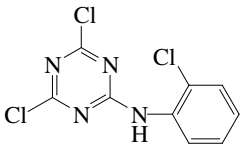
19 Fungicides

CONTENTS

19.1 List of Chemicals and Data Compilations (by Functional Group)

19.1 LIST OF CHEMICALS AND DATA COMPILATIONS

19.1.1 ANILAZINE



Common Name: Anilazine
Synonym: Botrysan, Direz, Dyrene, Kemate, Triasyn, triazine, Zinochlor
Chemical Name: 2-chloro-*N*-(4,6-dichloro-1,3,5-triazin-2-yl)aniline; 2,4-dichloro-6-(*o*-chloro-anilino)-*s*-triazine; 4,6-dichloro-*N*-(2-chlorophenyl)-1,3,5-triazin-2-amine
Uses: as fungicide to control early and late blights of potatoes and tomatoes; anthracnose in cucurbits; leaf spot diseases in many crops; glume blotch of wheat; also used on vegetables, ornaments, berry fruits, melons, coffee and tobacco, etc.
CAS Registry No: 101-05-3
Molecular Formula: $C_9H_5Cl_3N_4$
Molecular Weight: 275.522
Melting Point (°C):
160 (Lide 2003)
Boiling Point (°C):
Density (g/cm^3 at 20°C): 1.80 (Hartley & Kidd 1987; Tomlin 1994)
Molar Volume (cm^3/mol):
252.8 (calculated-Le Bas method at normal boiling point)
153.1 (calculated-density)
Dissociation Constant pK_a:
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
Entropy of Fusion, ΔS_{fus} (J/mol K):
Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F: 0.0474 (mp at 160°C)

Water Solubility (g/m^3 or mg/L at 25°C or as indicated):
8.00 (20°C, Hartley & Kidd 1987; Worthing & Hance 1991; Tomlin 1994; Milne 1995)
8.00 (20–25°C, selected, Wauchope et al. 1992; Hornsby et al. 1996)
8.00 (selected, Lohninger 1994)

Vapor Pressure (Pa at 25°C or as indicated):
negligible (20°C, Hartley & Kidd 1987)
8.20×10^{-7} (20°C, Worthing & Hance 1991; Tomlin 1994)
8.26×10^{-7} (20–25°C, selected, Wauchope et al. 1992; Hornsby et al. 1996)

Henry's Law Constant (Pa·m^3/mol at 25°C or as indicated):
2.82×10^{-5} (20°C, calculated-P/C, this work)

Octanol/Water Partition Coefficient, log K_{OW}:
4.39 (calculated, Chiou 1981)
3.79 (calculated-CLOGP program, Biagi et al. 1991)
3.01 (20°C, Worthing & Hance 1991; Tomlin 1994)
3.88 (RP-HPLC-RT correlation, Saito et al. 1993)
1.91 (at pH 7, Milne 1995)
3.00 (selected, Hansch et al. 1995)

Bioconcentration Factor, log BCF:
2.28 (calculated-S as per Kenaga 1980, this work)

Sorption Partition Coefficient, log K_{OC}:

3.00 (20–25°C, estimated, Wauchope et al. 1992; Hornsby et al. 1996)
3.00 (estimated-chemical structure, Lohninger 1994)
3.14 (calculated-S as per Kenaga 1980, this work)
3.00, 2.53, 3.30 (soil, quoted obs.; estimated-class-specific model, estimated-general model using molecular descriptors, Gramatica et al. 2000)

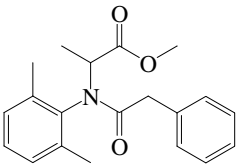
Environmental Fate Rate Constants, k, or Half-Lives, $t_{½}$:

Hydrolysis: stable in neutral and slightly acidic media, $t_{½}$ = 730 h at pH 4, $t_{½}$ = 790 h at pH 7, $t_{½}$ = 22 h at pH 9, 22°C (Tomlin 1994).

Half-Lives in the Environment:

Air:
Surface water:
Groundwater:
Sediment:
Soil: $t_{½}$ ~ 12 h in damp soil (Hartley & Kidd 1987; Tomlin 1994);
field $t_{½}$ = 1 d (20–25°C, selected, Wauchope et al. 1992; Hornsby et al. 1996).
Biota:

19.1.2 BENALAXYL



Common Name: Benalaxyl
Synonym: Galben, M 9834, Tairel
Chemical Name: methyl *N*-phenylacetyl-*N*-2,6-xylyl-*DL*-alaninate; methyl *N*-(2,6-dimethylphenyl)-*N*-(phenylacetyl)-*DL*-alaninate
CAS Registry No: 71626-11-4
Uses: as fungicide to control late blights of potatoes and tomatoes; downy mildews of hops, vines, lettuce, onions, soybeans and other crops; many diseases in flowers and ornamentals; and often used in combination with other fungicides, etc.
Molecular Formula: $C_{20}H_{23}NO_3$
Molecular Weight: 325.402
Melting Point (°C):
79 (Lide 2003)
Boiling Point (°C):
Density (g/cm^3 at 20°C):
1.27 (25°C, Hartley & Kidd 1987; Milne 1995)
Molar Volume (cm^3/mol):
390.8 (calculated-Le Bas method at normal boiling point)
256.2 (calculated-density)
Dissociation Constant pK_a:
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
Entropy of Fusion, ΔS_{fus} (J/mol K):
Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F: 0.295 (mp at 79°C)

Water Solubility (g/m^3 or mg/L at 25°C):
37.0 (Hartley & Kidd 1987; Worthing & Hance 1991; Tomlin 1994; Milne 1995)
37.0 (20–25°C, Augustijn-Beckers et al. 1994; Hornsby et al. 1996)

Vapor Pressure (Pa at 25°C or as indicated):
6.7×10^{-4} (Hartley & Kidd 1987; Worthing & Hance 1991; Tomlin 1994)
1.33×10^{-3} (20–25°C, Augustijn-Beckers et al. 1994; Hornsby et al. 1996)

Henry's Law Constant (Pa·m^3/mol):
0.0117 (calculated-P/C, this work)

Octanol/Water Partition Coefficient, log K_{OW}:
3.40 (Worthing & Hance 1991; Milne 1995)
3.40 (Tomlin 1994)
3.40 (selected, Hansch et al. 1995)
3.24 (RP-HPLC-RT correlation using short ODP column, Donovan & Pescatore 2002)

Bioconcentration Factor, log BCF:
1.91 (calculated-S as per Kenaga 1980, this work)

Sorption Partition Coefficient, log K_{OC}:
3.44–3.86 (soil, Tomlin 1994)
3.00 (soil, estimated, Augustin-Beckers et al. 1994; Hornsby et al. 1996)

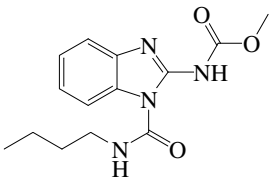
Environmental Fate Rate Constants, k, or Half-Lives, $t_{½}$:

Hydrolysis: $t_{½}$ = 86 d at pH 9, 25°C, but stable in aqueous solutions at pH 4–9 (Tomlin 1994).

Half-Lives in the Environment:

Air:
Surface water:
Groundwater:
Sediment:
Soil: $t_{½}$ = 20–71 d in soil (Tomlin 1994);
field $t_{½}$ = 30 d (Augustijn-Beckers et al. 1994; Hornsby et al. 1996).
Biota:

19.1.3 Benomyl



Common Name: Benomyl
Synonym: Arilate, BBC, Benex, Benlate, Benosan, Fibenzo, Fundazol
Chemical Name: methyl *N*-(1-butylcarbamoyl-2-benzimidazole)carbamate; methyl 1-(butyl-carbamoyl)benzimidazol-2-ylcarbamate; methyl 1-[(butylamino)carbonyl]-1*H*-benz-imidazol-2-ylcarbamate
Uses: as fungicide to control a wide range of diseases of fruit, nuts, vegetables, mushrooms, field crops, ornamentals, turf and trees; also provides secondary acaricidal control, principally as an ovicide, etc.
CAS Registry No: 17804-35-2
Molecular Formula: $C_{14}H_{18}N_4O_3$
Molecular Weight: 290.318
Melting Point (°C):
140 (dec., Tomlin 1994)
dec (Lide 2003)
Boiling Point (°C):
Density (g/cm^3 at 20°C):
Molar Volume (cm^3/mol):
320.0 (calculated-Le Bas method at normal boiling point)
Dissociation Constant pK_a:
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
Entropy of Fusion, ΔS_{fus} (J/mol K):
Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F: 0.0744 (mp at 140°C)

Water Solubility (g/m^3 or mg/L at 25°C or as indicated):
3.8 (Austin et al. 1976; quoted, Kenaga 1980; Howard 1991)
18.2, 4.0, 3.6, 2.8, 3.0, 1.9, 1.8, 8.8, 4.5 (pH 1, 3, 5,7, 8, 9, 10, 11, 12, room temperature, shake flask-HPLC/UV, Singh & Chiba 1985)
2.8 (shake flask-HPLC/UV at pH 7, Singh & Chiba 1985; quoted, Howard 1991)
2.0 (Hartley & Kidd 1987; Milne 1995)
4.0 (pH 3–10, Worthing & Hance 1991)
2.0 (20–25°C, selected, Wauchope et al. 1992; Hornsby et al. 1996)
2.0 (stable only at pH 7, Montgomery 1993)
4.0 (selected, Lohninger 1994)
4.0 (pH 3–10, very soluble at pH 1, decomposes at pH 13, Tomlin 1994)

Vapor Pressure (Pa at 25°C or as indicated):
$< 1.00 \times 10^{-5}$ (20°C, Hartley & Kidd 1987)
$< 1.33 \times 10^{-8}$ (20–25°C, selected, Wauchope et al. 1992; Hornsby et al. 1996)
$< 4.90 \times 10^{-6}$ (Tomlin 1994)

Henry's Law Constant (Pa·m^3/mol at 25°C):
$< 1.93 \times 10^{-6}$ (calculated-P/C)

Octanol/Water Partition Coefficient, log K_{OW}:
2.12 (20°C, shake flask-UV, Austin & Briggs 1976)
2.42 (Rao & Davidson 1982; Hansch & Leo 1985; 1987)
3.11 (Garten & Trabalka 1983; Travis & Arms 1988)
2.12 (Hansch & Leo 1985)

2.42 (Sangster 1993)
1.40–3.11 (Montgomery 1993)
2.12 (recommended, Hansch et al. 1995)
1.33 (RP-HPLC-RT correlation using short ODP column, Donovan & Pescatore 2002)

Bioconcentration Factor, log BCF:

2.46 (estimated-S, Kenaga 1980; quoted, Howard 1991)
–0.47 (vegetation, Popov & Sboeva 1974; Jalali & Anderson 1976)

Sorption Partition Coefficient, log K_{OC}:

3.32 (estimated-S, Kenaga 1980; quoted, Howard 1991)
3.28 (soil, 20–25°C, selected, Wauchope et al. 1992; Hornsby et al. 1996)
3.28 (soil, calculated, Montgomery 1993)
3.28 (selected, Lohninger 1994)
3.28 (soil, Tomlin 1994)
2.71 (soil, calculated-MCI $^1\chi$, Sabljic et al. 1995)
2.73, 1.92 (soil, estimated-class-specific model, estimated-general model using molecular descriptors, Gramatica et al. 2000)

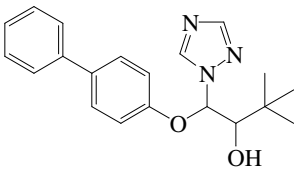
Environmental Fate Rate Constants, k, or Half-Lives, $t_{½}$:

Volatilization:
Photolysis:
Oxidation: photooxidation $t_{½}$ = 1.6 h in air, based on estimated rate constant for the vapor-phase reaction with hydroxyl radicals in air (Atkinson 1987; quoted, Howard 1991).
Hydrolysis: very significant in water with $t_{½}$ < 1 wk (Howard 1991).
Biodegradation:
Biotransformation:
Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants:

Half-Lives in the Environment:

Air: estimated $t_{½}$ ~ 1.6 h, based on the vapor-phase reaction with hydroxyl radicals in air (Atkinson 1987; quoted, Howard 1991).
Surface water: $t_{½}$ = 2 h (Tomlin 1994).
Groundwater:
Sediment:
Soil: degradation occurred within 15 d in unsterilized soil (Hine et al. 1969);
$t_{½}$ = 6–12 months (Hartley & Kidd 1987);
field $t_{½}$ = 67 d (20–25°C, selected, Wauchope et al. 1992; Hornsby et al. 1996);
$t_{½}$ = 19 h in soil (Tomlin 1994).
Biota: $t_{½}$ = 3–7 d on foliage (quoted, Montgomery 1993).

19.1.4 BITERTANOL



Common Name: Bitertanol
Synonym: Baycor, Baymat, Biloxazol, Sibutol
Chemical Name: 1-(biphenyl-4-yloxy)-3,3-dimethyl-1-(1*H*-1,2,4-triazol-1-yl)butan-2-ol; β-([1,1′-biphenyl]-4-yloxy)-α-(1,1-dimethylethyl)-1*H*-1,2,4-triazole-1-ethanol
Uses: as fungicide to control scab on apples and pears; rusts and powdery mildews on ornamentals; black spot on roses; and leaf spot and other diseases of vegetables, cucurbits, cereals, deciduous fruit, bananas, groundnuts, soy beans, etc.
CAS Registry No: 70585-38-5 (diastereoisomer A), 55179-31-2 (diastereoisomer B)
Molecular Formula: $C_{20}H_{23}N_3O_2$
Molecular Weight: 337.415
Melting Point (°C):

139.8	(diastereoisomer A, Hartley & Kidd 1987)
146.3	(diastereoisomer B, Hartley & Kidd 1987)
118.0	(eutectic mixture of the two diastereoisomers, Hartley & Kidd 1987; Worthing & Hance 1991)
136.7	(diastereoisomer A, Worthing & Hance 1991; Tomlin 1994)
145.2	(diastereoisomer B, Worthing & Hance 1991; Tomlin 1994)

Boiling Point (°C):
Density (g/cm^3 at 20°C):
Molar Volume (cm^3/mol):

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

Dissociation Constant pK_a:
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
Entropy of Fusion, ΔS_{fus} (J/mol K):
Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F: 0.122 (eutectic mixture, mp at 118° C)

Water Solubility (g/m^3 or mg/L at 25°C or as indicated):

5.0	(20°C, eutectic mixture; Hartley & Kidd 1987; Worthing & Hance 1991)
2.9	(20°C, diastereoisomer A, Worthing & Hance 1991; Tomlin 1994)
1.6	(20°C, diastereoisomer B, Worthing & Hance 1991; Tomlin 1994)

Vapor Pressure (Pa at 25°C or as indicated):

1.0×10^{-6}	(20°C, Hartley & Kidd 1987)
0.0038	(100°C, diastereoisomer A, Worthing & Hance 1991)
0.0032	(100°C, diastereoisomer B, Worthing & Hance 1991)
2.2×10^{-10}	(20°C, diastereoisomer A, Tomlin 1994)
2.5×10^{-10}	(20°C, diastereoisomer B, Tomlin 1994)

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

8.45×10^{-5}	(20°C, eutectic mixture, calculated-P/C, this work)

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

4.10	(20°C, diastereoisomer A, Worthing & Hance 1991; Tomlin 1994)
4.40	(20°C, diastereoisomer B, Worthing & Hance 1991; Tomlin 1994)
4.16	(Schreiber & Schönherr 1992)
4.16	(selected, Hansch et al. 1995)

Bioconcentration Factor, log BCF:

2.40 (20°C, eutectic mixture, calculated-S as per Kenaga 1980, this work)

Sorption Partition Coefficient, log K_{OC}:

2.25 (20°C, eutectic mixture, calculated-S as per Kenaga 1980, this work)

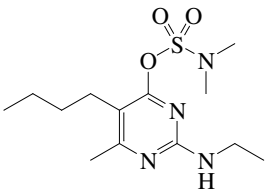
Environmental Fate Rate Constants, k, or Half-Lives, $t_{½}$:

Volatilization:
Photolysis:
Oxidation:
Hydrolysis: stable in neutral, acidic and alkaline media, hydrolytic $t_{½}$ > 1 yr at 25°C and pH 4, 7 and 9 (Tomlin 1994).
Biodegradation: degradation in soil is rapid (Tomlin 1994).
Biotransformation:
Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants:

Half-Lives in the Environment:

Surface water: environmental $t_{½}$ = 1 month to 1 yr (Tomlin 1994).

19.1.5 BUPIRIMATE



Common Name: Bupirimate
Synonym: Nimrod, PP 588
Chemical Name: 5-butyl-2-ethylamino-6-methylpyrimidin-4-yl dimethylsulfamate; 5-butyl-2-(ethylamino)-6-methyl-4-pyrimidinyl dimethylsulfamate
Uses: as fungicide to control powdery mildews of apples and pears, stone fruit, strawberries, gooseberries, vines, roses and other ornamentals, cucurbits, hops, beet, and other crops, etc.
CAS Registry No: 41483-43-6
Molecular Formula: $C_{13}H_{24}N_4O_3S$
Molecular Weight: 316.419

Melting Point (°C):
50–51 (Hartley & Kidd 1987; Worthing & Hance 1991; Tomlin 1994)
Boiling Point (°C):
Density (g/cm^3 at 20°C):

Molar Volume (cm^3/mol):
368.9 (calculated-Le Bas method at normal boiling point, this work)
Dissociation Constant pK_a:
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
Entropy of Fusion, ΔS_{fus} (J/mol K):
Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F:

Water Solubility (g/m^3 or mg/L at 25°C):
22.0 (Martin & Worthing 1977)
22.0 (Hartley & Kidd 1987; Worthing & Hance 1991; Tomlin 1994)
23.0 (at pH 5.2, Worthing & Hance 1991)

Vapor Pressure (Pa at 25°C or as indicated):
6.7×10^{-5} (20°C, Hartley & Kidd 1987; Worthing & Hance 1991)
1.0×10^{-4} (Tomlin 1994)

Henry's Law Constant (Pa·m^3/mol at 25°C):
9.64×10^{-3} (calculated-P/C, this work)

Octanol/Water Partition Coefficient, log K_{OW}:
2.70 (shake flask, pH 7, Stevens et al. 1988)
3.70 (Worthing & Hance 1991)
3.90 (Tomlin 1994)
2.70 (selected, Sangster 1993; Hansch et al. 1995)

Bioconcentration Factor, log BCF:
2.02 (calculated-S, Kenaga 1980)
2.56 (calculated-K_{OW} as per Kenaga 1980, this work)

Sorption Partition Coefficient, log K_{OC}:
2.90 (calculated-S, Kenaga 1980)

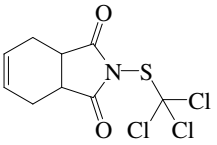
Environmental Fate Rate Constants, k, or Half-Lives, $t_{½}$:

Volatilization:
Photolysis: rapidly decomposed by ultraviolet irradiation in aqueous solutions (Tomlin 1994).
Oxidation:
Hydrolysis: stable in dilute alkalis, but readily hydrolyzed by dilute acids (Tomlin 1994).
Biodegradation:
Biotransformation:
Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants:

Half-Lives in the Environment:

Soil: $t_{½}$ = 35–90 d for nonsterile flooded or non-flooded soil, pH 5.1 to pH 7.3 (Tomlin 1994).

