temperatures see reference:

$t_{1/2} = 4\text{--}5$ d for the vapor-phase reaction with hydroxyl radicals (Howard 1991)

$k(aq.) = 8 \times 10^8 \text{ M}^{-1} \text{ s}^{-1}$ for the reaction (Fenton with reference to lindane) with hydroxyl radical in aqueous solutions at pH 1.9 ± 0.1 and at $24 \pm 1^\circ\text{C}$ (Buxton et al. 1988; quoted, Faust & Hoigné 1990; Haag & Yao 1992)

$k(aq.) < 1.3 \text{ M}^{-1} \text{ s}^{-1}$ 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).

$k(aq.) = (1.2\text{--}8.1) \times 10^8 \text{ M}^{-1} \text{ s}^{-1}$ for the reaction (Fenton with reference to lindane) with hydroxyl radical in aqueous solutions at pH 1.9 ± 0.1 and at $24 \pm 1^\circ\text{C}$ (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:

$k_2 = 0.016 \text{ d}^{-1}$ with $t_{1/2} = 43$ d and $k_2 = 0.022 \text{ d}^{-1}$ 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)

$k_2 = 0.007 \text{ d}^{-1}$ with $t_{1/2} = 95$ d and $k_2 = 0.016 \text{ d}^{-1}$ 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)

$k_2 = 0.008 \text{ d}^{-1}$ with $t_{1/2} = 83 \text{ d}$ and $k_2 = 0.017 \text{ d}^{-1}$ with $t_{1/2} = 42 \text{ d}$ for food concn of 17 ng/g and 134 ng/g, respectively, in a 30-d uptake followed by 160-d depuration studies for C₉-CHB toxaphene congener (juvenile rainbow trout, Fisk et al. 1998)

$k_2 = 0.068 \text{ yr}^{-1}$, 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)

$k_2 = 0.085 \text{ yr}^{-1}$, 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: $t_{1/2} = 4\text{--}5 \text{ d}$ for the vapor-phase reaction with hydroxyl radicals (GEMS 1986; quoted, Howard 1991).

Surface water: measured $k < 1.3 \text{ M}^{-1} \text{ s}^{-1}$ for direct reaction with ozone in water at pH 2 and 21°C, with $t_{1/2} > 7 \text{ h}$ at pH 7 (Yao & Haag 1991);

half-lives in lake water: $t_{1/2} = 18\text{--}31 \text{ yr}$ in Lake Superior, $t_{1/2} = 5\text{--}8 \text{ yr}$ in Lake Michigan, $t_{1/2} \sim 8.5 \text{ yr}$ in Lake Huron and $t_{1/2} \sim 6 \text{ yr}$ in Lake Ontario (Glassmeyer et al. 2000).

Ground water:

Sediment:

Soil: very persistent with reported half-life from $t_{1/2} = 0.8 \text{ yr}$ (Adams 1967; quoted, Howard 1991) to 14 yr (Nash & Woolson 1967; quoted, Howard 1991);

$t_{1/2} > 50 \text{ d}$ when subject to plant uptake via volatilization (Callahan et al. 1979; quoted, Ryan et al. 1988) measured dissipation rate $k = 0.010 \text{ d}^{-1}$ (Seiber et al. 1979; quoted, Nash 1988);

$t_{1/2} = 9 \text{ d}$ in screening model calculations (Jury et al. 1987b);

estimated dissipation rate $k = 0.0011$ and 0.013 d^{-1} (Nash 1988);

$t_{1/2} = 3650 \text{ d}$ for volatilization to atmosphere from chemical below soil surface (Jury et al. 1990);

field $t_{1/2} = 9 \text{ d}$ (20–25°C, selected, Hornsby et al. 1996)

$t_{1/2} = 0.8\text{--}14 \text{ yr}$ in soil, $t_{1/2} = 10\text{--}18 \text{ yr}$ in the environment (Geyer et al. 2000)

Biota: field $t_{1/2} = 15.6 \text{ d}$ in fruit tree leaves (Decker et al. 1950; quoted, Nash 1983);

microagroecosystem $t_{1/2} = 19 \text{ d}$ in cotton leaves (Nash & Harris 1977; quoted, Nash 1983);

field $t_{1/2}$ ca. 6.3 d in cotton canopy (Willis et al. 1980; quoted, Nash 1983);

$t_{1/2} = 524 \text{ d}$ for white suckers, and $t_{1/2} = 232$ to 322 d for lake trout (total toxaphene, Delorme et al. 1993);

average fish half-lives in the Great Lakes. $t_{1/2} = 9.1 \text{ yr}$ in Lake Michigan, $t_{1/2} = 7.7 \text{ yr}$ in Lake Huron and $t_{1/2} = 4.3 \text{ yr}$ in Lake Ontario (lake trout, Glassmeyer et al. 2000)

Depuration $t_{1/2} = 32\text{--}96 \text{ d}$ 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

$t/^\circ\text{C}$	$H/(\text{Pa m}^3/\text{mol})$
10	0.10
20	0.36
30	0.69
35	0.86
40	1.50
$\log H = A - B/(T/K)$	
	$H/(\text{Pa m}^3/\text{mol})$
A	10.42 ± 0.54
B	3209 ± 162

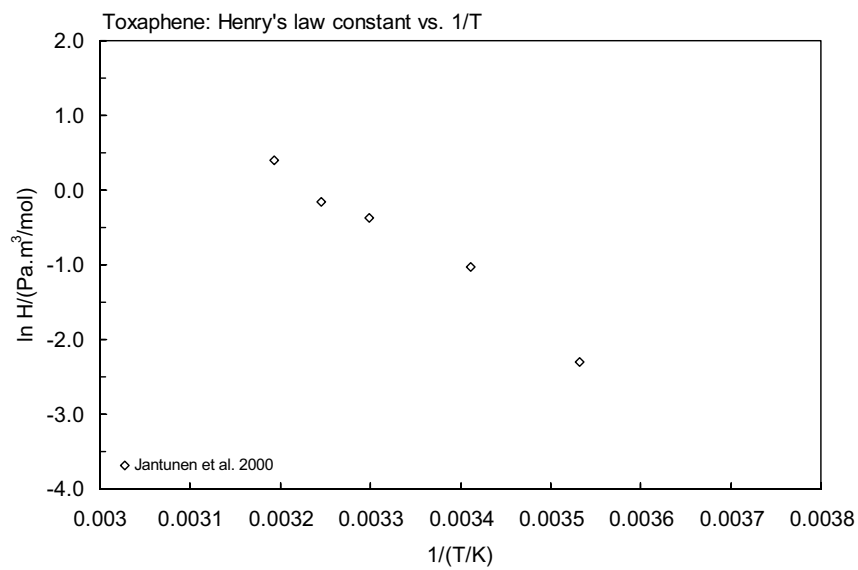
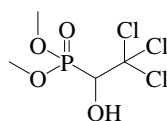


FIGURE 18.1.1.76.1 Logarithm of Henry's law constant versus reciprocal temperature for toxaphene.

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, Comboto, Danex, DEP, Dephton, 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, Trichlorophene, 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 ($^{\circ}C$):

77 (Lide 2003)

Boiling Point ($^{\circ}C$):

100 (at 0.1 mmHg, Spencer 1973; Montgomery 1993; Milne 1995)

Density (g/cm^3 at $20^{\circ}C$):

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 $25^{\circ}C$ (assuming $\Delta S_{fus} = 56 J/mol K$), F: 0.309 (mp at $77^{\circ}C$)

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$ or as indicated):

154000 (Spencer 1973, 1982; Martin & Worthing 1977; Worthing 1979)

> 5000 ($20^{\circ}C$, shake flask-GC, Bowman & Sans 1983a)

150000 (Davies & Lee 1987)

120000 ($20^{\circ}C$, Worthing & Hance 1991; Tomlin 1994)

120000 (20 – $25^{\circ}C$, 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 $25^{\circ}C$ or as indicated):

0.00095 ($20^{\circ}C$, vapor density, MacDougall 1964)

0.00104 ($20^{\circ}C$, Eichler 1965; Melnikov 1971; Spencer 1973; Hartley & Graham-Bryce 1980)

0.0640 ($20^{\circ}C$, GC-RT correlation without mp correction, Kim et al. 1984; Kim 1985)