19.1.6 CAPTAN



Common Name: Captan
Synonym: Aacaptan, Amercide, Captab, Captaf, Captane, Captex, Flit 406, Glyodex 37-22, Malipur, Merpan, Orthocide, Pillarcap, Vondcaptan
Chemical Name: *N*-(trichloromethylthio)cyclohex-4-ene-1,2-dicarboximide; 1,2,3,6-tetrahydro-*N*-(trichloromethylthio)phthalimide; 3a,4,7,7a-tetrahydro-[(trichloromethyl)thio]-1*H*-isoindole-1,3(2*H*)-dione
CAS Registry No: 133-06-2
Uses: as fungicide to control a wide range of fungal diseases; also used as seed treatment on maize, ornamentals, vegetables, oilseed rape, and other crops.
Molecular Formula: $C_9H_8Cl_3NO_2S$
Molecular Weight: 300.590

Melting Point (°C):

178	(Hartley & Kidd 1987; Howard 1991; Worthing & Hance 1991; Tomlin 1994; Milne 1995)
172.5	(Lide 2003)

Boiling Point (°C):
Density (g/cm^3 at 20°C):

1.74	(Hartley & Kidd 1987; Tomlin 1994; Milne 1995)

Molar Volume (cm^3/mol):

250.5	(calculated-Le Bas method at normal boiling point)
172.8	(calculated-density)

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

44.35	(DSC method, Plato 1972)

Entropy of Fusion, ΔS_{fus} (J/mol K):
Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F: 0.0357 (mp at 172.5°C)

Water Solubility (g/m^3 or mg/L at 25°C or as indicated):

8.70	(colorimetric, Burchfield 1959)
< 0.5	(Martin & Worthing 1977)
0.50	(Briggs 1981)
3.30	(Hartley & Kidd 1987; Worthing & Hance 1991; Tomlin 1994)
0.50	(20°C, selected, Suntio et al. 1988; quoted, Howard 1991; Majewski & Capel 1995)
5.10	(20–25°C, selected, Wauchope et al. 1992; Hornsby et al. 1996)
1.44	(calculated, Patil 1994)

Vapor Pressure (Pa at 25°C or as indicated):

< 0.0013	(Khan 1980)
< 0.0013	(Hartley & Kidd 1987; Worthing & Hance 1991; Tomlin 1994)
0.0010	(20°C, selected, Suntio et al. 1988; quoted, Howard 1991; Majewski & Capel 1995)
1.1×10^{-5}	(20–25°C, selected, Wauchope et al. 1992; Hornsby et al. 1996)

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

0.60	(20°C, calculated-P/C, Suntio et al. 1988)

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

2.35	(Leo et al. 1971)
1.52	(Rao & Davidson 1980)
2.54	(shake flask-UV, Lord et al. 1980; Briggs 1981)
2.35	(Hansch & Leo 1985)
2.79	(Worthing & Hance 1991; Milne 1995)
2.35	(RP-HPLC-RT correlation, Saito et al. 1993)
2.60	(RP-HPLC-RT correlation, Sicbaldi & Finizio 1993)
2.35	(recommended, Sangster 1993)
2.35	(recommended, Hansch et al. 1995)
2.60	(RP-HPLC-RT correlation, Finizio et al. 1997)

Bioconcentration Factor, log BCF:

> 2.96	(estimated-S, Kenaga 1980a; quoted, Howard 1991)
2.67	(earthworms, Lord et al. 1980)
1.30	(activated sludge, Freitag et al. 1984, 1985)
1.30	(algae, Freitag et al. 1984,85)
1.00	(golden ide, Freitag et al. 1985)
1.56	(regression-log K_{OW}, Hansch & Leo 1985)

Sorption Partition Coefficient, log K_{OC}:

2.30	(soil, converted from K_{OM} multiplied by 1.724, Briggs 1981)
2.29	(Lyman et al. 1982; quoted, Howard 1991)
1.52	(estimated, Jury et al. 1987)
1.52	(screening model calculations, Jury et al. 1987b)
2.30	(soil, quoted exptl., Meylan et al. 1992)
2.94	(soil, calculated-MCI χ and fragments contribution, Meylan et al. 1992)
2.30	(soil, 20–25°C, selected, Wauchope et al. 1992; Hornsby et al. 1996)
2.30	(selected, Lohninger 1994)
2.30	(soil, quoted or calculated-MCI $^1\chi$, Sabljic et al. 1995)

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

Volatilization:

Photolysis: photolysis $t_{½}$ = 37 min in isopropanol, $t_{½}$ = 420 min in cyclohexene and $t_{½}$ = 380 min in cyclohexane by UV-irradiation ($\lambda > 280$ nm): (Schwack & Flöβer-Müller 1990).

Oxidation: photooxidation $t_{½}$ = 3.2–32 h in air, based on estimated rate constant for the vapor-phase reaction with hydroxyl radicals in air (Atkinson 1987; quoted, Howard et al. 1991)

Hydrolysis: pseudo-first-order hydrolysis $t_{½}$ = 0.1 d (Burchfield 1959; quoted, Freed 1976);

$t_{½}$ = 1.8 h, based on first-order rate constant $k = 6.5 \times 10^{-3}$ s^{-1} at pH 7.1 and 28°C (Wolfe et al. 1976; quoted, Howard et al. 1991);

$t_{½}$ = 10.3 h, based on first-order rate constant $k = 1.87 \times 10^{-5} \cdot s^{-1}$ at pH 5.2 and 28°C (Wolfe et al. 1976; quoted, Howard et al. 1991);

$t_{½}$ = 10.5 minutes, based on first-order rate constant $k = 1.10 \times 10^{-3} \cdot s^{-1}$ at pH 8.3 and 28°C (Wolfe et al. 1976; quoted, Howard et al. 1991);

$t_{½}$ = 170 min in a river water sample at pH 7 and 28°C (Wolfe et al. 1976; quoted, Howard 1991);

over rate constant $k = 6.5 \times 10^{-5}$ s^{-1} with $t_{½}$ = 3 h at 25°C and pH 7 (Mabey & Mill 1978)

$t_{½}$ = 7 h in Lake Superior water at pH 7.6 and 12°C, $t_{½}$ = 1 h at pH 7.6 and 25°C, $t_{½}$ = 40 h at pH 6.7 and 12°C, and $t_{½}$ = 8 h at pH 6.7 and 23°C (Wolfe et al. 1976; quoted, Howard 1991).

Biodegradation: unacclimated aqueous aerobic degradation $t_{½}$ = 48–1440 h, based on unacclimated and acclimated soil grab sample data (Agnihotri 1970; Foschi et al. 1970; quoted, Howard et al. 1991); unacclimated aqueous anaerobic degradation $t_{½}$ = 192–5760 h, based on unacclimated aqueous aerobic half-life (Howard et al. 1991);

rate constant $k = 0.231$ d^{-1} with a biodegradation $t_{½}$ = 3 d in soil (Rao & Davidson 1980).

Biotransformation:

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

Half-Lives in the Environment:

Air: $t_{½}$ = 2.6 h and 1.4 h for the vapor-phase reaction with photochemically produced hydroxyl radicals and ozone (Atkinson 1985; quoted, Howard 1991);
photooxidation $t_{½}$ = 3.2–32 h in air, based on estimated rate constant for the vapor-phase reaction with hydroxyl radicals in air (Atkinson 1987; quoted, Howard et al. 1991);
atmospheric transformation lifetime was estimated to be < 1 d (Kelly et al. 1994).

Surface water: hydrolysis $t_{½}$ = 170 min in a river water sample at pH 7 and 28°C (Wolfe et al. 1976; quoted, Howard 1991);
$t_{½}$ = 7 h in Lake Superior water at pH 7.6 and 12°C, $t_{½}$ = 1 h at pH 7.6 and 25°C, $t_{½}$ = 40 h at pH 6.7 and 12°C, and $t_{½}$ = 8 h at pH 6.7 and 23°C (Wolfe et al. 1976; quoted, Howard 1991).

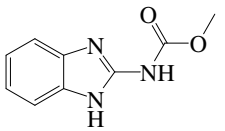
Groundwater: $t_{½}$ = 10.5 min at pH 8.3 to $t_{½}$ = 10.3 h at pH 5.2, based on first-order hydrolysis rate constants in surface waters (Wolfe et al. 1976; quoted, Howard et al. 1991).

Sediment:

Soil: $t_{½}$ = 48–1440 h, based on unacclimated and acclimated soil grab sample data (Agnihotri 1970; Foschi et al. 1970; quoted, Howard et al. 1991);
rate constant k = 0.231 d^{-1} with a biodegradation $t_{½}$ = 3 d (Rao & Davidson 1980);
$t_{½}$ = 2.5 d in soil (Halfon et al. 1996);
field $t_{½}$ = 2.5 d (20–25°C, selected, Wauchope et al. 1992; Hornsby et al. 1996);
$t_{½}$ = 1 d at pH 7.2 (Tomlin 1994).

Biota: biochemical $t_{½}$ = 3 d from screening model calculations (Jury et al. 1987b).

19.1.7 CARBENDAZIM



Common Name: Carbendazim
Synonym: Bavistin, BCM, BMK, Carbendazime, Carbendazol, Carbendazym, G 665, Kemdazin, Mecarzole
Chemical Name: carbamic acid, methyl 1*H*-benzimidazol-2-yl, methyl ester; methyl benzimidazole-2-ylcarbamate; methyl 1*H*-benzimidazol-2-ylcarbamate
Uses: as fungicide for control of a wide range of fungal diseases in cereals, fruit, vines, hops, ornamentals, vegetables, rice coffee, cotton, mushrooms, and other crops; also used by trunk injection to give some control of Dutch elm disease.
CAS Registry No: 10605-21-7
Molecular Formula: $C_9H_9N_3O_2$
Molecular Weight: 191.186
Melting Point (°C):
302–307 (with dec., Hartley & Kidd 1987; Worthing & Hance 1991; Tomlin 1994; Milne 1995)
300 (dec, Lide 2003)
Boiling Point (°C):
Density (g/cm^3 at 20°C):
1.45 (Hartley & Kidd 1987; Tomlin 1994; Milne 1995)

Molar Volume (cm^3/mol):
194.8 (calculated-Le Bas method at normal boiling point)
131.9 (calculated-density)

Dissociation Constant pK_a:
4.48 (Austin & Briggs 1976)
4.24 (Sangster 1993)
4.20 (Tomlin 1994)
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
Entropy of Fusion, ΔS_{fus} (J/mol K):
Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F: 0.002 (mp at 300°C)

Water Solubility (g/m^3 or mg/L at 25°C or as indicated):
8.0 (24°C at pH 7, Hartley & Kidd 1987; Worthing & Hance 1991; Milne 1995)
29, 8.0, 7.0 (24°C, at pH 4, 7, 8, Tomlin 1994)
8.0 (20–25°C at pH 7, selected, Augustijn-Beckers et al. 1994; Hornsby et al. 1996)

Vapor Pressure (Pa at 25°C or as indicated):
6.50×10^{-8} (20°C, Hartley & Kidd 1987)
$< 9.0 \times 10^{-5}$ (20°C, Worthing & Hance 1991)
9.0×10^{-5}, 1.5×10^{-4}, 0.0013 (20, 25, 50°C, quoted, Tomlin 1994)
$< 1.0 \times 10^{-7}$ (20°C, quoted, Tomlin 1994)
6.50×10^{-8} (20–25°C, selected, Augustijn-Beckers et al. 1994; Hornsby et al. 1996)

Henry's Law Constant (Pa·m^3/mol at 25°C):
1.55×10^{-6} (calculated-P/C, this work)

Octanol/Water Partition Coefficient, log K_{OW}:
1.52 (shake flask, Austin & Briggs 1976)
1.40 (shake flask-UV, Lord et al. 1980)
1.34 (shake flask at pH 5, Barak et al. 1983)

1.56 (Worthing & Hance 1991; Milne 1995)
1.43 (recommended, Sangster 1993)
1.38, 1.505, 1.49 (pH 5, 7, 9, Tomlin 1994)
1.56, 1.77 (pH 6, 7, Tomlin 1994)
1.52 (recommended, Hansch et al. 1995)
1.80 (Pomona-database, Müller & Kördel 1996)
1.35 (RP-HPLC-RT correlation using short ODP column, Donovan & Pescatore 2002)

Bioconcentration Factor, log BCF:

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

Sorption Partition Coefficient, log K_{OC}:

3.14 (soil, calculated-S, Kenaga 1980)
2.35 (soil, HPLC-screening method, mean value of different stationary and mobile phases, Kördel et al. 1993, 1995)
2.30–2.40 (soil, Tomlin 1994)
2.35 (soil, calculated-MCI $^1\chi$, Sabljic et al. 1995)
2.69 (soil, 20–25°C at pH 7, selected, Augustijn-Beckers et al. 1994; Hornsby et al. 1996)
2.35; 2.25 (HPLC-screening method; calculated-PCKOC fragment method, Müller & Kördel 1996)
4.00, 2.09, 2.41, 2.28, 2.83 (first generation Eurosoils ES-1, ES-2, ES-3, ES-4, ES-5, shake flask/batch equilibrium-HPLC/UV, Gawlik et al. 1998)
2.318, 2.346, 2.091, 2.198 (second generation Eurosoils ES-2, ES-3, ES-4, ES-5, shake flask/batch equilibrium-HPLC/UV and HPLC-k′ correlation, Gawlik et al. 2000)

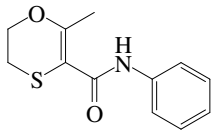
Environmental Fate Rate Constants, k, or Half-Lives, $t_{½}$:

Hydrolysis: $t_{½}$ > 35 d (pH 5 and 7 at 22°C, Worthing & Hance 1991);
slowly decomposed in alkaline solution, $t_{½}$ > 350 d at pH 5, 7, 124 d at pH 9 (Tomlin 1994).

Half-Lives in the Environment:

Air:
Surface water: $t_{½}$ = 2 and 25 months in water under aerobic and anaerobic conditions, respectively (Tomlin 1994).
Groundwater:
Sediment:
Soil: $t_{½}$ = 8–32 d under outdoor conditions, decomposes with $t_{½}$ = 6–12 months on bare soil, $t_{½}$ = 3 to 6 months on turf (Tomlin 1994);
field $t_{½}$ = 120 d (20–25°C, selected, Augustijn-Beckers et al. 1994; Hornsby et al. 1996).
Biota:

19.1.8 CARBOXIN



Common Name: Carboxin
Synonym: Carbathiin, D 735, Kemikar, Kisvax, Vitavax
Chemical Name: 5,6-dihydro-2-methyl-1,4-oxathi-ine-3-carboxanilide; 2,3-dihydro-6-methyl-5-phenylcarbamoyl-1,4-oxathi-ine
CAS Registry No: 5234-68-4
Uses: as fungicide in seed treatment for control of seed diseases of barley, wheat, oats, rice, groundnuts, soybeans, cotton, vegetables, maize, and other crops, etc.
Molecular Formula: $C_{12}H_{13}NO_2S$
Molecular Weight: 235.302
Melting Point (°C):
91.5–92.5 (Spencer 1982; Harley & Kidd 1987; Worthing & Hance 1991; Tomlin 1994)
98.0–100 (dimorphic, Spencer 1982; Hartley & Kidd 1987; Worthing & Hance 1991; Tomlin 1994)
94 (Lide 2003)
Boiling Point (°C):
Density (g/cm^3 at 20°C):
1.30 (Worthing & Hance 1991; Montgomery 1993; Tomlin 1994)
Molar Volume (cm^3/mol):
246.6 (calculated-Le Bas method at normal boiling point)
173.0 (calculated-density)
Dissociation Constant pK_a:
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
22.175 (DSC method, Plato 1972)
Entropy of Fusion, ΔS_{fus} (J/mol K):
Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F: 0.210 (mp at 94°C)

Water Solubility (g/m^3 or mg/L at 25°C or as indicated):
170 (Martin & Worthing 1977)
170 (Spencer 1982; Hartley & Kidd 1987; Montgomery 1993; Milne 1995)
199 (Worthing & Hance 1991; Tomlin 1994)
215 (calculated-group contribution fragmentation method, Kühne et al. 1995)
195 (20–25°C, selected, Wauchope et al. 1992; Hornsby et al. 1996)
195 (selected, Lohninger 1994)

Vapor Pressure (Pa at 25°C or as indicated):
$< 1.0 \times 10^{-3}$ (20°C, Hartley & Kidd 1987)
2.5×10^{-5} (Worthing & Hance 1991; Tomlin 1994)
1.3×10^{-5} (20–25°C, selected, Wauchope et al. 1992; Hornsby et al. 1996)
2.5×10^{-5} (20°C, Montgomery 1993)

Henry's Law Constant (Pa·m^3/mol at 25°C):
3.45×10^{-5} (calculated-P/C, Montgomery 1993)
1.57×10^{-5} (calculated-P/C, this work)

Octanol/Water Partition Coefficient, log K_{OW}:
2.17 (Worthing & Hance 1991; Montgomery 1993; Milne 1995)
2.18 (Tomlin 1994)
2.14 (selected, Hansch et al. 1995)
2.60 (RP-HPLC-RT correlation using short ODP column, Donovan & Pescatore 2002)

Bioconcentration Factor, log BCF:

1.53 (calculated-S, Kenaga 1980)

Sorption Partition Coefficient, log K_{OC}:

2.41 (soil, calculated-S, Kenaga 1980)
2.41 (soil, 20–25°C, selected, Wauchope et al. 1992; Hornsby et al. 1996)
2.41 (calculated, Montgomery 1993)
2.41 (estimated-chemical structure, Lohninger 1994)
2.57 (soil, Tomlin 1994)

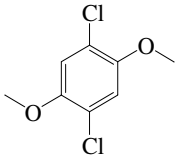
Environmental Fate Rate Constants, or Half-Lives, $t_{½}$:

Volatilization:
Photolysis: $t_{½} < 3$ h when exposed to light in aqueous solutions at pH 7 (Tomlin 1994).
Oxidation:
Hydrolysis: hydrolysis $t_{½} < 3$ d when exposed to light (Montgomery 1993).
Biodegradation:
Biotransformation:
Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants:

Half-Lives in the Environment:

Soil: $t_{½} \sim 24$ h (Worthing & Hance 1991; quoted, Montgomery 1993; Tomlin 1994);
field $t_{½} = 3$ d (20–25°C, selected, Wauchope et al. 1992; Hornsby et al. 1996).

19.1.9 CHLORONEB



Common Name: Chloroneb
Synonym: Demosan; Tersan SP
Chemical Name: 1,4-dichloro-2,5-dimethoxybenzene
CAS Registry No: 2675-77-6
Uses: as fungicide applied to soil or used as seed treatment for control of seedling diseases of beans, cotton, soybeans, and beet; also used for control of snow mold (*Typhula* spp.) and Pythium blight on turf grass.
Molecular Formula: $C_8H_8Cl_2O_2$
Molecular Weight: 207.055

Melting Point (°C):
134 (Lide 2003)
Boiling Point (°C):
268 (Spencer 1982; Hartley & Kidd 1987; Worthing & Hance 1991; Tomlin 1994; Milne 1995)
Density (g/cm^3 at 20°C):
1.66 (Spencer 1982)
Molar Volume (cm^3/mol):
200.4 (calculated-Le Bas method at normal boiling point)
124.8 (calculated-density)
Dissociation Constant pK_a:
Enthalpy of Vaporization, ΔH_V (kJ/mol):
71.91 (Rordorf 1989)
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
30.54 (DSC method, Plato & Glasgow 1969)
29.1 (Rordorf 1989)
Entropy of Fusion, ΔS_{fus} (J/mol K):
72.0 (Rordorf 1989)
Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F: 0.0852 (mp at 134°C)

Water Solubility (g/m^3 or mg/L at 25°C or as indicated):
8 (Martin & Worthing 1977; Spencer 1982)
8 (Hartley & Kidd 1987; Worthing & Hance 1991; Tomlin 1994; Milne 1995)
8 (20–25°C, selected, Wauchope et al. 1992; Hornsby et al. 1996)

Vapor Pressure (Pa at 25°C or as indicated and reported temperature dependence equations):
0.40 (Spencer 1982)
0.40 (Hartley & Kidd 1987; Worthing & Hance 1991; Tomlin 1994)
0.017, 0.43, 6.90, 77.0, 630 (25, 50, 70, 100, 125°C, gas saturation-GC, Rordorf 1989)
log (P_S/Pa) = 16.452 – 5436/(T/K); measured range 32.5–135°C (solid, gas saturation-GC, Rordorf 1989)
log (P_L/Pa) = 12.303 – 3757.8/(T/K); measured range 136–151°C (liquid, gas saturation-GC, Rordorf 1989)
0.40 (20–25°C, selected, Wauchope et al. 1992; Hornsby et al. 1996)

Henry's Law Constant (Pa·m^3/mol):

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

Bioconcentration Factor, log BCF:

Sorption Partition Coefficient, log K_{OC}:

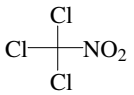
3.06	(soil, Hamaker & Thompson 1972)
3.10	(soil, quoted exptl., Meylan et al. 1992)
2.36	(calculated-MCI χ and fragments contribution, Meylan et al. 1992)
3.22	(soil, 20–25°C, selected, Wauchope et al. 1992; Hornsby et al. 1996)
3.22	(selected, Lohninger 1994)

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

Half-Lives in the Environment:

Soil: $t_{½}$ ~ 24 h (Worthing & Hance 1991);
field $t_{½}$ = 130 d (20–25°C, selected, Wauchope et al. 1992; Hornsby et al. 1996).