0.0187 ($20^{\circ}C$, GC-RT correlation with mp correction, Kim et al. 1984; Kim 1985)

0.00021 ($20^{\circ}C$, Worthing & Hance 1991; Tomlin 1994)

0.00027 (20 – $25^{\circ}C$, selected, Wauchope et al. 1992; Hornsby et al. 1996)

0.00104 ($20^{\circ}C$, Montgomery 1993)

0.00051 (Tomlin 1994)

Henry's Law Constant ($Pa \cdot m^3/mol$ at $25^{\circ}C$ or as indicated):

1.7×10^{-6} ($20^{\circ}C$, 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: $k(\text{aerobic}) = 0.28 \text{ d}^{-1}$ 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 $k = 1.90 \times 10^{-4} \text{ min}^{-1}$ 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 $k = 1.90 \times 10^{-4} \text{ min}^{-1}$ 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 $k = 1.90 \times 10^{-5} \text{ min}^{-1}$ 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, Fat 25°C	pK _a
Acephate [30560-19-1]	Orthene	<i>O,S</i> -dimethyl acetylphosphoramidothioate	C ₄ H ₁₀ NO ₃ PS	183.166	88	0.241	
Aldicarb [116-06-3]	Temik	2-methyl-2-(methylthio)-propionaldehyde <i>O</i> -(methylcarbamoyl) oxime	C ₇ H ₁₄ N ₂ O ₂ S	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 ₈ Cl ₆	364.910	104	0.168	
Aminocarb [2032-59-9]	Matacil	4-dimethylamino- <i>m</i> -tolyl methylcarbamate	C ₁₁ H ₁₆ N ₂ O ₂	208.257	94	0.210	
Azinphos-methyl [86-50-0]	Guthion	<i>O,O</i> -dimethyl- <i>S</i> -[4-oxo-1,2,3-benzotriazin-3(4 <i>H</i>)-yl)methyl]phosphorodithioate	C ₁₀ H ₁₂ N ₃ O ₃ PS 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	<i>O</i> -4-bromo-2,5-dichlorophenyl- <i>O,O</i> -dimethyl phosphorothioate	C ₈ H ₈ BrCl ₂ PS	317.999	54	0.519	
Bromophos-ethyl [4824-78-6]	Nexagen, Filariol	<i>O</i> -(4-bromo-2,5-dichlorophenyl) <i>O,O</i> -diethyl phosphorothioate	C ₁₀ H ₁₂ Cl ₂ O ₃ PS	394.049			
Carbaryl [63-25-2]	Sevin	1-naphthyl- <i>N</i> -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	<i>S</i> -chlorophenylthio methyl <i>O,O</i> -diethyl phosphorothioate	C ₁₁ H ₁₆ ClO ₂ PS ₃	342.866	liquid	1	
Carbosulfan [55285-14-8]	Marshal, Advantage Posse, FMC 35001	2,3-dihydro-2,2-dimethylbenzofuran-7-yl(dibutylaminothio) methylcarbamate	C ₂₀ H ₃₂ N ₂ O ₃ S	380.544	liquid	1	
Chlordane [57-74-9]	Aspon-chlordane, Chlorindan, Octachlor	1,2,4,5,7,8,8-octachloro-3 <i>a</i> ,4,7,7 <i>a</i> -tetrahydro-4,7-methanoindane	C ₁₀ H ₆ Cl ₈	409.779	106	0.160	
	cis- or α-chlordane [5103-71-9]		C ₁₀ H ₆ Cl ₈	409.799	107–109	0.153	
	trans- or β-chlordane [5103-74-2]		C ₁₀ H ₆ Cl ₈	409.799	103–105	0.168	
	γ-chlordane [5564-34-7]		C ₁₀ H ₆ Cl ₈	409.799	131	0.0912	
	technical grade ^a [12789-03-6]						
Chlorfenvinphos [470-90-6]	Birlane, Sapecron	2-chloro-1-(2,4-dichlorophenyl) vinyl diethyl phosphate	C ₁₂ H ₁₄ Cl ₃ O ₄ P	359.569	B19	1	
Chlorpyrifos [2921-88-2]	Brodan, Dursban, Dowco 179	<i>O,O</i> -diethyl <i>O</i> -3,5,6-trichloro 2-pyridyl phosphorothioate	C ₉ H ₁₁ Cl ₃ NO ₃ PS	350.586	42	0.681	
Chlorpyrifos-methyl [5598-13-0]	Reldan, Dowco 214	<i>O,O</i> -dimethyl <i>O</i> -3,5,6-trichloro-2-pyridyl phosphorothioate	C ₇ H ₇ Cl ₃ NO ₃ PS	322.534	43	0.666	

Crotoxyphos [7700-17-6]	Ciodrin	dimethyl(<i>E</i>)-1-methyl-2-(1-phenyl-ethoxycarbonyl)vinyl phosphate	C ₁₄ H ₁₉ O ₆ P	314.271	liquid	1
Cyhalothrin [68085–85–8]	Cyhalothrin	(<i>RS</i>)- α -cyano-3-phenoxybenzyl(<i>Z</i>)-(1 <i>RS</i> ,3 <i>RS</i>)-2-chloro-3,3,3-trifluoropropanyl)-2,2-dimethylcyclopropanecarboxylate	C ₂₃ H ₁₉ ClF ₃ NO ₃	449.850		
lambda-Cyhalothrin [91465–08–6]			C ₂₃ H ₁₉ ClF ₃ NO ₃	449.850	49.2	0.579
Cypermethrin [52315-07-8]	Polytrin, Ambush C, Kakfil Super, BSI, draft E-ISO	(<i>RS</i>)- α -cyano-3-phenoxybenzyl (1 <i>RS</i> ,3 <i>RS</i> ; 1 <i>RS</i> ,3 <i>RS</i>)-3-(2,2-dichlorovinyl)-2,2=dimethylcyclopropanecarboxylate	C ₂₂ H ₁₉ Cl ₂ NO ₃	416.297	70	0.362
	α -cypermethrin [67375-30-8]		C ₂₂ H ₁₉ Cl ₂ NO ₃	416.297	78-81	0.292
	β -cypermethrin [65731–84–2]		C ₂₂ H ₁₉ Cl ₂ NO ₃	416.297	64–71	
	ζ -cypermethrin [52315–07–8]		C ₂₂ H ₁₉ Cl ₂ NO ₃	416.297	–22.4	1
DDD						
<i>p,p'</i> -DDD [72-54-8]	<i>p,p'</i> -TDE	1,1-Dichloro-2,2-bis (4-chlorophenyl)ethane	C ₁₄ H ₁₀ Cl ₄	320.041	109.5	0.148
<i>o,p'</i> -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						
<i>p,p'</i> -DDE [72-55-9]	<i>p,p'</i> -DDE	1,1-dichloro-2,2-bis-(<i>p</i> -chlorophenyl)-ethylene	C ₁₄ H ₈ Cl ₄	318.026	89	0.236
<i>o,p'</i> -DDE [3424-82-6]	<i>o,p'</i> -DDE	1,1-Dichloro-2(2-chlorophenyl)-2-(4-chlorophenyl)ethylene	C ₁₄ H ₈ Cl ₄	318.026	88-90	0.236
DDT	Agritan		C ₁₄ H ₉ Cl ₅	354.486	108.5	0.152
<i>p,p'</i> -DDT [50-29-3]		1,1,1-trichloro-2,2-bis-(4-chlorophenyl)-ethane				
<i>o,p'</i> -DDT [789-02-6]		1,1,1-trichloro-2-(chlorophenyl)-2-(4-chlorophenyl)-ethane	C ₁₄ H ₉ Cl ₅	354.486		
Deltamethrin [62918-63-5]	Decis, K-Othrine Butox, Butoflin	(<i>S</i>)- α -cyano-3-phenoxybenzyl(1 <i>R</i> ,3 <i>R</i>)-3-(2,2-dibromovinyl)-2,2-dimethylcyclo-propanecarboxylate	C ₂₂ H ₁₉ Br ₂ NO ₃	505.199	98-101	0.186
Demeton [8065-48-3]	Systox	<i>O,O</i> -diethyl <i>O</i> -2-ethylthioethyl phosphorothioate	C ₈ H ₁₉ O ₃ PS ₂	258.339	liquid	1
Demeton-S-methyl [919-86-8]	Metasystoxi	<i>S</i> -2-ethylthioethyl <i>O,O</i> -dimethyl phosphorothioate	C ₆ H ₁₅ O ₃ PS ₂	230.285	liquid	1
Dialifor [10311-84-9]	Torak	<i>S</i> -2-chloro-1-phthalimidoethyl <i>O,O</i> -diethylphosphorodithioate	C ₁₄ H ₁₇ ClNO ₄ PS ₂	393.846	68	0.379
Diamidaphos [1754-58-1]	Nellite	phenyl <i>N,N'</i> -dimethylphosphoro-diamidate	C ₈ H ₁₃ N ₂ O ₂ P	200.175	103.5	0.170
Diazinon [333-41-5]	Basudin, Diazide, Spectracide	<i>O,O</i> -diethyl <i>O</i> -2-isopropyl-6-methyl-pyrimidin-4-yl phosphorothioate	C ₁₂ H ₂₁ N ₂ O ₃ PS	304.345	liquid	1