19.1.10 CHLOROPICRIN



Common Name: Chloropicrin
Synonym: Acquinite, Nemax, Nitrochloroform, Picfume
Chemical Name: Trichloronitromethane
CAS Registry No: 76-06-2
Uses: fungicide/herbicide/insecticide/nematicide/rodenticide; used as a soil disinfectant for control of nematodes, soil insects, soil fungi, and weed seeds; also used for fumigation of stored grain to control insects and rodents, for glasshouse and mushroom-house fumigation, etc.
Molecular Formula: CCl_3NO_2
Molecular Weight: 164.376
Melting Point (°C):
–64.0 (Spencer 1982; Hartley & Kidd 1987; Tomlin 1994; Lide 2003)
Boiling Point (°C):
112.4 (Spencer 1982; Hartley & Kidd 1987; Tomlin 1994)
Density (g/cm^3 at 20°C):
1.65659, 1.64756 (20°C, 25°C, Dreisbach 1961)
1.656 (20°C, Spencer 1982; Tomlin 1994)
1.6558, 1.6483 (20°C, 25°C, Montgomery 1993)
Molar Volume (cm^3/mol):
113.9 (calculated-Le Bas method at normal boiling point)
99.3 (calculated-density)
Dissociation Constant pK_a:
Enthalpy of Vaporization, ΔH_V (kJ/mol):
39.40, 33.12 (25°C, bp, Dreisbach 1961)
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
11.68 (Dreisbach 1961)
Entropy of Fusion, ΔS_{fus} (J/mol K):
Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F: 1.0

Water Solubility (g/m^3 or mg/L at 25°C or as indicated):
2270 (Martin & Worthing 1977; Kenaga 1980; Montgomery 1993; Lohninger 1994)
2270 (0°C, Spencer 1982; quoted, Howard 1991; Tomlin 1994)
2270, 1620 (0, 25°C, Hartley & Kidd 1987)
2300 (Davies & Lee 1987)
1621 (Howard 1991)
2270 (20–25°C, selected, Wauchope et al. 1992; Hornsby et al. 1996)
1620 (Tomlin 1994)

Vapor Pressure (Pa at 25°C or as indicated and the reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section.):
3174* (gas saturation, measured range 0–35°C, Baxter et al. 1920)
log (P/mmHg) = 8.2424 – 2045.1/(273 + t/°C); temp range 0–35°C (gas saturation, Baxter et al. 1920)
2666* (20°C, summary of literature data, temp range –25.5 to 111.9°C, Stull 1947)
3324 (calculated by formula, Dreisbach 1961)
log (P/mmHg) = 7.03335 – 1369.70/(218.0 + t/°C), temp range 28–176°C, (Antoine eq. for liquid state, Dreisbach 1961)
760, 3173 (0, 25°C, Spencer 1982)
3200 (Hartley & Kidd 1987)
3173 (Howard 1991)
2253, 3173, 4400 (20, 25, 30°C, Montgomery 1993)

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

208.0 (Kawamoto & Urano 1989)

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

1.03 (HPLC-RT correlation, Kawamoto & Urano 1989)
2.09 (shake flask, Hansch & Leo 1987)
2.07 (Howard 1991)
1.03, 2.09 (Montgomery 1993)
2.09 (selected, Sangster 1993; Hansch et al. 1995)

Bioconcentration Factor, log BCF:

0.90 (calculated, Kenaga 1980; quoted, Howard 1991)

Sorption Partition Coefficient, log K_{OC}:

1.79 (calculated, Kenaga 1980)
1.91 (soil, correlated-Freundlich Isotherm, Kawamoto & Urano 1989)
1.79 (soil, Wauchope et al. 1992; Hornsby et al. 1996)
1.79 (selected, Lohninger 1994)

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

Volatilization: $t_{½}$ = 4.3 h for evaporation from a body of water 1 m deep with a current of 1 m/s and a wind of 3 m/s (Howard 1991).

Photolysis: $t_{½}$ = 20 d in simulated atmosphere, $t_{½}$ = 3 d in aqueous solution with sunlight irradiation (Montgomery 1993).

Oxidation:

Hydrolysis:

stable in neutral aqueous solution and with a minimum $t_{½}$ = 11 yr (Howard 1991).

Biodegradation: rate constant k(aerobic) = 1.5 d^{-1} with $t_{½}$ = 0.46 d at 20°C by aerobic activated sludge and k(anaerobic) = 1.5 d^{-1} with $t_{½}$ = 0.46 d at 20°C by anaerobic microorganisms cultivated an artificial sewage (Kawamoto & Urano 1990)

k(anaerobic) = 12 d^{-1} and $t_{½}$ = 0.058 d (corrigendum, Kawamoto & Urano 1991)

Biotransformation:

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

Half-Lives in the Environment:

Air: $t_{½}$ = 20 d by photodegradation (Howard 1991).

Surface water: biodegradation $t_{½}$ = 0.46 d at 20°C by aerobic activated sludge or anaerobic microorganisms (Kawamoto & Urano 1990)

volatilization $t_{½}$ = 4.3 h from a model river and photodegradation $t_{½}$ = 3 d in the surface layer of water (Howard 1991).

Groundwater:

Sediment:

Soil: field $t_{½}$ ~ 1 d (estimated, Wauchope et al. 1992; Hornsby et al. 1996).

Biota:

TABLE 19.1.10.1
Reported vapor pressures of chloropicrin at various temperatures and the coefficients for the vapor pressure equations

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

Baxter et al. 1920		Stull 1947		Spencer 1982		Montgomery 1993	
gas saturation		summary of literature data		handbook		handbook	
t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa
–20	200	–25.5	133.3	0	760	20	2253
–19	226.6	–3.30	666.6	25	3173	25	3173
–18	253.3	7.80	1333			30	4400
0	760.3	20.0	2666	Dreisbach eq.2			
10	1383	33.8	5333	A	7.03335		
15	1843	42.3	7999	B	1369.7		
20	2441	53.8	13332	C	218		
25	3174	71.8	26664	temp range 28–176°C			
30	4146	91.8	53329				
35	5352	111.9	101325				
eq. 2	P/mmHg	mp/°C	–64				
A	8.2424						
B	2045.1						
C	273						

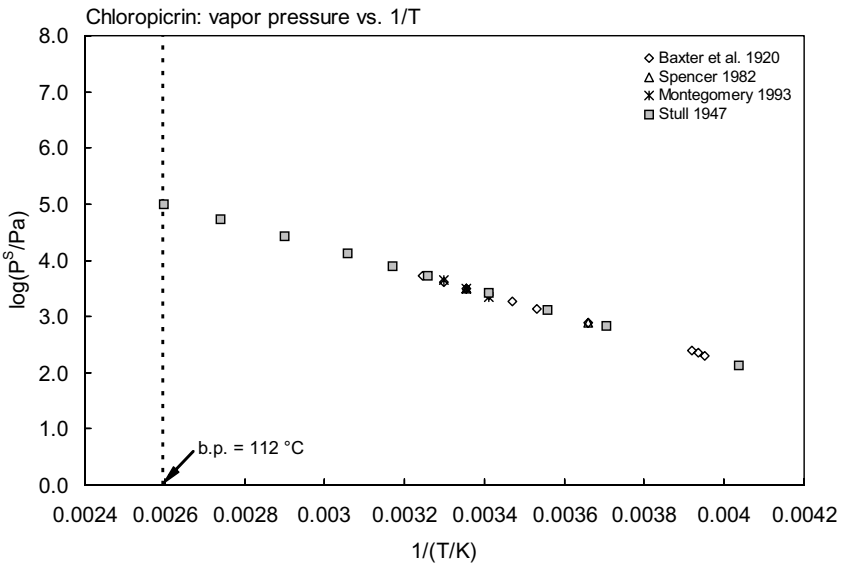
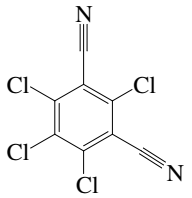


FIGURE 19.1.10.1 Logarithm of vapor pressure versus reciprocal temperature for chloropicrin.

19.1.11 CHLOROTHALONIL



Common Name: Chlorothalonil
Synonym: Bravo, chlorthalonil, Daconil, DAC 2787, Exotherm, Forturf, Nopcocide N 96, TPN
Chemical Name: tetrachloroisophthalonitrile; 2,4,5,6-tetrachloro-1,3-benzenedicarbonitrile; 2,4,5,6-tetrachloro-1,3-dicyanobenzene
CAS Registry No: 1897-45-6
Uses: fungicide, fumigant, soil insecticide
Molecular Formula: $C_8Cl_4N_2$
Molecular Weight: 265.911
Melting Point (°C):
250 (Lide 2003)
Boiling Point (°C):
350 (Hartley & Kidd 1987; Worthing & Hance 1991; Montgomery 1993; Tomlin 1994; Milne 1995)
Density (g/cm^3 at 20°C): 1.80 (Montgomery 1993; Tomlin 1994)
Molar Volume (cm^3/mol):
233.0 (calculated-Le Bas method at normal boiling point)
147.7 (calculated-density)
Dissociation Constant pK_a:
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
Entropy of Fusion, ΔS_{fus} (J/mol K):
Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F: 0.0062 (mp at 250°C)

Water Solubility (g/m^3 or mg/L at 25°C or as indicated):
0.60 (Martin & Worthing 1977; Kenaga 1980; Spencer 1982; Hartley & Kidd 1987; Worthing 1987, 1991)
0.30 (Davies & Lee 1987)
0.50 (calculated-group contribution fragmentation method, Kühne et al. 1995)
0.60 (20–25°C, selected, Wauchope et al. 1992; Hornsby et al. 1996)
0.90 (Tomlin 1994)

Vapor Pressure (Pa at 25°C or as indicated):
< 1.30 (40°C, Hartley & Kidd 1987; Worthing & Hance 1991)
232 (Worthing & Walker 1987; quoted, Majewski & Capel 1995)
0.133 (20–25°C, estimated, Wauchope et al. 1992; Hornsby et al. 1996)
1.3×10^{-3} (40°C, Montgomery 1993)
8.1×10^{-3} (selected, Brouwer et al. 1994)
7.6×10^{-5} (Tomlin 1994)

Henry's Law Constant (Pa·m^3/mol at 25°C or as indicated):
576 (calculated-P/C as per Worthing 1987, Majewski & Capel 1995)
0.0194 (20°C, Kawamoto & Urano 1989)
0.0151 (20°C, calculated-bond contribution method, Meylan & Howard 1991)
0.02 (Montgomery 1993)

Octanol/Water Partition Coefficient, log K_{OW}:
0.14 (screening model calculations, Jury et al. 1987b)

2.64 (HPLC-RT correlation, Kawamoto & Urano 1989)
2.64 (recommended, Sangster 1993)
2.89 (RP-HPLC-RT correlation, Saito et al. 1993)
2.90 (recommended, Hansch et al. 1995)
3.80 (RP-HPLC-RT correlation, Nakamura et al. 2001)

Bioconcentration Factor, log BCF:

1.92 (calculated-S, Kenaga 1980)
1.66 (calculated-K_{OW} as per Kenaga 1980, this work)

Sorption Partition Coefficient, log K_{OC}:

3.76 (soil, calculated, Kenaga 1980)
3.14 (soil, screening model calculations, Jury et al. 1987b)
3.14 (soil, Gustafson et al. 1989)
3.26 (soil, correlated-Freundlich Isotherm, Kawamoto & Urano 1989)
3.14 (soil, 20–25°C, selected, Wauchope et al. 1992; Hornsby et al. 1996)
2.76, 3.14 (soil, Montgomery 1993)
3.00 (sand, quoted, Montgomery 1993)
3.14 (estimated-chemical structure, Lohninger 1994)
3.20, 4.15 (sand, silt, Tomlin 1994)
3.26 (soil, calculated-MCI $^1\chi$, Sabljic et al. 1995)

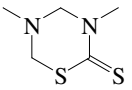
Environmental Fate Rate Constants, or Half-Lives, $t_{½}$:

Volatilization:
Photolysis:
Oxidation:
Hydrolysis:
Biodegradation: biochemical $t_{½}$ = 70 d (Jury et al. 1987b);
first-order rate constants in biotic and abiotic shake-flask tests k = –0.0161 and –0.0155 d^{-1} in nonsterile sediment/estuarine water and k = –0.00574 d^{-1} in sterile sediment/estuarine water and k = –0.00355 and –0.00329 d^{-1} in nonsterile estuarine water and k = –0.00283 d^{-1} in sterile estuarine water both at Davis Bayou (Walker et al. 1988);
rate constant k(aerobic) = 1.7 d^{-1} with $t_{½}$ = 0.41 d at 20°C by aerobic activated sludge and k(anaerobic) = 1.7 d^{-1} with $t_{½}$ = 0.41 d at 20°C by anaerobic microorganisms cultivated an artificial sewage (Kawamoto & Urano 1990)
Biotransformation:
Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants:

Half-Lives in the Environment:

Air:
Surface water: biodegradation $t_{½}$ = 0.41 d at 20°C by aerobic activated sludge or anaerobic microorganisms cultivated by an artificial sewage (Kawamoto & Urano 1990)
Groundwater:
Sediment:
Soil: $t_{½}$ = 70 d from screening model calculations (Jury et al. 1987b);
$t_{½}$ ~ 1.5–3 months (Hartley & Kidd 1987; Worthing & Hance 1991);
soil $t_{½}$ = 68 d (Gustafson 1989);
field $t_{½}$ = 30 d (20–25°C, selected, Wauchope et al. 1992; Hornsby et al. 1996);
$t_{½}$ = 4.1 d and 1.5–3 months (Montgomery 1993);
$t_{½}$ = 5–35 d in aerobic and anaerobic soil studies and from a few hours to a few days in aerobic and anaerobic aquatic soil studies (Tomlin 1994).
Biota: biochemical $t_{½}$ = 70 d from screening model calculations (Jury et al. 1987b).

19.1.12 DAZOMET



Common Name: Dazomet
Synonym: tiazon, Mylone, Crag Fungicide 974, Salvo, Basamid, Fongosan
Chemical Name: 3,5-dimethyl-1,3,5-thiadiazinane-2-thione
Uses: soil fumigant, nematicide, fungicide, herbicide, insecticide
CAS Registry No: 533-74-4
Molecular Formula: $C_5H_{10}N_2S_2$
Molecular Weight: 162.276
Melting Point (°C):
106 (Lide 2003)
Boiling Point (°C):
Density (g/cm^3): 1.37 (Montgomery 1993; Tomlin 1994)
Acid Dissociation Constant, pK_a:
Molar Volume (cm^3/mol):
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
Entropy of Fusion, ΔS_{fus} (J/mol K):
Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F: 0.160 (mp at 106°C)

Water Solubility (g/m^3 or mg/L at 25°C or as indicated):
1200 (Spencer 1982)
3000 (20°C, Worthing & Walker 1983, 1987; Hartley & Kidd 1987; Montgomery 1993; Tomlin 1994)
2000 (Herbicide Handbook 1989, quoted, Augustijn-Beckers et al. 1994)
3000 (20–25°C, selected, Augustijn-Beckers et al. 1994; Hornsby et al. 1996)

Vapor Pressure (Pa at 25°C or as indicated):
3.7×10^{-4} (20°C, Hartley & Kidd 1987; Worthing & Walker 1983, 1987; Montgomery 1993; Tomlin 1994)
4.0×10^{-4}, 3.73×10^{-4} (20°C, quoted, Augustijn-Beckers et al. 1994)
4.0×10^{-4} (20–25°C, selected, Augustijn-Beckers et al. 1994; Hornsby et al. 1996)

Henry's Law Constant (Pa·m^3/mol at 25°C or as indicated):
2.03 (20°C, calculated-P/C, Montgomery 1993)

Octanol/Water Partition Coefficient, log K_{OW}:
0.15 (Montgomery 1993)
1.40 (at pH 7, Tomlin 1994)

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

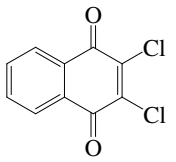
Bioconcentration Factor, log BCF or log K_B:

Sorption Partition Coefficient, log K_{OC}:
0.48 (calculated, Montgomery 1993)
–0.046 at pH 9, 0.778 (quoted values, Augustijn-Beckers et al. 1994)
1.0 (estimated, Augustijn-Beckers et al. 1994; Hornsby et al. 1996)

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

Half-Lives in the Environment:
Soil: field $t_{½}$ = 7 d (Augustijn-Beckers et al. 1994; Hornsby et al. 1996).

19.1.13 DICHLONE



Common Name: Dichlone
Synonym: Algistat, Compound 604, Ent 3776, Phygon, Quintar, Sanquinon
Chemical Name: 2,3-dichloro-1,4-naphthoquinone; 2,3-dichloro-1,4-naphthalenedione
CAS Registry No: 117-80-6
Uses: fungicide/algicide; as fungicide for control of blossom blights, scab on apples and pears and brown spot on stone fruit, etc.; also used to control blue-green algae in ponds, lakes, and swimming pools.
Molecular Formula: $C_{10}H_4Cl_2O_2$
Molecular Weight: 227.044
Melting Point (°C):
195 (Lide 2003)
Boiling Point (°C):
275 (at 2 mmHg, Hartley & Kidd 1987; Howard 1991; Montgomery 1993)
Density (g/cm^3 at 20°C):
Molar Volume (cm^3/mol):
196.8 (calculated-Le Bas method at normal boiling point)
Dissociation Constant pK_a:
Enthalpy of Vaporization, ΔH_V (kJ/mol):
78.30 (Rordorf 1989)
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
27.0 (Rordorf 1989)
Entropy of Fusion, ΔS_{fus} (J/mol K):
58 (Rordorf 1989)
Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F: 0.0215 (mp at 195°C)

Water Solubility (g/m^3 or mg/L at 25°C as indicated):
0.10 (Kenaga 1980)
8.00 (20°C, Hodnett et al. 1983)
0.10 (Hartley & Kidd 1987; Worthing & Hance 1991; Tomlin 1994; Milne 1995)
1.00 (Montgomery 1993)
0.10 (20–25°C, selected, Augustijn-Beckers et al. 1994; Hornsby et al. 1996)

Vapor Pressure (Pa at 25°C or as indicated and reported temperature dependence):
3.30×10^{-4}, 8.80×10^{-3}, 0.15, 1.70, 14.0 (25, 50, 70, 100, 125°C, gas saturation-GC, Rordorf 1989)
$\log (P_S/Pa) = 14.965 - 5500.9/(T/K)$; measured range 40.4–191°C (solid, gas saturation-GC, Rordorf 1989)
$\log (P_L/Pa) = 13.396 - 4803.6/(T/K)$; measured range 40.4–191°C (liquid, gas saturation-GC, Rordorf 1989)
1.47×10^{-4} (calculated from S and Henry's law constant, Howard 1991)
10930 (20–25°C, estimated, Augustijn-Beckers et al. 1994; Hornsby et al. 1996)

Henry's Law Constant (Pa·m^3/mol at 25°C):
6.51×10^{-5} (Hine & Mookerjee 1975)

Octanol/Water Partition Coefficient, log K_{OW}:
3.16 (estimated, Hodnett et al. 1983)
5.62 (calculated, Montgomery 1993)

Bioconcentration Factor, log BCF:

3.35 (estimated-S, Kenaga 1980; quoted, Howard 1991)

Sorption Partition Coefficient, log K_{OC}:

4.19 (estimated-S, Kenaga 1980; quoted, Howard 1991)
4.00 (20–25°C, estimated, Augustijn-Beckers et al. 1994; Hornsby et al. 1996)
4.19 (calculated, Montgomery 1993)

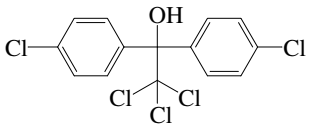
Environmental Fate Rate Constants, k, or Half-Lives, $t_{½}$:

Volatilization:
Photolysis:
Oxidation: estimated photooxidation $t_{½}$ = 3.87 d in air, based on the vapor-phase reaction with hydroxyl radicals in air (Atkinson 1987; quoted, Howard 1991).
Hydrolysis: $t_{½}$ = 5 d at pH 7 (Howard 1991).
Biodegradation:
Biotransformation:
Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants:

Half-Lives in the Environment:

Air: estimated $t_{½}$ = 3.87 d, based on the vapor-phase reaction with hydroxyl radicals in air (Atkinson 1987; quoted, Howard 1991).
Surface water:
Groundwater:
Sediment:
Soil: $t_{½}$ = 1 d in moist and slightly under three months in dry silt loam soil at pH 6.2–6.4 and 29°C, respectively (Burchfield 1959; quoted, Howard 1991);
field $t_{½}$ = 10 d (20–25°C, estimated, Augustijn-Beckers et al. 1994; Hornsby et al. 1996).
Biota:

19.1.14 DICOFOL



Common Name: Dicofol
Synonym: kelthane, kelthan
Chemical Name: 2,2,2-trichloro-1,1-bis(4-chlorophenyl)ethenol, 4-chloro-α-(4-chlorophenyl)-α-(trichloromethyl)-benzenemethanol
Uses: acaricide
CAS Registry No: 115-32-2
Molecular Formula: $C_{14}H_9Cl_5O$
Molecular Weight: 370.485
Melting Point (°C):
77.5 (Lide 2003)
Boiling Point (°C):
180 (0.1 mmHg, Hartley & Kidd 1987)
193 (360 mmHg, tech., Tomlin 1994)
Density (g/cm^3): 1.45 (Worthing & Walker 1987; Tomlin 1994)
Acid Dissociation Constant, pK_a:
Molar Volume (cm^3/mol):
Enthalpy of Vaporization, ΔH_V (kJ/mol):
104.0 (Rordorf 1989)
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
19.8 (Rordorf 1989)
Entropy of Fusion, ΔS_{fus} (J/mol K):
57 (Rordorf 1989)
Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F: 0.305 (mp at 77.5°C)

Water Solubility (g/m^3 or mg/L at 25°C or as indicated):
1.32 (generator column-GC/ECD, Weil et al. 1974)
1.20 (24°C, 99% purity, Verschueren 1983)
0.80 (20°C, in distilled water, Verschueren 1983)
0.80 (selected, Wauchope et al. 1992; Hornsby et al. 1996)
0.80 (Tomlin 1994)

Vapor Pressure (Pa at 25°C or as indicated and reported temperature dependence equations):
2.40×10^{-5}, 1.20×10^{-3}, 0.032, 0.56, 68.0 (25, 50, 70, 100, 125°C, gas saturation-GC, Rordorf 1989)
log (P_S/Pa) = 17.084 – 6470.1/(T/K); measured range 85.5–145°C (solid, gas saturation-GC, Rordorf 1989)
log (P_L/Pa) = 14.104 – 5354.8/(T/K); measured range 85.5–145°C (liquid, gas saturation-GC, Rordorf 1989)
5.33×10^{-5} (selected, Wauchope et al. 1992; Hornsby et al. 1996)
5.30×10^{-5} (tech., Tomlin 1994)

Henry's Law Constant (Pa·m^3/mol at 25°C):
5.66×10^{-5} (calculated-bond contribution method, Howard 1991)

Octanol/Water Partition Coefficient, log K_{OW}:
3.54 (Rao & Davidson 1980)
3.54 (Nigg et al. 1986)
4.28 (Tomlin 1994)
3.54 (Hansch & Leo 1987; quoted, Sangster 1993)

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

Bioconcentration Factor, log BCF or log K_B:

4.18–4.27 (fathead minnow, Howard 1991)
3.98–4.16 (in presence of suspended clay, Howard 1991)
2.75, 3.54 (calculated-S, calculated-K_{OW}, Howard 1991)

Sorption Partition Coefficient, log K_{OC}:

3.60, 3,30 (estimated-S, calculated-K_{OW}, Howard 1991)
3.46–3.91 (range of reported data, Wauchope et al. 1992)
3.70 (soil, recommended, Wauchope et al. 1992; Hornsby et al. 1996)
3.92, 3.91, 3.79, 3.77 (sand, sandy loam, silty loam, clay loam, Tomlin 1994)

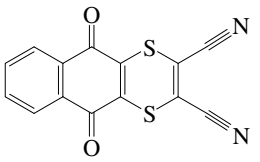
Environmental Fate Rate Constants, k, and Half-Lives, $t_{½}$:

Volatilization:
Photolysis: direct photolysis $t_{½}$ = 2.92 d in the atmosphere for reaction with OH radicals; $t_{½}$ = 6 d for exposure of thin film of dicofol to sunlight at 300 nm (Howard 1991).
Photooxidation:
Hydrolysis: $t_{½}$ = 60 min at pH 8.2 and 3 min at pH 10.2 with an initial concn of 0.4 mg/L (Verschueren 1983); stable to acids, but unstable in alkaline media, $t_{½}$ = 85 d at pH 5, 64–99 h at pH 7, 26 min at pH 9 (Tomlin 1994).
Biodegradation: degradation in anaerobic sewage to 4,4′-dichlorobenzophenone (DBP); 88–94% conversion to DBP for filtered river water, 47–56% for unfiltered river water of pH 7.5 in a 24-h expt. (Verschueren 1983); $t_{½}$ = 61 d and 16 d under aerobic and anaerobic conditions in silt loam (Tomlin 1994).
Biotransformation:
Bioconcentration and Uptake and Elimination Rate Constants (k_1 and k_2):

Half-Lives in the Environment:

Air: vapor phase $t_{½}$ ~ 2.92 s life in the atmosphere for reaction with OH radicals (estimated, Howard 1991)
Surface water: hydrolysis $t_{½}$ = 60 min at pH 8.2 and 3 min at pH 10.2 with an initial concn of 0.4 mg/L; degradation in anaerobic sewage to 4,4′-dichlorobenzophenone (DBP); 88–94% conversion to DBP for filtered river water, 47–56% for unfiltered river water of pH 7.5 in a 24-h expt. (Verschueren 1983)
aqueous photodegradation $t_{½}$ = 1–4 d at pH 5 in sensitized conditions and $t_{½}$ = 15–93 d in unsensitized conditions; stable to acids, but unstable in alkaline media, $t_{½}$ = 85 d at pH 5, 64–99 h at pH 7, 26 min at pH 9 (Tomlin 1994).
Ground water:
Sediment:
Soil: field $t_{½}$ = 45 d (Wauchope et al. 1992; Hornsby et al. 1996);
soil photodegradation $t_{½}$ = 30 d in silt loam, soil metabolism $t_{½}$ = 61 d under aerobic conditions and $t_{½}$ = 16 d under anaerobic conditions in silt loam; field dissipation $t_{½}$ = 60–100 d (Tomlin 1994).
Biota:

19.1.15 DITHIANON



Common Name: Dithianon
Synonym: Delan, Delan-Col
Chemical Name: 2,3-dicyano-1,4-dithia-anthraquinone; 5,10-dihydro-5,10-dioxonaphtho[2,3-b]-*p*-dithin-2,3-dicarbonitrile
CAS Registry No: 3347-22-6
Uses: as fungicide for control of many foliar diseases.
Molecular Formula: $C_{14}H_4N_2O_2S_2$
Molecular Weight: 296.324
Melting Point (°C):
220 (Lide 2003)
Boiling Point (°C):
Density (g/cm^3 at 20°C):
1.580 (Tomlin 1994)
Molar Volume (cm^3/mol):
264.0 (calculated-Le Bas method at normal boiling point)
187.6 (calculated-density)
Dissociation Constant pK_a:
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
Entropy of Fusion, ΔS_{fus} (J/mol K):
Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F: 0.0122 (mp at 220°C)

Water Solubility (g/m^3 or mg/L at 25°C or as indicated):
0.50 (20°C, Hartley & Kidd 1987; Worthing & Hance 1991; Tomlin 1994)

Vapor Pressure (Pa at 25°C):
6.6×10^{-5} (Hartley & Kidd 1987; Worthing & Hance 1991; Tomlin 1994)

Henry's Law Constant (Pa·m^3/mol at 25°C):
0.0391 (calculated-P/C, this work)

Octanol/Water Partition Coefficient, log K_{OW}:
2.84 (Worthing & Hance 1991)
3.20 (Tomlin 1994)
2.84 (selected, Hansch et al. 1995)

Bioconcentration Factor, log BCF:
2.96 (calculated-S per Kenaga 1980, this work)

Sorption Partition Coefficient, log K_{OC}:
3.81 (soil, calculated-S per Kenaga 1980, this work)

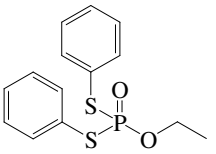
Environmental Fate Rate Constants, k, or Half-Lives, $t_{½}$:
Volatilization:
Photolysis: $t_{½}$ = 19 h when exposed to artificial sunlight in 0.1 mg/L aqueous solution (Tomlin 1994).
Oxidation:
Hydrolysis: $t_{½}$ = 12.2 h at pH 7 (Tomlin 1994).

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

Half-Lives in the Environment:

Surface water: hydrolysis $t_{½}$ = 12.2 h at pH 7 and photolytic $t_{½}$ = 19 h when exposed to artificial sunlight in 0.1 mg/L aqueous solutions (Tomlin 1994).

19.1.16 EDIFENPHOS



Common Name: Edifenphos
Synonym: EDDP, Hinosan, edifenfos
Chemical Name: *O*-ethyl *S,S*-diphenyl phosphorodithioate
CAS Registry No: 17109-49-8
Uses: as fungicide for control of blast and blight diseases in rice, etc.
Molecular Formula: $C_{14}H_{15}O_2PS_2$
Molecular Weight: 310.371
Melting Point (°C):
–25 (Tomlin 1994)
Boiling Point (°C):
154 (at 0.01 mmHg, Hartley & Kidd 1987; Worthing & Hance 1991)
Density (g/cm^3 at 20°C):
1.230 (Hartley & Kidd 1987; Worthing & Hance 1991)
1.251 (Tomlin 1994)
Molar Volume (cm^3/mol):
250.5 (calculated from density)
Dissociation Constant pK_a:
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
Entropy of Fusion, ΔS_{fus} (J/mol K):
Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F: 1.0

Water Solubility (g/m^3 or mg/L at 25°C or as indicated):
56.0 (20°C, Hartley & Kidd 1987; Tomlin 1994)
insoluble (Worthing & Hance 1991)

Vapor Pressure (Pa at 25°C or as indicated):
0.013 (20°C, Hartley & Kidd 1987)
0.013 (20°C, Tomlin 1994)

Henry's Law Constant (Pa·m^3/mol at 25°C or as indicated):
0.0721 (20°C, calculated-P/C, this work)

Octanol/Water Partition Coefficient, log K_{OW}:
3.48 (RP-HPLC-RT correlation, Saito et al. 1993)
4.20 (RP-HPLC-RT correlation, Nakamura et al. 2001)

Bioconcentration Factor, log BCF:
1.81 (calculated-S as per Kenaga 1980, this work)

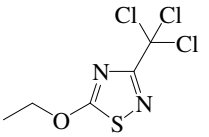
Sorption Partition Coefficient, log K_{OC}:
2.68 (calculated-S as per Kenaga 1980, this work)

Environmental Fate Rate Constants, k, or Half-Lives, $t_{½}$:
Hydrolysis: hydrolyzed by strong acids and alkalis, at 25°C, $t_{½}$ = 19 d at pH 7 and $t_{½}$ = 2 d at pH 9 (Tomlin 1994).

Half-Lives in the Environment:
Air:
Surface water: hydrolysis $t_{½}$ = 19 d at pH 7 and $t_{½}$ = 2 d at pH 9 (Tomlin 1994).

Groundwater:
Sediment:
Soil: half-life in soil in the range of few days to a few weeks (Tomlin 1994).
Biota:

19.1.17 ETRIDIAZOLE



Common Name: Etridiazole
Synonym: Aaterra, Banrot, Dwell, Echlomezol, ETCMTD, Ethazole, ETMT, Koban, MF-344, OM 2425, Pansoil, Terracoat, Terrazole, Truban
Chemical Name: 5-ethoxy-3-(trichloromethyl)-1,2,4-thiadiazole; ethyl 3-trichloromethyl-1,2,4-thiadiazolyl ether
Uses: as fungicide for control of *Phytophthora* and *Pythium* spp. in cotton, ornamentals, vegetables, groundnuts, cucurbits, tomatoes, and other crops; also used as a nitrification inhibitor in maize, cotton and wheat.
CAS Registry No: 2593-15-9
Molecular Formula: $C_5H_5Cl_3N_2OS$
Molecular Weight: 247.530
Melting Point (°C):
19.9 (Tomlin 1994; Milne 1995; Lide 2003)
Boiling Point (°C):
95.0 (at 1 mmHg, Hartley & Kidd 1987; Tomlin 1994; Milne 1995)
Density (g/cm^3 at 20°C):
1.503 (25°C, Hartley & Kidd 1987; Tomlin 1994)
Molar Volume (cm^3/mol):
219.0 (calculated-Le Bas method at normal boiling point)
164.7 (calculated-density)
Dissociation Constant pK_a:
2.77 (Tomlin 1994)
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
Entropy of Fusion, ΔS_{fus} (J/mol K):
Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F: 1.0

Water Solubility (g/m^3 or mg/L at 25°C or as indicated):
50.0 (Hartley Kidd 1987; Worthing & Hance 1991; Milne 1995; selected, Lohninger 1994)
50.0 (20–25°C, selected, Wauchope et al. 1992; Hornsby et al. 1996)

Vapor Pressure (Pa at 25°C or as indicated):
0.013 (20°C, Hartley & Kidd 1987)
0.013 (rm. temp., Worthing & Hance 1991)
0.013 (20–25°C, selected, Wauchope et al. 1992; Hornsby et al. 1996)

Henry's Law Constant (Pa·m^3/mol at 25°C):
0.0644 (calculated-P/C, this work)

Octanol/Water Partition Coefficient, log K_{OW}:
2.48–2.60 (Worthing & Hance 1991; Milne 1995)
3.36 (Tomlin 1994)
2.55 (selected, Hansch et al. 1995)

Bioconcentration Factor, log BCF:
1.83 (calculated-S as per Kenaga 1980, this work)
1.22 (calculated-K_{OW} as per Kenaga 1980, this work)

Sorption Partition Coefficient, log K_{OC}:
0.725 (sandy soil, Worthing & Hance 1991)
0.149 (silt loam, Worthing & Hance 1991)

3.00 (soil, 20–25°C, estimated, Wauchope et al. 1992; Hornsby et al. 1996)
3.00 (selected, Lohninger 1994)

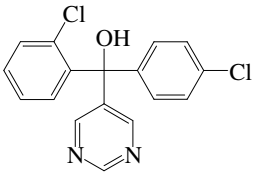
Environmental Fate Rate Constants, k, or Half-Lives, $t_{½}$:

Volatilization:
Photolysis:
Oxidation:
Hydrolysis: $t_{½}$ = 103 d at pH 6 (Worthing & Hance 1991);
$t_{½}$ = 12 d at pH 6, 45°C, $t_{½}$ = 103 d at pH 6, 25°C (Tomlin 1994).
Biodegradation: soil $t_{½}$ = 9.5 d under aerobic conditions and $t_{½}$ = 3 d under anaerobic conditions (Tomlin 1994).
Biotransformation:
Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants:

Half-Lives in the Environment:

Soil: $t_{½}$ = 9.5 d under aerobic, $t_{½}$ = 3 d under anaerobic conditions, field dissipation $t_{½}$ = 1 wk in sandy clay loam (Tomlin 1994);
field $t_{½}$ = 103 d (20–25°C, selected, Hornsby et al. 1996).

19.1.18 FENARIMOL



Common Name: Fenarimol
Synonym: Bloc, EL-222, Rimidin, Rubigan
Chemical Name: (±)-2,4′-dichloro-α-(pyrimidin-5-yl)benzhydryl alcohol; α-(2-chlorophenyl)-α-(4-chlorophenyl)-5-pyrimidinemethanol
CAS Registry No: 60168-88-9
Uses: as fungicide for control of powdery mildews in pome fruit, strawberries, vines, cucurbits, roses, and beet; also for control of scab on pome fruit, brown patch and snow mold of turf.
Molecular Formula: $C_{17}H_{12}Cl_2N_2O$
Molecular Weight: 331.195
Melting Point (°C):
118 (Lide 2003)
Boiling Point (°C):
Density (g/cm^3 at 20°C):
Molar Volume (cm^3/mol):
338.8 (calculated-Le Bas method at normal boiling point)
Dissociation Constant pK_a:
2.58 (Sangster 1993)
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
Entropy of Fusion, ΔS_{fus} (J/mol K):
Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F: 0.122 (mp at 118°C)

Water Solubility (g/m^3 or mg/L at 25°C or as indicated):
13.7 (Martin & Worthing 1977)
13.7 (at pH 7, Hartley & Kidd 1987; Worthing & Hance 1991; Tomlin 1994; Milne 1995)
14.0 (20–25°C, selected, Wauchope et al. 1992; Hornsby et al. 1996)
14.0 (selected, Lohninger 1994)

Vapor Pressure (Pa at 25°C or as indicated):
$< 1.3 \times 10^{-5}$ (Hartley & Kidd 1987)
1.30×10^{-5} (Worthing & Hance 1991)
2.93×10^{-5} (20–25°C, selected, Wauchope et al. 1992; Hornsby et al. 1996)
6.5×10^{-5} (vapor pressure balance, Tomlin 1994)

Henry's Law Constant (Pa·m^3/mol at 25°C or as indicated):
6.93×10^{-4} (20–25°C, calculated-P/C, this work)

Octanol/Water Partition Coefficient, log K_{OW}:
0.67 (shake flask, at pH 5.3, Martin & Edgington 1981)
–1.59 (shake flask-UV at pH 5, Barak et al. 1983)
3.70 (Stevens et al. 1988)
3.60 (shake flask-HPLC, Bateman et al. 1990)
3.69 (pH 7, Worthing & Hance 1991; Tomlin 1994; Milne 1995)
3.60 (selected, Hansch et al. 1995)
3.61 (RP-HPLC-RT correlation using short ODP column, Donovan & Pescatore 2002)

Bioconcentration Factor, log BCF:

2.16 (calculated-S, Kenaga 1980)

Sorption Partition Coefficient, log K_{OC}:

3.01 (calculated-S, Kenaga 1980)
2.78 (soil, 20–25°C, selected, Wauchope et al. 1992; Hornsby et al. 1996)
0.176–1.08 (soil, Tomlin 1994)
2.78 (estimated-chemical structure, Lohninger 1994)

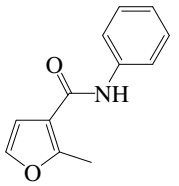
Environmental Fate Rate Constants, k, or Half-Lives, $t_{½}$:

Volatilization:
Photolysis: decomposed readily by sunlight (Tomlin 1994).
Oxidation:
Hydrolysis: $t_{½}$ = 28 d at 52°C and pH 3, 6 and 9 (Tomlin 1994).
Biodegradation: $t_{½}$ > 365 d under aerobic conditions in soil, and microbial degradation is accelerated by light (Tomlin 1994).
Biotransformation:
Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants:

Half-Lives in the Environment:

Soil: $t_{½}$ > 365 d under aerobic conditions in soil (28% sand, 14.7% clay, 57.3% silt and pH 6 (Tomlin 1994) field $t_{½}$ = 360 d (20–25°C, selected, Wauchope et al. 1992; Hornsby et al. 1996).