Dicapthon [2463-84-5]	Dicaptan	<i>O</i> -(2-chloro-4-nitrophenyl)- <i>O,O</i> -dimethyl phosphorothioate	C ₈ H ₉ ClNO ₅ PS	297.653	53	0.531
Dichlofenthion [97-17-6]	Mobilawn	<i>O</i> -2,4-dichlorophenyl <i>O,O</i> =diethyl phosphorothioate	C ₁₀ H ₁₃ Cl ₂ O ₃ PS	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, Fat 25°C	pK _a
Dichlorvos [62-73-7]	Vapona, Nuvan, DDVP, Dede vap	2,2-dichlorovinyl- <i>O,O</i> -dimethyl phosphate	C ₄ H ₇ Cl ₂ O ₄ P	220.976	liquid	1	
Dicrotophos [141-66-2]	Carbicon, Ektafos, Bidrin	(<i>E</i>)-2-dimethylcarbamoyl-1-methylvinyl dimethyl phosphate	C ₈ H ₁₆ NO ₅ P	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- <i>exo</i> -1,4- <i>endo</i> -5,8-dimethanonaphthalene	C ₁₂ H ₈ Cl ₆ O	380.909	175.5	0.0334	
Diflubenzuron [35367-38-5]	Deflubenzon, Dimilin	1-(4-chlorophenyl)-3-(2,6-difluoro-benzol) urea	C ₁₄ H ₉ ClF ₂ N ₂ O ₂	310.683	239	0.00795	
Dimethoate [60-51-5]	Cygon	<i>O,O</i> -dimethyl- <i>S</i> -(<i>N</i> -methyl-carbamoyl-methyl phosphorodithioate	C ₅ H ₁₂ NO ₃ PS ₂	229.258	52	0.543	
Dinoseb [88-85-7]	Antox, Aretit, BNP 30, DNBP	2- <i>sec</i> -butyl-4,6-dinitrophenol	C ₁₀ H ₁₂ N ₂ O ₅	240.212	40	0.713	
Disulfoton [298-04-4]	Di-Syston, Dithiosystox	<i>O,O</i> -diethyl- <i>S</i> -(ethylthio)-ethyl phosphorodithioate	C ₈ H ₁₉ O ₂ PS ₃	274.405	-25	1	
Endosulfan [115-29-7]	Thiodan, Cyclo dan, Malix, Thifor	5-norbornene-2,3-dimethanol-1,4,5,6,7,7-hexachlorocyclic sulfite	C ₉ H ₆ Cl ₆ O ₃ S	406.925	106	0.160	
	α-Endosulfan [959-98-8]		C ₉ H ₆ Cl ₆ O ₃ S	406.925	106	0.160	
	β-Endosulfan [33213-65-9]		C ₉ H ₆ Cl ₆ O ₃ S	406.925	207-209	0.0160	
Endosulfan sulfate [1031-07-8]			C ₉ H ₆ Cl ₆ O ₄ S	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- <i>exo</i> -1,4- <i>exo</i> -5,8-dimethanonaphthalene	C ₁₂ H ₈ Cl ₆ O	380.909	dec 245	0.00694	
Ethiofencarb [29973-13-5]	Croneton, Bay-Hox-1901	α-ethylthio- <i>o</i> -tolyl methylcarbamate	C ₁₁ H ₁₅ NO ₂ S	225.307	33.4	0.827	
Ethion [563-12-2]	Nialate, diethion	<i>O,O,O',O'</i> -tetraethyl- <i>S,S'</i> -methylene bis(phosphorodithioate)	C ₉ H ₂₂ O ₄ P ₂ S ₄	384.476	-13	1	
Ethoprophos [13194-48-4]	Mocap, ethoprop	<i>O</i> -ethyl- <i>S,S</i> -dipropyl-phosphorodithioate	C ₈ H ₁₉ O ₂ PS ₂	242.340	liquid	1	
Fenitrothion [122-14-5]	Sumithion, Folithion Cyfen	<i>O,O</i> -dimethyl <i>O</i> -4-nitro- <i>m</i> -tolyl phosphorothioate	C ₉ H ₁₂ NO ₅ PS	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	(<i>R,S</i>)- <i>O</i> -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	<i>O,O</i> -diethyl <i>O</i> -4-methylsulphinylphenyl phosphorothioate	C ₁₁ H ₁₇ O ₄ PS ₂	308.354			