19.1.19 FENFURAM



Common Name: Fenfuram
Synonym: Panoram
Chemical Name: 2-methylfuran-3-carboxanilide; 2-methyl-3-furanilide; 2-methyl-N-phenyl-3-furancarboxamide
CAS Registry No: 24691-80-3
Uses: as fungicide for control of bunts and smuts (*Tilletie* and *Ustilago* spp.) in cereals, when applied as a seed treatment.
Molecular Formula: $C_{12}H_{11}NO_2$
Molecular Weight: 201.221
Melting Point (°C):
109–110 (Worthing & Hance 1991)
Boiling Point (°C):
Density (g/cm^3 at 20°C):
1.36 (Worthing & Hance 1991)
Molar Volume (cm^3/mol):
217.1 (calculated-Le Bas method at normal boiling point)
148.0 (calculated-density)
Dissociation Constant pK_a:
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
Entropy of Fusion, ΔS_{fus} (J/mol K):
Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F:

Water Solubility (g/m^3 or mg/L at 25°C or as indicated):
100 (Martin & Worthing 1977; Kenaga 1980)
100 (20°C, Hartley & Kidd 1987; Worthing & Hance 1991; Tomlin 1994)
100 (20–25°C, selected, Hornsby et al. 1996)

Vapor Pressure (Pa at 25°C or as indicated):
2.0×10^{-5} (20°C, Hartley & Kidd 1987)
2.0×10^{-5} (extrapolated to 20°C, Worthing & Hance 1991; Tomlin 1994)
2.0×10^{-5} (20–25°C, selected, Hornsby et al. 1996)

Henry's Law Constant (Pa·m^3/mol):

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

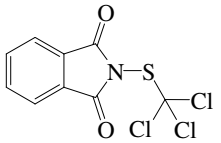
Bioconcentration Factor, log BCF:
1.66 (calculated-S, Kenaga 1980)

Sorption Partition Coefficient, log K_{OC}:
2.54 (calculated-S, Kenaga 1980)
2.48 (20–25°C, estimated, Hornsby et al. 1996)

Environmental Fate Rate Constants, k, or Half-Lives, $t_{½}$:
Hydrolysis: stable in neutral media, but hydrolyzed by strong acids and alkalis (Tomlin 1994).

Half-Lives in the Environment:
Soil: $t_{½}$ ~ 42 d (Hartley & Kidd 1987; Tomlin 1994);
field $t_{½}$ = 42 d (20–25°C, selected, Hornsby et al. 1996).

19.1.20 FOLPET



Common Name: Folpet
Synonym: ENT-26539, Faltan, Folpan, Folpel, Ftalan, Fungitrol, Orthophaltan, Phaltan, Spolacid, Thiophal, Vinicoll
Chemical Name: *N*-(trichloromethylthio)phthalimide; 2-[(trichloromethylthio]-1*H*-isoindole-1,3(2*H*)-dione
CAS Registry No: 133-07-3
Uses: fungicide for control of downy/powdery mildews, leaf spot diseases, etc.
Molecular Formula: $C_9H_4Cl_3NO_2S$
Molecular Weight: 296.558
Melting Point (°C):
177 (Worthing & Hance 1991; Tomlin 1994; Milne 1995; Lide 2003)
Boiling Point (°C):
Density (g/cm^3 at 20°C):
Molar Volume (cm^3/mol):
246.2 (calculated-Le Bas method at normal boiling point)
Dissociation Constant pK_a:
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
8.50 (DSC method, Plato 1972)
Entropy of Fusion, ΔS_{fus} (J/mol K):
Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F: 0.0323 (mp at 177°C)

Water Solubility (g/m^3 or mg/L at 25°C or as indicated):
1.0 (Martin & Worthing 1977)
1.0 (rm. temp., Hartley & Kidd 1987; Worthing & Hance 1991; Tomlin 1994; Milne 1995)

Vapor Pressure (Pa at 25°C or as indicated):
< 0.0013 (20°C, Hartley & Kidd 1987)
0.0013 (20°C, Worthing & Hance 1991; Tomlin 1994)

Henry's Law Constant (Pa·m^3/mol):

Octanol/Water Partition Coefficient, log K_{OW}:
3.63 (shake flask-UV, Briggs 1981)
2.85 (selected, Yoshioka et al. 1986)
2.85 (shake flask, log P database, Hansch & Leo 1987)
2.85 (recommended, Sangster 1993)
3.11 (Tomlin 1994)
2.85 (recommended, Hansch et al. 1995)

Bioconcentration Factor, log BCF:
1.91 (calculated-S, Kenaga 1980)
3.32 (earthworms, Lord et al. 1980)

Sorption Partition Coefficient, log K_{OC}:
1.78 (calculated-S, Kenaga 1980)
3.03 (reported as log K_{OM}, Briggs 1981)
3.27, 2.16 (soil, quoted exptl., calculated-fragment contribution method, Meylan et al. 1992)
3.27 (soil, calculated-MCI $^1\chi$, Sabljic et al. 1995)

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

Volatilization:

Photolysis: $t_{½}$ = 101 min in isopropanol, $t_{½}$ = 144 min in cyclohexene and $t_{½}$ = 1620 min in cyclohexane by UV-irradiation ($\lambda > 280$ nm): (Schwack & Flöβer-Müller 1990).

Oxidation:

Hydrolysis: hydrolyze at pH 7 with rates similar to captan, i.e., first-order rate constant $k = 6.5 \times 10^{-5}$ s^{-1} with $t_{½}$ = 2.96 h in a phosphate buffer solution at pH 7.07 and 28°C (Wolfe et al. 1976).

Biodegradation:

Biotransformation:

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

Half-Lives in the Environment:

Air:

Surface water: $t_{½}$ = 4.3 d (Tomlin 1994).

Groundwater:

Sediment:

Soil: $t_{½}$ = 4.3 d (Tomlin 1994).

Biota:

19.1.21 Formaldehyde

Common Name: Formaldehyde
Synonym: formalin, methanal, oxomethane
Chemical Name: formaldehyde
Uses: fungicide/bactericide; used as soil sterilant in mushroom houses and other areas; also used as a silage preservative.
CAS Registry No: 50-00-0
Molecular Formula: HCHO
Molecular Weight: 30.026
Melting Point (°C):
–92 (Weast 1982–83; Dean 1985: Lide 2003)
Boiling Point (°C):
–19.1 (Lide 2003)
Density (g/cm^3):
0.815 (Weast 1982–83)
0.815 (–20°C, Verschueren 1983; Dean 1985)
Acid Dissociation Constant, pK_a:
Molar Volume (cm^3/mol):
29.6 (calculated-Le Bas method at normal boiling point)
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
Entropy of Fusion, ΔS_{fus} (J/mol K):
Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F: 1.0

Water Solubility (g/m^3 or mg/L at 25°C):
1,220,000 (Dean 1985)
very soluble, up to 55% (Howard 1989)

Vapor Pressure (Pa at 25°C or as indicated):
1333 (–88°C, Verschueren 1983)
451030 (> 1 atmospheric pressure, Howard 1989)

Henry's Law Constant (Pa·m^3/mol at 25°C):
0.0331 (Dong et al. 1986)
0.0169 (Gaffney et al. 1987)
0.0298 (gas stripping-HPLC, Zhou & Mopper 1990)

Octanol/Water Partition Coefficient, log K_{OW}:
–0.75 (calculated-f const. per Rekker 1977, Deneer et al. 1988)
0.00 (calculated, Verschueren 1983)
0.35 (Howard 1989)
0.35 (recommended, Sangster 1989, 1993)

Bioconcentration Factor, log BCF:
no bioconcentration in fish and shrimp observed (Howard 1989)

Sorption Partition Coefficient, log K_{OC}:
0.365 (estimated-S as per Kenaga 1980, this work)

Environmental Fate Rate Constants, k, and Half-Lives, $t_{½}$:
Volatilization:
Photolysis: sunlight photolysis $t_{½}$ = 1.25–6.0 h, based on measured gas-phase photolysis by simulated sunlight (Calvert et al. 1972; Su et al. 1979; quoted, Howard et al. 1991).

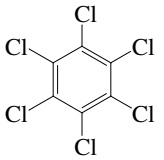
Oxidation: rate constant k = 3.2×10^{-16} cm^3 $molecule^{-1}$ s^{-1} for the vapor-phase reaction with NO_3 radicals in the atmosphere at (298 ± 1) K (Atkinson & Lloyd 1984; quoted, Carlier et al. 1986);
rate constant k = 4.50×10^{-14} cm^3 $molecule^{-1}$ s^{-1} for the vapor-phase reaction with HO_2 radicals in the atmosphere at 298 K (Baulch et al. 1984; quoted, Carlier et al. 1986);
rate constant k = 111.1×10^{-11} cm^3 $molecule^{-1}$ s^{-1} for the vapor-phase reaction with OH radicals in the atmosphere at 298 K (Baulch et al. 1984; quoted, Carlier et al. 1986);
atmospheric photooxidation $t_{½}$ = 7.13–71.3 h, based on measured rate constant for the vapor-phase reaction with OH radicals in air (Atkinson 1985; quoted, Howard et al. 1991);
aqueous photooxidation $t_{½}$ = 4,813–190,000 h, based on measured rate constant for the reaction with OH radicals in water (Dorfman & Adams 1973; quoted, Howard et al. 1991).
Hydrolysis: no hydrolyzable group (Howard et al. 1991).
Biodegradation: aqueous aerobic $t_{½}$ = 24–168 h, based on unacclimated aqueous aerobic biodegradation screening test data (Gellman & Heukelekian 1950; Heukelekian & Rand 1955; quoted, Howard et al. 1991); aqueous anaerobic $t_{½}$ = 96–672 h, based on unacclimated aqueous aerobic biodegradation half-life (Howard et al. 1991).
Biotransformation:
Bioconcentration Uptake (k_1) and Elimination (k_2) Rate Constants:

Half-Lives in the Environmental Compartments:

Air: photooxidation $t_{½}$ = 7.13–71.3 h, based on measured rate constant for the vapor-phase reaction with hydroxyl radicals in air (Atkinson 1985; quoted, Howard et al. 1991);
$t_{½}$ = 1.26–6.0 h, based on photolysis half-life in air (Howard et al. 1991).
Surface water: $t_{½}$ = 24–168 h, based on unacclimated aqueous aerobic biodegradation half-life (Howard et al. 1991).
Ground water: $t_{½}$ = 48–336 h, based on unacclimated aqueous aerobic biodegradation half-life (Howard et al. 1991).
Sediment:
Soil: $t_{½}$ = 24–168 h, based on unacclimated aqueous aerobic biodegradation half-life (Howard et al. 1991).
Biota:

19.1.22 HEXACHLOROBENZENE

(See also Chapter 6. Chlorobenzenes and other Halogenated Mononuclear Aromatics)



Common Name: Hexachlorobenzene
Synonym: HCB, perchlorobenzene, anticarie, Bunt-cure, Bunt-no-more, Julin's carbon chloride
Chemical Name: hexachlorobenzene
Uses: as fungicide for seed treatment to control common bunt and dwarf bunt of wheat.
CAS Registry No: 118-74-1
Molecular Formula: C_6Cl_6
Molecular Weight: 284.782
Melting Point (°C):
230.0 (Weast 1982–83)
228.83 (Lide 2003)
Boiling Point (°C):
322 (sublime, Weast 1982–83)
325 (Lide 2003)
Density (g/cm^3):
1.5691 (23.6°C, Weast 1982–83; Horvath 1982)
Molar Volume (cm^3/mol):
181.5 (23.6°C, calculated-density, Weast 1972–73; Horvath 1982)
221.4 (calculated-Le Bas method at normal boiling point)
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
28.744 (Tsonopoulos & Prausnitz 1971)
22.40 (Miller et al. 1984)
Entropy of Fusion, ΔS_{fus} (J/mol K):
57.32 (Tsonopoulos & Prausnitz 1971)
44.77 (Miller et al. 1984)
Fugacity Ratio (assuming ΔS_{fusion} = 56 J/mol K), F: 0.010 (mp at 228.83°C)
0.0090 (25°C, Miller et al. 1985)
0.0075, 0.0094 (20°C, 25°C, Suntio et al. 1988)

Water Solubility (g/m^3 or mg/L at 25°C):
0.005 (generator column-GC/ECD, Weil et al. 1974)
0.006 (shake flask-LSC/^{14}C, Lu & Metcalf 1975)
0.110 (shake flask-nephelometry, Hollifield 1979)
0.005 (shake flask-UV, Yalkowsky et al. 1979)
0.0034 (calculated-K_{OW}, Yalkowsky et al. 1979; Yalkowsky & Valvani 1980)
0.0035 (selected, Neely 1980)
0.036 (selected, Briggs 1981)
0.0039 (shake flask-GC, Könemann 1981)
0.0054 (generator column-GC/ECD, Hashimoto et al. 1982)
0.0012–0.014 (shake flask-GC/ECD, Hashimoto et al. 1982)
0.005 (recommended, Horvath 1982)
0.0051 (Deutsche Forschungsgemeinschaft 1983; Fischer et al. 1991)
0.0066 (selected, Yoshida et al. 1983b)
0.047 (generator column-GC/ECD, Miller et al. 1984; 1985)
0.0162 (calculated-UNIFAC activity coeff., Banerjee 1985)
0.005 (recommended, IUPAC 1985)

0.0146 (calculated-K_{OW} and HPLC-RT, Chin et al. 1986)
0.006–0.2 (calculated-K_{OW}, Anliker & Moser 1987)
0.00537 (calculated-UNIFAC activity coeff., Banerjee et al. 1990)

Vapor Pressure (Pa at 25°C or as indicated):
0.00028 (Sears & Hopke 1949)
0.0015 (Callahan et al. 1979)
0.0026 (selected, OECD 1979)
0.00145 (20°C, Kiltzer et al. 1979)
0.0023 (gas saturation-GC, Farmer et al. 1980)
0.0013 (selected, Neely 1980; Suntio et al. 1988; Nash 1989)
0.000453; 0.000167 (Klein et al. 1981)
0.00046 (evaporation rate, Dobbs & Cull 1982)
0.00121 (extrapolated, Antoine eq., Gückel et al. 1982)
0.0006 (20°C, evaporation rate & gravimetric, Gückel et al. 1982)
0.0024 (20°C, Deutsche Forschungsgemeinschaft 1983; Fischer et al. 1991)
0.00147 (selected, Yoshida et al. 1983b)
0.303; 0.159; 0.121 (supercooled liquid P_L, selected; GC-RT, Bidleman 1984)
0.0031 (selected, Mackay et al. 1985)
0.00147, 0.187 (20°C, selected, solid, supercooled liquid, Bidleman & Foreman 1987)
0.245 (selected, Suntio et al. 1988; quoted, Ballschmiter & Wittlinger 1991)
0.303, 0.127 (supercooled liquid, selected, Hinckley et al. 1990)
0.0023 (selected from Mackay et al. 1992, Mortimer & Connell 1995)
0.034; 0.141 (liquid P_L, GC-RT correlation; quoted lit., Donovan 1996)

Henry's Law Constant (Pa·m^3/mol at 25°C or as indicated):
68.2 (20°C, Callahan et al. 1979)
5.07 (calculated-P/C, Mackay & Shiu 1981)
131.3 (batch stripping, Atlas et al. 1982)
68.9 (20°C, calculated, Mabey et al. 1982)
12.16 (calculated-P/C, Calamari et al. 1983)
62.0 (calculated-P/C, Yoshida et al. 1983b)
139 (calculated-P/C, Bobra et al. 1985)
48.6 (20°C, batch stripping, Oliver 1985)
133, 115.9 (observed, calculated-QSAR, Nirmalakhandan & Speece 1988)
7.12 (20°C, calculated-P/C, Suntio et al. 1988)
11.0 (calculated, Nash 1989)
139.0 (calculated-P/C, Fischer et al. 1991)

Octanol/Water Partition Coefficient, log K_{OW}:
6.18 (Neely et al. 1974; selected, McKim et al. 1985)
4.13 (radioisotope tracer-^{14}C, Lu & Metcalf 1975)
6.51 (calculated-f const., Rekker 1977; quoted, Harnish et al. 1983)
6.18 (selected, Callahan et al. 1979; Neuhauser et al. 1985)
4.13 (Hansch & Leo 1979)
5.0, 6.27 (shake flask-GC, HPLC-k′ correlation, Könemann et al. 1979; selected, Figueroa & Simmons 1991)
6.44 (calculated-f constant, Könemann et al. 1979; Könemann 1981; selected, Opperhuizen 1986)
5.23 (HPLC-RT correlation, Veith et al. 1979a; selected, Mackay 1982; Freitag et al. 1985)
6.18 (HPLC-RT, Veith et al. 1979b; quoted, Veith & Kosian 1982; Ryan et al. 1988; Saito et al. 1992)
6.53 (calculated-f const., Yalkowsky et al. 1979,1983; Yalkowsky & Valvani 1980; Valvani & Yalkowsky 1980; selected, Miller et al. 1984)
5.23 (selected, Kenaga & Goring 1980; selected, Yoshida et al. 1983b)
5.44 (selected, Briggs 1981)
6.22 (HPLC-RT correlation, McDuffie 1981)

5.50 (shake flask-GC, Chiou et al. 1982; Chiou 1985; selected, Oliver & Niimi 1983; Oliver & Charlton 1984; Bobra et al. 1985; Hawker & Connell 1985; Oliver 1987a,b & c; Geyer et al. 1987; Suntio et al. 1988; Connell & Hawker 1988; Thomann 1989; Hawker 1990; Ballschmiter & Wittlinger 1991; Fischer et al. 1991)
5.66 (HPLC-RT correlation, Hammers et al. 1982)
5.40 (shake flask-GC, Watarai et al. 1982; quoted, Suntio et al. 1988)
6.13–6.27, 5.66 (range, mean, shake flask method, Eadsforth & Moser 1983)
6.27–6.48, 6.38 (range, mean, HPLC method, Eadsforth & Moser 1983)
5.0, 5.19 (selected, calculated, Kaiser 1983; Kaiser et al. 1984)
5.89 (selected, Calamari et al. 1983)
6.42 (calculated-f const., Veith et al. 1983)
5.23, 4.61 (selected, calculated-molar refraction, Yoshida et al. 1983)
5.47 (generator column-GC/ECD, Miller et al. 1984, 1985; Kerler & Schönherr 1988; Mackay & Paterson 1991)
5.75; 5.70–5.79 (quoted lit.; HPLC-RV correlation, Garst & Wilson 1984; Garst 1984)
5.20, 5.23, 5.44, 5.50, 5.55 (reported lit. values, Geyer et al. 1984)
5.47 (Sarna et al. 1984)
5.47, 6.86, 6.42 (selected, HPLC/MS, calculated-π const., Burkhard et al. 1985)
5.61 (selected, Mackay et al. 1985)
5.75 (selected OECD value, Brooke et al. 1986)
5.6, 5.9 (HPLC-RV correlation, Brooke et al. 1986)
6.51, 6.18 (selected, calculated-K_{OW} & HPLC-RT, Chin et al. 1986)
6.92 (HPLC-k′ correlation, De Kock & Lord 1987)
5.64 (HPLC-k′ correlation, Mailhot 1987)
5.45 (selected, Gobas et al. 1987, 1989; Travis & Arms 1988)
5.66 (correlated, Isnard & Lambert 1988, 1989)
5.47; 6.42, 6.55, 6.22, 5.34, 4.86, 4.75 (selected exptl.; calculated-π const., f const., HPLC-RT correlation, MW, MCI χ, TSA, Doucette & Andren 1988)
5.47; 5.37 (selected; calculated-V_I and solvatochromic parameters, Kamlet et al. 1988)
5.50 (shake flask-GC, Pereira et al. 1988)
5.31, 6.58 (selected, calculated-UNIFAC activity coeff., Banerjee & Howard 1988)
6.68 (calculated-f const., De Bruijn et al. 1989)
5.73 (shake flask/slow stirring-GC, De Bruijn et al. 1989; De Bruijn & Hermens 1990; quoted, Bintein & Devillers 1994; Sijm et al. 1995)
5.44 (recommended, Sangster 1993)
5.73 (recommended, Hansch et al. 1995)
6.42 (quoted Pomona-database, Müller & Kördel 1996)

Bioconcentration Factor, log BCF:

3.89 (rainbow trout, calculated-k_1/k_2, Neely et al. 1974)
3.09 (fish, Körte et al. 1978)
4.27, 3.73, 4.34 (fathead minnow, rainbow trout, green sunfish, Veith et al. 1979)
5.46 (guppy, lipid basis, Könemann & van Leeuwen 1980; selected, Chiou 1985)
4.27 (fish, Giam et al. 1980)
1.20 (rats, adipose tissue, Geyer et al. 1980)
3.93, 2.46 (fish, flowing water, static water, Kenaga & Goring 1980; Kenaga 1980a)
3.61, 2.45 (calculated from water solubility, K_{OC}, Kenaga 1980a)
4.39, 4.20 (algae, calculated, Geyer et al. 1981)
3.91 (fish, correlated, Mackay 1982)
4.27, 3.89 (fathead minnow, rainbow trout, selected, Bysshe 1982)
4.60 (guppy, calculated-MCI χ, Koch 1983)
4.08–4.30 (rainbow trout, Oliver & Niimi 1983)
5.16–5.37 (rainbow trout, lipid basis, Oliver & Niimi 1983; selected, Chiou 1985)
4.31 (calculated-K_{OW}, Calamari et al. 1983)
3.93 (calculated-K_{OW}, Yoshida et al. 1983b)

4.39, 3.36, 4.54 (algae, fish, activated sludge, Klein et al. 1984)
4.39, 3.83 (algae: exptl., calculated, Geyer et al. 1984; quoted, Wang et al. 1996)
4.27 (fathead minnow, 25°C, calculated, Davies & Dobbs 1984; Anliker & Moser 1987)
4.34, 3.74 (green sunfish, rainbow trout, 15°C, calculated, Davies & Dobbs 1984)
4.39, 3.36, 4.54 (algae, fish, sludge, Klein et al. 1984)
4.54 (activated sludge, Freitag et al. 1984; Halfon & Reggiani 1986)
4.39, 3.41, 4.54 (algae, fish, activated sludge, Freitag et al. 1985)
3.05 (fish, selected, Hawker & Connell 1986)
2.62–2.97 (human fat, lipid basis, Geyer et al. 1987)
2.44–2.79 (human fat, wet weight, Geyer et al. 1987)
4.41 (algae, Mailhot 1987)
4.34 (fathead minnow, Carlson & Kosian 1987)
4.38, 4.30 (worms, fish, Oliver 1987a)
3.48 (fish-normalized, Tadokoro & Tomita 1987)
4.19 (guppy, calculated, Gobas et al. 1987)
5.46 (guppy-lipid phase, calculated-K_{OW}, Gobas et al. 1987, 1989)
6.42, 6.71, 5.96, 5.98 (field data-lipid base: Atlantic croakers, blue crabs, spotted sea trout, blue catfish, Pereira et al. 1988)
–1.35 (beef, reported as biotransfer factor log B_b, Travis & Arms 1988)
–2.07 (milk, reported as biotransfer factor log B_m, Travis & Arms 1988)
–0.32 (vegetable, reported as biotransfer factor log B_v, Travis & Arms 1988)
5.30 (guppy-lipid phase, calculated-K_{OW}, Gobas et al. 1989)
3.90, 4.19 (fish, selected, Connell & Hawker 1988; Hawker 1990)
5.30 (guppy, correlated, Gobas et al. 1989)
3.53 (picea omorika, Reischl et al. 1989)
3.57 (fish, calculated, Figueroa & Simmons 1991)
4.37, 4.16 (rainbow trout, guppy, Saito et al. 1992)
4.27, 4.37 (fathead minnows, Saito et al. 1992)
4.25 (*Chlorella pyrenoidosa*, Sijm et al. 1995)
4.39, 3.18 (*Chlorella fusca, Myriophyllum spicatum*, Wang et al. 1996)

Sorption Partition Coefficient, log K_{OC}:

3.59 (Kenaga & Goring 1980; Kenaga 1980a; selected, Lyman 1982; Yoshida 1983b; Nash 1989)
4.45 (Kenaga 1980a)
4.44, 4.21, 3.59 (estimated-S, K_{OW}, BCF, Lyman 1982)
6.08 (calculated, Mabey et al. 1982)
3.59 (selected, Bysshe 1982; Lyman et al. 1982)
2.56 (shake flask-GC/ECD, Speyer soil, Freundlich isotherm, Rippen et al. 1982)
2.70 (shake flask-GC/ECD, Alfisol, Freundlich isotherm, Rippen et al. 1982)
4.58 (calculated-K_{OW}, Calamari et al. 1983)
5.90 (field data, Oliver & Charlton 1984)
4.90 (bottom sediment, Karickhoff & Morris 1985a)
5.10 (calculated-K_{OW}, Oliver & Charlton 1984)
5.2–6.7, 6.1 (suspended sediment, average, Oliver 1987c)
5.80 (algae > 50 μm, Oliver 1987c)
6.0–6.5, 6.3; 5.1 (Niagara River plume, range, mean; calculated-K_{OW}, Oliver 1987b)
4.77 (HPLC-k′, Hodson & Williams 1988)
4.70; 3.53 (HPLC-screening method; calculated-PCKOC fragment method, Müller & Kördel 1996)

Sorption Partition Coefficient, log K_{OM}:

4.25 (shake flask-GC, soil-organic matter, Briggs 1981)
5.50 (Niagara River-organic matter, Oliver & Charlton 1984)

Sorption Partition Coefficient, log K_P:

3.04–4.51 (sediment suspensions, Karickhoff & Morris 1985b; selected, Brusseau & Rao 1989)
5.11 (simulation of Oliver 1985, Brusseau & Rao 1989)

Half-Lives in the Environment:

Air: degradation rate constant of 0.0144 h^{-1} (Mackay et al. 1985; quoted, Mackay & Paterson 1991); 3753–37530 h, based on estimated photooxidation half-life (Atkinson 1987); 17000 h (selected from Mackay et al. 1992, Mortimer & Connell 1995).

Surface Water: 23256–50136 h, based on estimated unacclimated aqueous aerobic biodegradation half-life (Beck & Hansen 1974); 1.4–50 d estimated, 0.3–3 d for river water and 30–300 d for lakes, estimated from persistence (Zoeteman et al. 1980); 55000 h (selected from Mackay et al. 1992, Mortimer & Connell 1995).

Ground Water: 46512–100272 h, based on unacclimated aqueous aerobic biodegradation half-life (Beck & Hansen 1974); 30–300 d, estimated from persistence (Zoeteman et al. 1980).

Soil: 23256–50136 h, based on unacclimated aerobic soil grab sample data (Beck & Hansen, 1974); > 50 d (Ryan et al. 1988).

Sediment: 55000 h (selected from Mackay et al. 1992, Mortimer & Connell 1995).

Biota: half-life in rainbow trout, > 224 d (Niimi & Cho 1980); in subadult rainbow trout-calculated to be 210 d at 4°C, 80 d at 12°C and 70 d at 18°C (Niimi & Palazzo 1985); in worms at 8°C, 27 d (Oliver 1987a); picea omorika, 30 d (Reischl et al. 1989); 163 h, clearance from fish (Neely 1980).

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

Volatilization/Evaporation: 3.45×10^{-10} mol/m^2·h (Gückel et al. 1982).

Photolysis:

Oxidation: rate constant in air, 1.44×10^{-2} h^{-1} (Brown et al. 1975; selected, Mackay et al. 1985); photooxidation half-life in air: 3753–37530 h, based on estimated rate constant for the vapor-phase reaction with hydroxyl radicals in air (Atkinson 1987).

Hydrolysis: not expected to be important, based on $k_h = 0$, observed after 13 d at pH 3, 7, 11 and 85°C (Ellington et al. 1987).

Biodegradation: aqueous aerobic biodegradation half-life: 23256–50136 h, based on unacclimated aerobic soil grab sample data (Beck & Hansen 1974); anaerobic aqueous biodegradation half-life: 93024–200544 h, based on estimated unacclimated aqueous aerobic biodegradation half-life (Beck & Hansen 1974) and degradation rate constant in soil, 1.9×10^{-5} h^{-1} (Beck & Hansen 1974; selected, Mackay et al. 1985; Mackay & Paterson 1991); not significant in an aerobic environment, and no significant degradation rate (Tabak et al. 1981; Mills et al. 1982).

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

k_1: 18.76 h^{-1} (trout muscle, Neely et al. 1974)
k_2: 0.00238 h^{-1} (trout muscle, Neely et al. 1974)
k_1: 10000 d^{-1} (guppy, Könemann & van Leeuwen 1980)
k_1: 22.5 h^{-1} (guppy, selected, Hawker & Connell 1985)
k_1: 18.8 h^{-1} (trout, selected, Hawker & Connell 1985)
k_1: 540.0 d^{-1} (fish, selected, Opperhuizen 1986)
k_2: 0.00510, 0.00818, 0.00640, 0.0047 d^{-1} (rainbow trout, calculated-fish mean body weight, Barber et al. 1988)
$1/k_2$: 420 h (trout, selected, Hawker & Connell 1985)
log k_1: 2.73 d^{-1} (fish, selected, Connell & Hawker 1988)
log k_1: 2.65 d^{-1} (fish, selected, Connell & Hawker 1988)
log $1/k_2$: 1.24 d^{-1}(fish, selected, Connell & Hawker 1988)
log k_2: –1.24 d^{-1} (fish, calculated-K_{OW}, Thomann 1989)
k_1: 0.049 h^{-1} (uptake of mayfly-sediment model II, Gobas et al. 1989b)
k_2: 0.023 h^{-1} (depuration of mayfly-sediment model II, Gobas et al. 1989b)
k_1 10489 h^{-1} (*Chlorella fusca*, Wang et al. 1996)
k_2: 0.424 h^{-1} (*Chlorella fusca*, Wang et al. 1996)

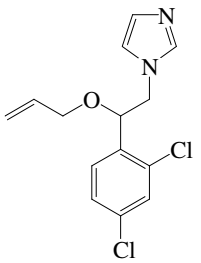
k_1: 6.558 h^{-1} (*Myriophyllum spicatum*, Wang et al. 1996)
k_2: 0.00429 h^{-1} (*Myriophyllum spicatum*, Wang et al. 1996)

Sediment Exchange Rate Constant:
0.026–1.2 d^{-1} (natural sediment, Karickhoff & Morris 1985).

Sediment Burial Rate Constant:
4.6×10^{-6} h^{-1} (Di Toro et al. 1981; selected, Mackay et al. 1985)

Stratospheric Diffusion Rate Constant:
1.7×10^{-6} h^{-1} (Mackay et al. 1985)

19.1.23 IMAZALIL



Common Name: Imazalil
Synonym: Bromazil, Deccozil, Enilconazole, Fecundal, Freshgard, Fungaflor, Fungazil, R 23979
Chemical Name: 1-(β-allyloxy-2,4-dichlorophenylethyl)imidazole; 1-[2-(2,4-dichlorophenyl)-2-(2-propenyloxy)ethyl]-1*H*-imidazole
CAS Registry No: 35554-44-0
Uses: as fungicide for control of a wide range of fungal diseases on fruit, vegetables, and ornamentals; also used as a seed dressing, for control of diseases of cereal and cotton, etc.
Molecular Formula: $C_{14}H_{14}Cl_2N_2O$
Molecular Weight: 297.129
Melting Point (°C):
50.0 (Hartley & Kidd 1987; Milne 1995; Lide 2003)
Boiling Point (°C):
> 340 (Worthing & Hance 1991; Tomlin 1994)
dec (Lide 2003)
Density (g/cm^3 at 20°C):
1.243 (23°C, Hartley & Kidd 1987; Worthing & Hance 1991; Milne 1995)
1.348 (26°C, Tomlin 1994)
Molar Volume (cm^3/mol):
318.8 (calculated-Le Bas method at normal boiling point)
239.1 (calculated-density)
Dissociation Constant pK_a:
6.53 (Worthing & Hance 1991)
7.47 (pK_b Tomlin 1994)
Enthalpy of Vaporization, ΔH_V (kJ/mol):
96.53 (Rordorf 1989)
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
29.1 (Rordorf 1989)
Entropy of Fusion, ΔS_{fus} (J/mol K):
90 (Rordorf 1989)
Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F: 0.568 (mp at 50°C)

Water Solubility (g/m^3 or mg/L at 25°C or as indicated):
1400 (20°C, Hartley & Kidd 1987; Milne 1995)
180 (pH 7.6, Worthing & Hance 1991; Tomlin 1994)
1400 (20–25°C, selected, Augustijn-Beckers et al. 1994; Hornsby et al. 1996)

Vapor Pressure (Pa at 25°C or as indicated and reported temperature dependence equations.):
9.30×10^{-6} (20°C, Hartley & Kidd 1987)
1.60×10^{-4}, 8.0×10^{-3}, 0.230, 4.20, 53.0 (25, 50, 70, 100, 125°C, gas saturation-GC, Rordorf 1989)
log (P_S/Pa) = 18.21 – 6562.5/(T/K); measured range 53.–129°C (solid, gas saturation-GC, Rordorf 1989)
log (P_L/Pa) = 13.52 – 5042.4/(T/K); measured range 53.6–129°C (liquid, gas saturation-GC, Rordorf 1989)
1.60×10^{-4} (20°C, Worthing & Hance 1991)
1.58×10^{-4} (20°C, Tomlin 1994)
9.30×10^{-6} (20–25°C, selected, Augustijn-Beckers et al. 1994; Hornsby et al. 1996)

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

1.97×10^{-6} (20–25°C, calculated-P/C, this work)

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

3.82 (Worthing & Hance 1991; Milne 1995)
3.82 (pH 9.2, Tomlin 1994)
3.82 (recommended, Hansch et al. 1995)

Bioconcentration Factor, log BCF:

4.57 (calculated-S as per Kenaga 1980, this work)
2.70 (calculated-K_{OW} as per Kenaga 1980, this work)

Sorption Partition Coefficient, log K_{OC}:

2.26 (clay loam, Worthing & Hance 1991; Tomlin 1994)
2.32 (sandy loam, Worthing & Hance 1991; Tomlin 1994)
1.83 (sandy soil, Worthing & Hance 1991; Tomlin 1994)
3.60 (soil, 20–25°C, selected, Augustijn-Beckers et al. 1994; Hornsby et al. 1996)
3.73 (soil, calculated-MCI $^1\chi$, Sabljic et al. 1995)
3.73; 3.52 (soil, quoted obs.; estimated-general model using molecular descriptors, Gramatica et al. 2000)

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

Volatilization:
Photolysis: stable to light under normal storage conditions (Tomlin 1994).
Oxidation:
Hydrolysis: very stable to hydrolysis in dilute acids and alkalis at room temperature (Tomlin 1994).
Biodegradation:
Biotransformation:
Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants:

Half-Lives in the Environment:

Soil: $t_{½}$ = 30–170 d (Tomlin 1994);
field $t_{½}$ = 150 d (20–25°C, selected, Augustijn-Beckers et al. 1994; Hornsby et al. 1996).

19.1.24 MANCOZEB

Common Name: Mancozeb
Synonym: dithane ultra, Dithane M45, Dithane SPC, Fore, Manzate, Manseb, Maezin, Nemispor, Penncozeb, Vondozeb, Zimanat, zine manganese ethylenebis[dithiocarbamate]
Chemical Name: manganese ethylenebis(dithiocarbamate) (polymeric) complex with zinc salt
CAS Registry No: 8018-01-7
Uses: fungicide
Molecular Formula: $(C_4H_6MnN_2S_4)_x(Zn)_y$
Molecular Weight:
Melting Point (°C):
192–194 (dec., Hartley & Kidd 1987; Montgomery 1993; Milne 1995)
192–204 (dec., Tomlin 1994)
Boiling Point (°C):
Density (g/cm^3 at 20°C):
Molar Volume (cm^3/mol):
Dissociation Constant pK_a:
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
Entropy of Fusion, ΔS_{fus} (J/mol K):
Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F:

Water Solubility (g/m^3 or mg/L at 25°C or as indicated):
insoluble (Spencer 1982; Hartley & Kidd 1987; Milne 1995)
6–20 (Montgomery 1993)
6–20 (Tomlin 1994)
6.0 (20–25°C, selected, Wauchope et al. 1992; Hornsby et al. 1996)

Vapor Pressure (Pa at 25°C):
negligible (Hartley & Kidd 1987; Tomlin 1994)
0 (selected, Wauchope et al. 1992; Hornsby et al. 1996)

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

Octanol/Water Partition Coefficient, log K_{OW}:
3.12–3.70 (Montgomery 1993)

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

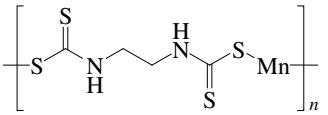
Bioconcentration Factor, log BCF:

Sorption Partition Coefficient, log K_{OC}:
2.93–3.21 (soil, calculated, Montgomery 1993)
> 3.30 (soil, Wauchope et al. 1992; Hornsby et al. 1996)
> 3.30 (soil, Tomlin 1994)

Environmental Fate Rate Constants, or Half-Lives:
Hydrolysis: unstable in acidic media (Hartley & Kidd 1987); $t_{½}$ = 20 d at pH 5, $t_{½}$ = 17 h at pH 7, $t_{½}$ = 34 h at pH 9 (Montgomery 1993; Tomlin 1994).

Half-Lives in the Environment:
Soil: field $t_{½}$ = 70 d (Wauchope et al. 1992; Hornsby et al. 1996);
$t_{½}$ ~. 6–15 d (Tomlin 1994).