Fenthion [55-38-9]	Baytex, Baycid, Mercaptophos,	<i>O,O</i> -dimethyl- <i>O</i> -(3-methyl-4-(methylthio)phenyl) phosphorothioate	C ₁₀ H ₁₅ O ₃ PS ₂	278.328	liquid	1
Fenvalerate [51630-58-1]	Sumicidin, Belmark, Pydrin	(<i>RS</i>)- α -cyano-3-phenoxybenzyl (<i>RS</i>)-2-(4-chlorophenyl)-3-methylbutyrate	C ₂₅ H ₂₂ ClNO ₂	419.901	liquid	1
Flucythrinate [70124-77-5]	Cybolt, Cythrin, Pay-Off	(<i>RS</i>)- α -cyano-3-phenoxybenzyl (<i>S</i>)-2-(4-difluoromethoxyphenyl)-3-methylbutyrate	C ₂₆ H ₂₃ F ₂ NO ₄	451.463	liquid	1
Fonofos [944-22-9]	Dyfonate, Fonophos	<i>O</i> -ethyl- <i>S</i> -phenyl (<i>RS</i>)-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- <i>endo</i> -methanoindene	C ₁₀ H ₅ Cl 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 ₅ Cl ₇ O	389.317	160	0.0474
Hexachlorocyclohexane	BHC, HCH	1,2,3,4,5,6-Hexachlorocyclohexane	C ₆ H ₆ Cl 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 ₆ H ₆ Cl ₆	290.830	112.5	0.139
δ -HCH'[319-86-8]	Δ -BHC	1,2,3,4,5,6-hexachlorocyclohexane	C ₆ H ₆ Cl ₆	290.830	141.5	0.0719
Iodofenphos [25311-71-1]	Nuvanol N	<i>O</i> -2,5-dichloro-4-iodophenyl <i>O,O</i> -dimethyl phosphorothioate	C ₈ H ₈ Cl ₂ IO ₃ PS	345.395	oil	1
Isophorone [78-59-1]	Isooctaphenone	3,5,5-trimethyl-2-cyclohexene-1-one	C ₉ H ₁₄ O	138.206	-8.1	1
Kepone [143-50-0]	Chlordecone	decachlorooctahydro-1,3,4-metheno-2 <i>H</i> -cyclobuta[<i>cd</i>]pentalen-2-one	C ₁₀ H ₁₀ O	490.636	350 dec	0.00065
Leptophos [21609-90-5]	Phosvel	<i>O</i> -(4-bromo-2,5-dichlorophenyl) <i>O</i> -methyl phenylphosphorothioate	C ₁₃ H ₁₀ BrCl ₂ O ₂ P S	412.066	71	0.345
Lindane [58-89-9]	γ -BHC, γ -HCH	1,2,3,4,5,6-hexachlorocyclohexane	C ₆ H ₆ Cl ₆	290.830	112.5	0.139
Malathion [121-75-5]	Karbofos, Cythion, mercaptothion	<i>S</i> -[1,2-bis(ethoxycarbenyl)ethyl]- <i>O,O</i> -dimethyl phosphorodithioate	C ₁₀ H ₁₉ O ₆ PS	330.358	1.4	1
Mecarbam [2595-54-2]	Afos	<i>S</i> -(<i>N</i> -ethyoxycarbonyl- <i>N</i> -methyl-carbamoylmethyl) <i>O,O</i> -diethyl	C ₁₀ H ₂₀ NO ₃ PS ₂	329.374	oil	1
Methamidophos [10265-92-6]	Monitor, Tamaron	<i>O,S</i> -dimethylphosphoramidothioate	C ₂ H ₈ NO ₂ PS	141.130	46	0.622
Methiocarb [2032-65-7]	Mesuroil, Draza	4-methylthio-3,5-xylyl methylcarbamate	C ₁₁ H ₁₅ NO ₂ S	225.308	120	0.117
Methomyl [16752-77-5]	Lannate	<i>S</i> -methyl- <i>N</i> -(methylcarbamoyl-oxy)-thioaceticimide	C ₅ H ₁₀ N ₂ O ₂ S	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 ₃ O ₂	345.648	87	0.246
Mevinphos [7786-34-7]	Apavinfos, Duraphos	2-carbomethoxy-1-methylvinyl dimethyl phosphate	C ₇ H ₁₃ O ₆ P	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 <i>H</i> -cyclobuta(<i>cd</i>)pentalene	C ₁₀ Cl ₁₂	545.543	485 dec	0.000031