19.1.25 MANEB



Common Name: Maneb
Synonym: MEB, Dithane, Bravo
Chemical Name: manganese ethylenebis(dithiocarbamate)
CAS Registry No: 12427-38-2
Uses: fungicide
Molecular Formula: $(C_4H_6MnN_2S_4)_x$
Molecular Weight: $(265.302)_x$
Melting Point (°C):
200 (dec, Lide 2003)
Boiling Point (°C):
Density (g/cm^3 at 20°C):
1.92 (Spencer 1982; Worthing & Walker 1983; Tomlin 1994)
Molar Volume (cm^3/mol):
Dissociation Constant pK_a:
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
Entropy of Fusion, ΔS_{fus} (J/mol K):
Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F:

Water Solubility (g/m^3 or mg/L at 25°C or as indicated):
slightly soluble (Spencer 1982)
insoluble (Worthing & Walker 1983; Hartley & Kidd 1987; Tomlin 1994; Milne 1995)
slight, 200, 6 (quoted, Wauchope et al. 1992)
6.0 (20–25°C, estimated and selected, Wauchope et al. 1992; Hornsby et al. 1996)

Vapor Pressure (Pa at 25°C or as indicated):
negligible (20°C, Worthing 1983; Hartley & Kidd 1987; Tomlin 1994)
0 (selected, Wauchope et al. 1992; Hornsby et al. 1996)

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

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

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

Bioconcentration Factor, log BCF:
2.40 (activated sludge, Freitag et al. 1983)
2.40, 2.26, < 1.0 (activated sludge, algae, *Golden ide*, Freitag et al. 1985)

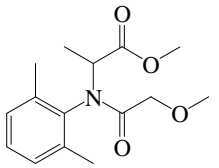
Sorption Partition Coefficient, log K_{OC}:
> 3.30 (soil, estimated, Wauchope et al. 1994; Hornsby et al. 1996)

Environmental Fate Rate Constants, k, or Half-Lives, $t_{½}$:
Volatilization:
Photolysis:
Oxidation:
Hydrolysis: rapidly hydrolyzed in acidic media (Hartley & Kidd 198);
$t_{½}$ < 24 h at pH 5.7 or 9 (Tomlin 1994).
Biodegradation:
Biotransformation:
Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants:

Half-Lives in the Environment:

Air: $t_{½}$ = 7–14 d, green house experiment in microagroecosystem chamber (Nash & Beall 1980).
Surface water: rapidly hydrolyzed in acidic media (Hartley & Kidd 1987).
Groundwater:
Sediment:
Soil: $t_{½}$ = 36 d in soil (sandy loam with pH 6.7),
green house experiment in microagroecosystem chamber (Nash & Beall 1980);
$t_{½}$ ~ 25 d in loamy sand in dark, aerobic conditions (Tomlin 1994);
field $t_{½}$ ~ 70 d (estimated, Wauchope et al. 1992; Hornsby et al. 1996).
Biota: $t_{½}$ = 6.4 d for beans, $t_{½}$ = 7.4 d for tomatoes (Nash & Beall 1980);
$t_{½}$ = 14 d on tomato leaves, green house experiment in microagroecosystem chamber (Nash & Beall 1980);
$t_{½}$ = 10 d for tomato fruit, $t_{½}$ = 4.5 d for tomato leaves in the field, $t_{½}$ = 3 d for tomatoes and soybean leaves in microagroecosystem (Nash 1983).

19.1.26 METALAXYL



Common Name: Metalaxyl
Synonym: Apron, CGA 48988, Ridomil, Subdue
Chemical Name: methyl *N*-(2-methoxyacetyl)-*N*-(2,6-xylyl)-DL-alaninate; methyl-*N*-(2,6-dimethylphenyl)-*N*-(methoxyacetyl)-DL-alaninate
CAS Registry No: 57837-19-1
Uses: fungicide to control of foliar and soil-borne diseases caused by *Peronosporates* on a wide range of crops; also used to treat seeds, etc.
Molecular Formula: $C_{15}H_{21}NO_4$
Molecular Weight: 279.333
Melting Point (°C):
71 (Lide 2003)
Boiling Point (°C):
Density (g/cm^3 at 20°C):
1.21 (Hartley & Kidd 1987; Worthing & Hance 1991; Montgomery 1993)
Molar Volume (cm^3/mol):
328.2 (calculated-Le Bas method at normal boiling point)
230.9 (calculated-density)
Dissociation Constant pK_a: << 0 (Tomlin 1994)
Enthalpy of Vaporization, ΔH_V (kJ/mol):
89.73 (Rordorf 1989)
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
27.4 (Rordorf 1989)
Entropy of Fusion, ΔS_{fus} (J/mol K):
79 (Rordorf 1989)
Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F: 0.354 (mp at 71°C)

Water Solubility (g/m^3 or mg/L at 25°C or as indicated):
7100 (quoted, Burkhard & Guth 1981)
7000 (shake flask-HPLC, Ellgehausen et al. 1981)
7100 (20°C, Hartley & Kidd 1987; Worthing & Hance 1991; Montgomery 1993)
7000 (quoted-Yalkowsky & Dannenfelser 1994, Pinsuwan et al. 1995)
8400 (20–25°C, selected, Wauchope et al. 1992; Hornsby et al. 1996)
8400 (selected, Lohninger 1994)
8400 (22°C, Tomlin 1994)

Vapor Pressure (Pa at 25°C or as indicated and reported temperature dependence equations):
2.93×10^{-4} (20°C, volatilization rate, Burkhard & Guth 1981)
2.93×10^{-4} (20°C, Hartley & Kidd 1987; Worthing & Hance 1991)
7.50×10^{-4}, 2.90×10^{-2}, 0.67, 10.0, 110 (25, 50, 70, 100, 125°C, gas saturation-GC, Rordorf 1989)
$\log (P_S/Pa) = 17.423 - 4687.6/(T/K)$; measured range 32.7–69.7°C (solid, gas saturation-GC, Rordorf 1989)
$\log (P_L/Pa) = 13.243 - 4687.6/(T/K)$; measured range 72.3–130°C (liquid, gas saturation-GC, Rordorf 1989)
7.5×10^{-4} (20–25°C, selected, Wauchope et al. 1992; Hornsby et al. 1996)
2.93×10^{-4} (20°C, Montgomery 1993)
7.5×10^{-4} (Tomlin 1994)

Henry's Law Constant (Pa·m^3/mol at 25°C or as indicated):
1.155 (20°C, evaporation rate, Burkhard & Guth 1981)
2.48×10^{-5} (calculated-P/C, this work)

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

1.65	(shake flask, Ellgehausen et al. 1980, 1981)
1.53	(shake flask, log P Database, Hansch & Leo 1987)
1.60	(shake flask at pH 7, Stevens et al. 1988)
1.70	(shake flask at pH 7, Baker et al. 1992)
1.59	(recommended value, Sangster 1993)
1.75	(Tomlin 1994)
1.693	(calculated-f const., Pinsuwan et al. 1995)
1.65	(recommended, Hansch et al. 1995)
1.40	(RP-HPLC-RT correlation using short ODP column, Donovan & Pescatore 2002)

Bioconcentration Factor, log BCF:

0.03	(*Daphnia magna,* wet wt. basis, Ellgehausen et al. 1980)

Sorption Partition Coefficient, log K_{OC}:

1.59	(av. of 3 soils, Sharom & Edgington 1982)
2.26	(av. of 7 soils, Carris 1983)
3.22	(av. of 12 soils, calculated-linearized Freundlich Isotherm, Sukop & Cogger 1992)
1.70	(soil, 20–25°C, estimated, Wauchope et al. 1992; Hornsby et al. 1996)
1.53–1.84	(soil, Montgomery 1993)
1.70	(estimated-chemical structure, Lohninger 1994)
1.57	(soil, calculated-MCI $^1\chi$, Sabljic et al. 1995)
1.57; 2.05	(soil, quoted obs.; estimated-general model using molecular descriptors, Gramatica et al. 2000)

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

Volatilization: k(calc) = 0.71 ng cm^{-2} h^{-1} and k(measured) = 0.35 ng cm^{-2} h^{-1} from moist soils at 20°C (Burkhard & Guth 1981).

Photolysis: irradiated by UV at 290 nm in the presence of hydrogen peroxide and titanium dioxide, respectively, in aqueous solution resulted in 29% and 84% transformation in 2.5 h (Moza et al. 1994).

Oxidation:

Hydrolysis: stable in neutral and acidic media at room temp., calculated $t_{½}$ > 200 d at 20°C and pH 1, $t_{½}$ = 115 d at pH 9 and $t_{½}$ = 12 d at pH 10 (Worthing & Hance 1991; Montgomery 1993; Tomlin 1994).

Biodegradation: overall degradation rate constant k = 0.0081 h^{-1} with $t_{½}$ = 85.5 h in sewage sludge and k = 0.0217 d^{-1} with $t_{½}$ = 31.9 d in garden soil (Müller & Buser 1995);

rate constant k = 0.060 d^{-1} for *R*-metalaxyl (fungicidally active) in soil expt incubated with *rac*-metalaxyl, k = 0.080 d^{-1} in soil expt incubated with *R*-metalaxyl; rate constant k = 0.015 d^{-1} for *S*-metalaxyl (fungicidally inactive) in soil expt incubated with *rac*-metalaxyl, k = 0.010/0.12 d^{-1} for in soil expt incubated with *S*-metalaxyl (Buser et al. 2002);

degradation rate constants for formulated racemic metalaxyl were found to be 0.039 d^{-1} with $t_{½}$ = 18 d for German soil, k = 0.018 d^{-1} with $t_{½}$ = 38 d for Cameroonian soil; for unformulated racemic metalaxyl rate constants were: k = 0.039 d^{-1} with $t_{½}$ = 18 d for German soil, k = 0.019 d^{-1} with $t_{½}$ = 17 d form Cameroonian soil; and for formulated R-metalaxyl rate constants were: k = 0.041 d^{-1} with $t_{½}$ = 17 d for German soil, k = 0.018 d^{-1} with $t_{½}$ = 38 d from Cameroonian soil. For soil incubated with metalaxyl enantiomers, R-metalaxyl degraded faster (k = 0.064 d^{-1}) than S-metalaxyl (k = 0.033 d^{-1}) in German soil when spiked with formulated racemic metalaxyl, while S-metalaxyl degraded faster (k = 0.026 d^{-1}) than R-metalaxyl (k = 0.014 d^{-1}) in Cameroonian soil when spiked with formulated racemic retalaxyl (Monkiedje et al. 2003).

Biotransformation:

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

Half-Lives in the Environment:

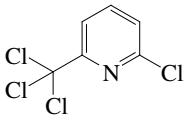
Soil: degradation $t_{½}$ = 39.5 d in garden soil (Müller & Buser 1995);

field $t_{½}$ = 70 d (20–25°C, selected, Wauchope et al. 1992; Hornsby et al. 1996);

residual activity in soil is about 70–90 d (Tomlin 1994);

degradation $t_{½}$ = 17–38 d of the racemic mixture and enantiomers of metalaxyl in controlled incubation experiments in typical soils from Germany and Cameroon. (Monkiedje et al. 2003).

19.1.27 NITRAPYRIN



Common Name: Nitrapyrin
Synonym: N-Serve
Chemical Name: 2-chloro-6-(trichloromethyl)pyridine
CAS Registry No: 1929-82-4
Uses: bactericide
Molecular Formula: $C_6H_3Cl_4N$
Molecular Weight: 230.907
Melting Point (°C):
63 (Lide 2003)
Boiling Point (°C):
136–137.5/11 mmHg (Tomlin 1994)
Density (g/cm^3 at 25°C):
1.744 (Montgomery 1993)
1.579 (Tomlin 1994)
Molar Volume (cm^3/mol):
Dissociation Constant pK_a:
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
Entropy of Fusion, ΔS_{fus} (J/mol K):
Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F: 0.424 (mp at 63°C)

Water Solubility (g/m^3 or mg/L at 25°C or as indicated):
40 (quoted, Briggs 1981)
40 (22°C, Spencer 1982; Worthing & Walker 1983, 1987; Montgomery 1993; Tomlin 1994)
92; 54 (generator column-RI; HPLC-RT correlation, Swann et al. 1983)
40 (20–25°C, selected, Wauchope et al. 1992; Hornsby et al. 1996)

Vapor Pressure (Pa at 25°C or as indicated):
0.37 (23°C, Spencer 1982; Worthing & Walker 1983, 1987)
0.373 (20°C, Montgomery 1993)
0.373 (20–25°C, Wauchope et al. 1992; Hornsby et al. 1996)

Henry's Law Constant (Pa·m^3/mol at 25°C):
216 (calculated-P/C, Montgomery 1993)

Octanol/Water Partition Coefficient, log K_{OW}:
3.02 (shake flask-UV, Briggs 1981)
3.02–3.41 (Montgomery 1993)
3.325 (Tomlin 1994)
3.41 (recommended, Hansch et al. 1995)
3.41 (LOGPSTAR or CLOGP data, Sabljic et al. 1995)

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

Bioconcentration Factor, log BCF or log K_B:
1.87, 1.36 (calcd-solubility, K_{OW}, Kenaga 1980b)

Sorption Partition Coefficient, log K_{OC}:
1.93–2.42; 2.19 (quoted: 10 soils range; mean, Briggs 1981)
2.0 (Cottenham soil, shake flask-GC, 20°C, Briggs 1981)

2.76 (calculated, Kenaga 1980b)
2.66 (average of 3 soils, HPLC-RT correlation, McCall et al. 1980)
2.64, 2.68, 2.66; 2.66 (Commeree soil, Tracy soil, Catlin soil; mean, HPLC-RT, Swann et al. 1981; quoted, McCall et al. 1981)
2.24–2.76 (quoted literature range, Wauchope et al. 1992)
2.76 (soil, Wauchope et al. 1992; Hornsby et al. 1996)
2.62–2.68 (soil, Montgomery 1993)
2.40–3.96 (soil, Tomlin 1994)
2.62 (soil, calculated-MCI $^{1}\chi$, Sabljic et al. 1995)

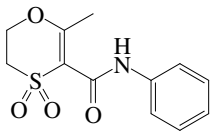
Environmental Fate Rate Constants, k, or Half-Lives, $t_{½}$:

Volatilization:
Photolysis: water photolysis $t_{½}$ = 2 h (Tomlin 1994).
Oxidation:
Hydrolysis: hydrolysis $t_{½}$ = 2 d at pH 7 (Tomlin 1994).
Biodegradation:
Biotransformation:
Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants:

Half-Lives in the Environment:

Air:
Surface water: hydrolysis $t_{½}$ = 2 d at pH 7, water photolysis $t_{½}$ = 2 h (Tomlin 1994).
Groundwater:
Sediment:
Soil: field $t_{½}$ = 10 d (Wauchope et al. 1992; Hornsby et al. 1992);
aerobic soil metabolism $t_{½}$ = 6.42 d, anaerobic metabolism $t_{½}$ ~ 2.5 h (Tomlin 1994).
Biota:

19.1.28 OXYCARBOXIN



Common Name: Oxycarboxin
Synonym: DCMOD, Oxycarboxine
Chemical Name: 5,6-dihydro-2-methyl-1,4-oxathi-ine-3-carboxanilide 4,4-dioxide; 5,6-dihydro-2-methyl-*N*-phenyl-1,4-oxathin-3-carboxamide 4,4-dioxide
CAS Registry No: 5259-88-1
Uses: as fungicide for control of rust diseases on ornamentals, cereals, and nursery trees, etc.
Molecular Formula: $C_{12}H_{13}NO_4S$
Molecular Weight: 267.301
Melting Point (°C):
129 (Lide 2003)
Boiling Point (°C):
Density (g/cm^3 at 20°C): 1.14 (Tomlin 1994)
Molar Volume (cm^3/mol):
261.4 (calculated-Le Bas method at normal boiling point)
234.5 (calculated-density)
Dissociation Constant pK_a:
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
Entropy of Fusion, ΔS_{fus} (J/mol K):
Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F: 0.054 (mp at 129°C)

Water Solubility (g/m^3 or mg/L at 25°C or as indicated):
1000 (Martin & Worthing 1977; quoted, Kenaga 1980)
1000 (Hartley & Kidd 1987; Worthing & Hance 1991; Tomlin 1994)
1000 (20–25°C, selected, Wauchope et al. 1992; Hornsby et al. 1996)
1000 (selected, Lohninger 1994)

Vapor Pressure (Pa at 25°C or as indicated):
0.0010 (20°C, Hartley & Kidd 1987)
< 133 (20°C, Worthing & Hance 1991)
5.60×10^{-6} (Tomlin 1994)
1.33×10^{-3} (20–25°C, selected, Wauchope et al. 1992; Hornsby et al. 1996)

Henry's Law Constant (Pa·m^3/mol at 25°C or as indicated):
3.56×10^{-4} (20–25°C, calculated-P/C, this work)

Octanol/Water Partition Coefficient, log K_{OW}:
0.74 (shake flask-UV, Mathre 1971)
0.74 (recommended, Sangster 1993)
0.772 (Tomlin 1994)
0.740 (selected, Hansch et al. 1995)
1.13 (RP-HPLC-RT correlation using short ODP column, Donovan & Pescatore 2002)

Bioconcentration Factor, log BCF:
1.11 (calculated-S, Kenaga 1980)

Sorption Partition Coefficient, log K_{OC}:
1.99 (calculated-S, Kenaga 1980)

1.98 (soil, estimated, Wauchope et al. 1992; Hornsby et al. 1996)
1.98 (selected, Lohninger 1994)

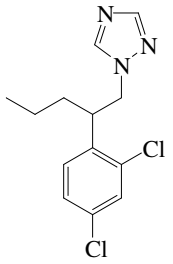
Environmental Fate Rate Constants, k, or Half-Lives, $t_{½}$:

Hydrolysis: $t_{½}$ = 44 d at pH 6, 25°C (Tomlin 1994).

Half-Lives in the Environment:

Soil: $t_{½}$ = 2.5–8 wk in sandy loam by aerobic soil metabolism (Tomlin 1994); field $t_{½}$ = 20 d (Wauchope et al. 1992; Hornsby et al. 1996).

19.1.29 PENCONAZOLE



Common Name: Penconazole
Synonym: Award, CGA 71818, Topas, Topaz, Topaze
Chemical Name: 1-(2,4-dichloro-β-propylphenylethyl)-1*H*-1,2,4-triazole;1-[2-(2,4-dichlorophenyl)pentyl]-1*H*-1,2,4-triazole
CAS Registry No: 66246-88-6
Uses: as fungicide for control of pathogenic *Ascomycetes, Basidiomycetes* and *Deuteromycetes* (especially powdery mildews) on vines, cucurbits, pome fruit, ornamentals and vegetables.
Molecular Formula: $C_{13}H_{15}Cl_2N_3$
Molecular Weight: 284.184
Melting Point (°C):
60.0 (Hartley & Kidd 1987; Worthing & Hance 1991)
62.1 (Rordorf 1989)
57.6–60.3 (Tomlin 1994)
Boiling Point (°C):
Density (g/cm^3 at 20°C): 1.30 (Tomlin 1994)
Molar Volume (cm^3/mol):
312.3 (calculated-Le Bas method at normal boiling point)
218.6 (calculated-density)
Dissociation Constant pK_a:
1.51 (Tomlin 1994)
Enthalpy of Vaporization, ΔH_V (kJ/mol):
91.45 (Rordorf 1989)
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
27.1 (Rordorf 1989)
Entropy of Fusion, ΔS_{fus} (J/mol K):
81 (Rordorf 1989)
Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F: 0.454 (mp at 60°C)

Water Solubility (g/m^3 or mg/L at 25°C or as indicated):
70 (20°C, Hartley & Kidd 1987; Worthing & Hance 1991)
73 (20°C, Tomlin 1994)

Vapor Pressure (Pa at 25°C or as indicated and reported temperature dependence equations):
0.00021 (20°C, Hartley & Kidd 1987; Worthing & Hance 1991; Tomlin 1994)
3.70×10^{-4}, 1.30×10^{-2}, 0.28, 4.0, 41.0 (25, 50, 70, 100, 125°C, gas saturation-GC, Rordorf 1989)
$\log (P_S/Pa) = 16.671 - 5995.1/(T/K)$; measured range 36.6–58.3°C (solid, gas saturation-GC, Rordorf 1989)
$\log (P_L/Pa) = 13.088 - 4777.0/(T/K)$; measured range 60.9–129°C (liquid, gas saturation-GC, Rordorf 1989)

Henry's Law Constant (Pa·m^3/mol at 25°C or as indicated):
0.00082 (20°C, calculated-P/C, this work)

Octanol/Water Partition Coefficient, log K_{OW}:
3.40 (shake flask-HPLC, Bateman et al. 1990)
3.20 (shake flask-HPLC, Chamberlain et al. 1991)

3.72 (pH 5.7, Tomlin 1994)
3.40, 3.20 (Sangster 1993)
3.40, 3.50 (Hansch et al. 1995)

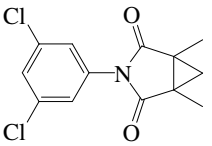
Bioconcentration Factor, log BCF:
1.75 (20°C, calculated-S as per Kenaga 1980, this work)

Sorption Partition Coefficient, log K_{OC}:
2.62 (20°C, calculated-S as per Kenaga 1980, this work)

Environmental Fate Rate Constants, k, or Half-Lives, $t_{½}$:
Hydrolysis: stable to hydrolysis pH 1–13, and to temperature up to 350°C (Tomlin 1994).