Monocrotophos [6923-22-4]	Nuvacron, Azodrin	dimethyl (<i>E</i>)-1-methyl-2-(methyl-carbamoyl)vinyl phosphate	C ₇ H ₁₄ NO ₅ P	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, Fat 25°C	pK _a
Naled [300-76-5]	Arthodibrom, Dibrom, Bromex, Bromchlophos	1,2-dibromo-2,2-dichloroethyl dimethyl phosphate	C ₄ H ₇ Br ₂ Cl ₂ O ₄ P	380.784	27	0.956	
Oxamyl [23135-22-0]	Vydate	<i>N,N'</i> -dimethyl-2-methylcarbamoyloxyimino-2-(methylthio)acetamine	C ₇ H ₁₃ N ₃ O ₃ S	219.261	109	0.150	
Parathion [56-38-2]	Folidol, Bladan, Niran	<i>O,O</i> -diethyl <i>O</i> -4-nitrophenyl phosphorothioate	C ₁₀ H ₁₄ NO ₅ PS	291.261	6.1	1	
Parathion-methyl [298-00-0]	Dalf, Nitrox	<i>O,O</i> -dimethyl <i>O</i> -(<i>p</i> -nitrophenyl) phosphorothioate	C ₈ H ₁₀ NO ₅ PS	263.208	38	0.746	
Pentachlorophenol [87-86-5]	PCP	pentachlorophenol	C ₆ H ₅ OH	266.336	174	0.0345	4.74
Pentachlorophenol sodium salt (Pentacon)							
Permethrin [52645-53-1]	Ambush, Kafil, Picket, Pramex	3-phenoxybenzyl(1 <i>RS</i> ,3 <i>RS</i> ;1 <i>RS</i> ,3 <i>RS</i>)-3(2,2-dichlorovinyl)-2,2=dimethylcyclo-prapanecarboxylate	C ₂₁ H ₂₀ Cl ₂ O ₃	391.288	34	0.816	
<i>cis</i> -Permethrin					63-65	0.414	
<i>trans</i> -Permethrin					44-47	0.629	
technical grade							
Phenthoate [2597-03-7]	Cidial, Elsan	ethyl 2-dimethoxythiophosphorythio-2-phenylacetate	C ₁₂ H ₁₇ O ₄ PS ₂	320.364	17-18	1	
Phorate [298-02-2]	Forsaath, Gramitox	<i>O,O</i> -diethyl- <i>S</i> -(ethylthio)methyl phosphordithioate	C ₇ H ₁₇ O ₂ PS ₃	260.378	<-15	1	
Phorate-sulfone				292.3			
Phorate-sulfoxide				276.4			
Phosmet [732-11-6]	Imidan	<i>S</i> -[(1,3-dihydro-1,3-dioxo-2 <i>H</i> -isoindol-2-yl)methyl]	C ₁₁ H ₁₂ NO ₄ PS ₂	317.321	72	0.346	
Phosphamidon [13171-21-6]	Dimecron	2-chloro-2-diethylcarbamoyl-1-methylvinyl dimethyl phosphate	C ₁₀ H ₁₉ ClNO ₅ P	299.689	-45	1	
Pirimicarb [23103-98-2]	Pirimor, Aphox	2-dimethylamino-5,6-dimethyl-pyrimidin-4-yl dimethylcarbamate	C ₁₁ H ₁₈ N ₄ O ₂	238.287	90.5	0.228	
Profenofos [41198-08-7]	Selecron	<i>O</i> -4-bromo-2-chlorophenyl <i>O</i> -ethyl <i>S</i> -propyl phosphorothioate	C ₁₁ H ₁₅ BrClO ₃ PS	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	<i>O,O</i> -dimethyl <i>O</i> -2,4,5-trichlorophenyl-phosphorothioate	C ₈ H ₈ Cl ₃ O ₃ PS	321.546	41	0.697	
Sulfotep [3689-24-5]	dithio, thiotep, ENT, Bladafum	<i>O,O,O',O'</i> -tetraethyl dithiopyrophosphate	C ₈ H ₂₀ O ₅ P ₂ S ₂	322.320	liquid	1	
Terbacil [5902-51-2]	Sinbar, Turbacil	5-chloro-3-(1,1-dimethyl)-6-methyl-2,4-(1 <i>H</i> ,3 <i>H</i>)-pyrimidine-dione	C ₉ H ₁₃ Cl ₂ N ₂ O ₃	216.664	176	0.0330	9.0

Terbufos [13071-79-9]	Contraven, Counter	<i>S-tert</i> -butylthiomethyl <i>O,O</i> -diethyl phosphorodithioate	C ₉ H ₂₁ O ₂ PS 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 <i>RS</i> ,3 <i>RS</i> ;1 <i>RS</i> ,3 <i>SR</i>)-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	<i>S</i> -(4-chlorophenyl)methyl diethyl-carbamothioate	C ₁₂ H ₁₆ ClNOS	257.779	1.7	1
Thiodicarb [59669-26-0]	Cicarbosulf, Larvin, Lepicron	dimethyl <i>N,N'</i> -thiobis(methylimino)-carbonyloxy bisethanimidothioate	C ₁₀ H ₁₈ N ₄ O ₄ S 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 ₄ H ₈ Cl ₃ O ₄ P	257.437	77	0.309
Zinophos [297-92-2]	Thionazin, Namafos Cynem	<i>O,O</i> -diethyl- <i>O</i> -pyrazin-2-yl phosphorothioate	C ₈ H ₁₃ N ₂ O ₃ PS	248.239	–1.69	1

TABLE 18.2.2
Summary of selected physical-chemical properties of insecticides at 25°C

Compound	Selected properties						Henry's law constant H/(Pa·m³/mol) calcd P/C	log K _{OC} reported
	Vapor pressure		Solubility			log K _{OW}		
	P ^s /Pa	P _L /Pa	S/(g/m³)	C ^s /(mol/m³)	C _L /(mol/m³)			
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								
<i>cis</i> - 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
<i>trans</i> - 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								
<i>p,p'</i> -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
<i>o,p'</i> -DDD	2.0 × 10 ⁻⁴ *	1.39 × 10 ⁻³	0.10*			6.0		
DDE								
<i>p,p'</i> -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
<i>o,p'</i> -DDE	8.0 × 10 ⁻⁴	3.44 × 10 ⁻³	0.1	3.14 × 10 ⁻⁴	1.35 × 10 ⁻³	5.8	2.54	
DDT								
<i>p,p'</i> -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
<i>o,p'</i> -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	$1.20 \times 10^{-6*}$	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)

Compound	Selected properties						Henry's law constant H/(Pa·m³/mol) calcd P/C	log K _{oc} reported
	Vapor pressure		Solubility			log K _{ow}		
	P ^S /Pa	P _L /Pa	S/(g/m³)	C ^S /(mol/m³)	C _L /(mol/m³)			
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
<i>p,p'</i> -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

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