Half-Lives in the Environment:
Soil: half-life is several months (Tomlin 1994).

19.1.30 PROCYMIDONE



Common Name: Procymidone
Synonym: S-7131, Sialex, Sumiboto, Sumilex, Sumisclex
Chemical Name: *N*-(3,5-dichlorophenyl)-1,2-dimethylcyclopropane-1,2-dicarboximide; 3-(3,5-dichlorophenyl)-1,5-dimethyl-3-azabicyclo[3,1,0]hexane-2,4-dione
CAS Registry No: 32809-16-8
Uses: as fungicide for control of *Botrytis, Sclerotinia, Monilia,* and *Helminthosporium* spp. on fruit, vines, vegetables, cereals and ornamentals, etc.
Molecular Formula: $C_{13}H_{11}Cl_2NO_2$
Molecular Weight: 284.138
Melting Point (°C):
166 (Lide 2003)
Boiling Point (°C):
Density (g/cm^3 at 20°C):
1.452 (25°C, Hartley & Kidd 1987; Tomlin 1994; Milne 1995)
Molar Volume (cm^3/mol):
225.9 (calculated-Le Bas method at normal boiling point)
195.7 (calculated-density)
Dissociation Constant pK_a:
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
Entropy of Fusion, ΔS_{fus} (J/mol K):
Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F: 0.0414 (mp at 166°C)

Water Solubility (g/m^3 or mg/L at 25°C or as indicated):
4.50 (Hartley & Kidd 1987; Worthing & Hance 1991; Tomlin 1994; Milne 1995)
4.50 (20–25°C, selected, Augustijn-Beckers et al. 1994; Hornsby et al. 1996)

Vapor Pressure (Pa at 25°C or as indicated):
0.018 (Hartley & Kidd 1987)
0.011 (20°C, Worthing & Hance 1991)
0.018, 0.0105 (20, 25°C, Tomlin 1994)
0.0187 (20–25°C, selected, Augustijn-Beckers et al. 1994; Hornsby et al. 1996)

Henry's Law Constant (Pa·m^3/mol at 25°C or as indicated):
1.181 (20–25°C, calculated-P/C, this work)

Octanol/Water Partition Coefficient, log K_{OW}:
3.14 (26°C, Worthing & Hance 1991; Tomlin 1994; Milne 1995)
3.0 (selected, Hansch et al. 1995)

Bioconcentration Factor, log BCF:
2.42 (calculated-S as per Kenaga 1980, this work)

Sorption Partition Coefficient, log K_{OC}:
3.18 (soil, estimated, Augustijn-Beckers et al. 1994; Hornsby et al. 1996)
3.28 (soil, calculated-S as per Kenaga 1980, this work)

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

Photolysis: when irradiation with UV light, $\lambda \geq 290$ nm, for procymidone solution (2 ppm): 9% and 11% photodegraded in 1 h, in the presence of 1 ppm humic acid and 1 ppm fulvic acid, respectively; rapid degradation with $t_{½}$ = 3 min in the presence of TiO_2 (20 ppm), but degraded slowly as 9% transformation in 2 h with Fe_2O_3 (100 ppm). (Hustert & Moza 1997)

Half-Lives in the Environment:

Air:

Surface water: photodegradation of procymidone solution (2 ppm), $t_{½}$ = 3 min in the presence of TiO_2 (20 ppm) when irradiated with UV light (Hustert & Moza 1997)

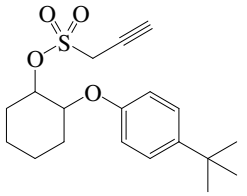
Groundwater:

Sediment:

Soil: persists for ca. 4–12 weeks (Hartley & Kidd 1987; Tomlin 1994);
field $t_{½}$ = 7 d (Augustijn-Beckers et al. 1994; Hornsby et al. 1996).

Biota:

19.1.31 PROPARGITE



Common Name: Propargite
Synonym: Comite, Omite
Chemical Name: 2-[4-(1,1-dimethylethyl)phenoxy]cyclohexyl 2-propynyl sulfite
CAS Registry No: 2312-35-8
Uses: acaricide
Molecular Formula: $C_{16}H_{26}O_4S$
Molecular Weight: 360.472
Melting Point (°C):
dark brown liquid (Hartley & Kidd 1987)
Boiling Point (°C):
Density (g/cm^3 at 25°C):
1.085–1.115 (Hartley & Kidd 1987; Worthing & Walker 1983, 1987)
Molar Volume (cm^3/mol):
Dissociation Constant pK_a:
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
Entropy of Fusion, ΔS_{fus} (J/mol K):
Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F: 1.0

Water Solubility (g/m^3 or mg/L at 25°C or as indicated):
practically insoluble in water (Worthing & Walker 1983, 1987)
0.5 (20°C, Hartley & Kidd 1987)
0.50 (20–25°C, selected, Wauchope et al. 1992; Hornsby et al. 1996)
0.5 (20–25°C, Majewski & Capel 1995)

Vapor Pressure (Pa at 25°C or as indicated):
400 (20°C, Worthing & Walker 1983, 1987; Hartley & Kidd 1987)
0.4 (20–25°C, selected, Wauchope et al. 1992; Hornsby et al. 1996)
0.4 (20–25°C, quoted, Majewski & Capel 1995)

Henry's Law Constant (Pa·m^3/mol at 25°C or as indicated)
280 (20–25°C, Majewski & Capel 1995)

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

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

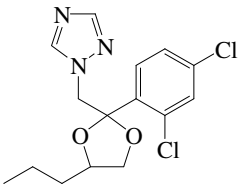
Bioconcentration Factor, log BCF or log K_B:

Sorption Partition Coefficient, log K_{OC}:
3.60 (soil, estimated, Wauchope et al. 1992; Hornsby et al. 1996)

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

Half-Lives in the Environment:
Soil: field $t_{½}$ = 40 and 56 d, the recommended $t_{½}$ = 56 d (Wauchope et al. 1992; Hornsby et al. 1996).

19.1.32 PROPICONAZOLE



Common Name: Propiconazole
Synonym: Alamo, Banner, CGA 64250, Desmel, Orbit, Practis, Radar, Spire, Tilt
Chemical Name: (±)-1-[2-(2,4-dichlorophenyl)-4-propyl-1,3-dioxalan-2-ylmethyl]-1H-1,2,4-triazole; 1-[2-(2,4-dichlorophenyl)-4-propyl-1,3-dioxalan-2-ylmethyl]-1H-1,2,4-triazole
CAS Registry No: 60207-90-1
Uses: as fungicide for control of mildews, rusts on cereals, ornamentals, fruits and other crops; and also used for other diseases of turf and grass seed crops, etc.
Molecular Formula: $C_{15}H_{17}Cl_2N_3O_2$
Molecular Weight: 342.221
Melting Point (°C): liquid
Boiling Point (°C):
180 (at 0.1 mmHg, Hartley & Kidd 1987; Worthing & Hance 1991; Tomlin 1994; Milne 1995)
Density (g/cm^3 at 20°C):
1.27 (Hartley & Kidd 1987; Worthing & Hance 1991; Milne 1995)
1.29 (20°C, Tomlin 1994)
Molar Volume (cm^3/mol):
358.6 (calculated-Le Bas method at normal boiling point)
267.3 (calculated-density)
Dissociation Constant pK_a:
1.09 (Tomlin 1994)
Enthalpy of Vaporization, ΔH_V (kJ/mol):
106.8 (Rordorf 1989)
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
Entropy of Fusion, ΔS_{fus} (J/mol K):
Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F: 1.0

Water Solubility (g/m^3 or mg/L at 25°C or as indicated):
110 (20°C, Hartley & Kidd; Worthing & Hance 1991; Milne 1995)
100 (20°C, Tomlin 1994)
110 (20–25°C, selected, Wauchope et al. 1992; Hornsby et al. 1996)
110 (selected, Lohninger 1994)
110 (20°C, quoted, Siebers et al. 1994)

Vapor Pressure (Pa at 25°C or as indicated and reported temperature dependence equations):
0.00013 (20°C, Hartley & Kidd 1987)
5.60×10^{-5}, 1.60×10^{-3}, 0.027, 0.32, 28.0 (25, 50, 70, 100, 125°C, gas saturation-GC, Rordorf 1989)
log (P_L/Pa) = 14.468 – 5581.2/(T/K); measured range 32.5–124°C (liquid, gas saturation-GC, Rordorf 1989)
0.000133 (20°C, Worthing & Hance 1991)
5.6×10^{-5} (20–25°C, Wauchope et al. 1992; Hornsby et al. 1996)
5.6×10^{-5} (Tomlin 1994)

Henry's Law Constant (Pa·m^3/mol at 25°C or as indicated):
4.0×10^{-4} (20°C, calculated-P/C, Siebers et al. 1994)
0.00017 (20–25°C, calculated-P/C, this work)

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

3.50	(Bateman et al. 1990; quoted, Sangster 1993)
3.72	(Siebers et al. 1994)
3.72	(pH 6.6, Tomlin 1994)
3.50	(selected, Hansch et al. 1995)
3.50	(LOGPSTAR or CLOGP data, Sabljic et al. 1995)
3.33	(RP-HPLC-RT correlation using short ODP column, Donovan & Pescatore 2002)

Bioconcentration Factor, log BCF:

Sorption Partition Coefficient, log K_{OC}:

2.81	(soil, selected, Wauchope et al. 1992; Hornsby et al. 1996)
2.52	(soil, calculated-S as per Kenaga 1980, this work)
2.81	(selected, Lohninger 1994)
3.39	(soil, calculated-MCI $^1\chi$, Sabljic et al. 1995)
3.39; 3.62	(soil, quoted obs.; estimated-general model using molecular descriptors, Gramatica et al. 2000)

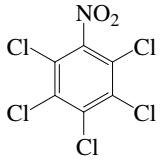
Environmental Fate Rate Constants, k, or Half-Lives, $t_{½}$:

Hydrolysis: no significant hydrolysis (Tomlin 1994).

Half-Lives in the Environment:

Air:
Surface water: $t_{½}$ = 25–85 d in aerobic aquatic systems at 25°C (Tomlin 1994).
Groundwater:
Sediment:
Soil: field $t_{½}$ = 110 d (Wauchope et al. 1992; Hornsby et al. 1996);
$t_{½}$ = 40–70 d in aerobic soils at 25°C (Tomlin 1994).
Biota:

19.1.33 QUINTOZENE



Common Name: Quintozene
Synonym: Avicol, Batrilex, Brassicol, Chinozan, earthcide, Fartox, Folosan, Fomac 2, Fungiclor, Kobutol, KOBU, KP 2, Marisan forte, Olpisan, PCNB, Pentagen, Phomasan, PKhNB, Quinosan, Quinocene, saniclor 30, Terraclor, Terrafun
Chemical Name: pentachloronitrobenzene
CAS Registry No: 82-68-8
Uses: as fungicide for seed and soil treatment, for control of *Botrytis, Rhizoctonia*, and *Sclerotinia* spp. on brassicas, vegetables, ornamentals and other crops, and *Telletia caries* of wheat.
Molecular Formula: $C_6Cl_5NO_2$
Molecular Weight: 295.335
Melting Point (°C):
144 (Lide 2003)
Boiling Point (°C):
328 (dec, Lide 2003)
Density (g/cm^3 at 20°C):
1.718 (25°C, Spencer 1982; Hartley & Kidd 1987; Worthing & Hance 1991; Milne 1995)
1.907 (21°C, Tomlin 1994)
Molar Volume (cm^3/mol):
207.3 (calculated-Le Bas method at normal boiling point)
154.9 (calculated-density)
Dissociation Constant pK_a:
Enthalpy of Vaporization, ΔH_V (kJ/mol):
77.3 (Rordorf 1989)
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
18 (Rordorf 1989)
Entropy of Fusion, ΔS_{fus} (J/mol K):
43 (Rordorf 1989)
Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F: 0.0680 (mp at 144°C)

Water Solubility (g/m^3 or mg/L at 25°C or as indicated):
practically insoluble (Spencer 1982; Worthing & Hance 1991; Milne 1995)
0.55 (20–25°C, shake flask-GC, Kanazawa 1981)
0.44 (20°C, Hartley & Kidd 1987; Pait et al. 1992; Milne 1995)
0.40 (Davies & Lee 1987)
0.44 (20–25°C, selected, Wauchope et al. 1992; Hornsby et al. 1996)
0.10 (selected, Lohninger 1994)
0.10 (20°C, Tomlin 1994)

Vapor Pressure (Pa at 25°C or as indicated and reported temperature dependence equations):
0.0151 (Spencer 1982)
6.60×10^{-3} (20°C, Hartley & Kidd 1987)
8.40×10^{-3}, 0.16, 1.90, 17.0, 110 (25, 50, 70, 100, 125°C, gas saturation-GC, Rordorf 1989)
$\log (P_S/Pa) = 14.34 - 4893.9/(T/K)$; measured range 49.9–140°C (solid, gas saturation-GC, Rordorf 1989)
$\log (P_L/Pa) = 12.234 - 4037.9/(T/K)$; measured range 150–196°C (liquid, gas saturation-GC, Rordorf 1989)
1.80 (Worthing & Hance 1991)
0.0147 (20–25°C, selected, Wauchope et al. 1992; Hornsby et al. 1996)
0.0127 (Tomlin 1994)

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

0.3718 (known LWAPC of Kawamoto & Urano 1989, Meylan & Howard 1991)
0.4812 (calculated-bond contribution method LWAPC, Meylan & Howard 1991)

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

4.22 (20°C, shake flask-GC, Kanazawa 1981)
5.21 (HPLC-RT correlation, McDuffie 1981)
5.00 (HPLC-RT correlation, Ohori & Ihashi 1987)
5.18 (HPLC-RT correlation, Kawamoto & Urano 1989)
4.77; 5.40 (shake flask-GC; calculated-fragment const., Niimi et al. 1989)
5.02 (RP-HPLC-RT correlation, Saito et al. 1993)
4.64 (recommended, Sangster 1993)
5.0–6.0 (Tomlin 1994)
4.22 (selected, Hansch et al. 1995)
4.89 (Pomona-database, Müller & Kördel 1996)
5.01 (RP-HPLC-RT correlation, Nakamura et al. 2001)
5.30 (RP-HPLC-RT correlation using short ODP column, Donovan & Pescatore 2002)

Bioconcentration Factor, log BCF:

2.38 (topmouth gudgeon, Kanazawa 1981)
3.49, 3.65, 3.06 (algae, activated sludge, fish, Freitag et al. 1985)
2.23 (rainbow trout, Niimi et al. 1989)
2.91 (quoted, Pait et al. 1992)

Sorption Partition Coefficient, log K_{OC}:

4.30 (correlated-Freundlich Isotherm, Kawamoto & Urano 1989)
4.30, 3.38 (soil, quoted exptl., calculated-MCI χ and fragments contribution, Meylan et al. 1992)
3.70 (soil, estimated, Wauchope et al. 1992; Hornsby et al. 1996)
4.34 (soil, HPLC-screening method, mean value of different stationary and mobile phases, Kördel et al. 1993, 1995)
3.78, 3.47 (for adsorption: silt loam, sand, Tomlin 1994)
3.98, 3.52 (for desorption: silt loam, sand, Tomlin 1994)
4.30 (estimated-chemical structure, Lohninger 1994)
4.34; 3.38 (HPLC-screening method; calculated-PCKOC fragment method, Müller & Kördel 1996)

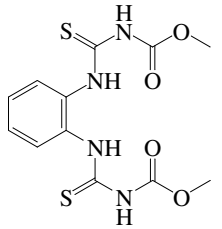
Environmental Fate Rate Constants, k, or Half-Lives, $t_{½}$:

Biodegradation: rate constant k(aerobic) = 0.16 d^{-1} with $t_{½}$ = 4.3 d at 20°C by aerobic activated sludge and k(anaerobic) = 0.16 d^{-1} with $t_{½}$ = 4.3 d at 20°C by anaerobic microorganisms cultivated an artificial sewage (Kawamoto & Urano 1990)
rate constant k = 6.5 d^{-1} with $t_{½}$ = 0.11 d (Corrigendum, Kawamoto & Urano 1991).

Half-Lives in the Environment:

Air:
Surface water: biodegradation $t_{½}$ = 4.3 d at 20°C by aerobic activated sludge or anaerobic microorganisms cultivated by an artificial sewage (Kawamoto & Urano 1990)
Groundwater:
Sediment:
Soil: $t_{½}$ ~ 4–10 months (Hartley & Kidd 1987; Tomlin 1994),
$t_{½}$ = 4 d (Pait et al. 1992);
field $t_{½}$ = 21 d (Wauchope et al. 1992; Hornsby et al. 1996).
Biota:

19.1.34 THIOPHANATE-METHYL



Common Name: Thiophanate-methyl
Synonym: Cerobin, Enovit, Fumidor, Fungitox, Fungo, Fungus Fighter, Labilite, Mildothane, Neotosin, NF-44, Pelt 44, Seal 7 Heal, Sigma, Sipcaplant, Sipcasan, Topsin M, Trevin
Chemical Name: dimethyl 4,4′-(*o*-phenylene)bis(3-thioallophanate; dimethyl [1,2-phenylene-bis(monocarbonothioyl)]-biscarbamate
Uses: fungicide/wound protectant
CAS Registry No: 23564-05-8
Molecular Formula: $C_{12}H_{14}N_4O_4S_2$
Molecular Weight: 342.394
Melting Point (C):
172 (dec., Worthing & Hance 1991; Tomlin 1994; Milne 1995; Lide 2003)
Boiling Point (°C):
Density (g/cm^3 at 20°C):
Molar Volume (cm^3/mol):
344.0 (calculated-Le Bas method at normal boiling point)
Dissociation Constant pK_a:
7.28 (Worthing & Hance 1991; Tomlin 1994)
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
Entropy of Fusion, ΔS_{fus} (J/mol K):
Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F: 0.0361 (mp at 172°C)

Water Solubility (g/m^3 or mg/L at 25°C or as indicated):
3.50 (20°C, Hartley & Kidd 1987)
26.6 (Worthing & Hance 1991)
3.50 (20–25°C, selected, Wauchope et al. 1992; Hornsby et al. 1996)
3.50 (selected, Lohninger 1994)
26.6 (20°C, Milne 1995)

Vapor Pressure (Pa at 25°C or as indicated):
$< 1.0 \times 10^{-5}$ (20°C, Hartley & Kidd 1987)
$< 1.33 \times 10^{-5}$ (20–25°C, selected, Wauchope et al. 1992; Hornsby et al. 1996)
9.50×10^{-6} (Tomlin 1994)

Henry's Law Constant (Pa·m^3/mol at 25°C):
0.0013 (calculated-P/C, this work)

Octanol/Water Partition Coefficient, log K_{OW}:
1.40 (Worthing & Hance 1991; Milne 1995)
1.50 (Tomlin 1994)
1.40 (selected, Hansch et al. 1995)
1.86 (RP-HPLC-RT correlation, pH 3.5, Hu et al. 1997)

Bioconcentration Factor, log BCF:

Sorption Partition Coefficient, log K_{OC}:

0.079	(Worthing & Hance 1991)
3.26	(20–25°C, estimated, Wauchope et al. 1992; Hornsby et al. 1996)
3.26	(selected, Lohninger 1994)

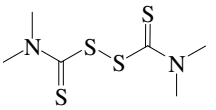
Environmental Fate Rate Constants, k, or Half-Lives, $t_{½}$:

Hydrolysis: stable neutral, aqueous solution, $t_{½}$ = 24.5 h at pH 9, 22°C (Tomlin 1994).

Half-Lives in the Environment:

Soil: field $t_{½}$ = 10 d (Wauchope et al. 1992; Hornsby et al. 1996);
persistence ca. 3–4 weeks (Tomlin 1994).

19.1.35 THIRAM



Common Name: Thiram
Synonym: Aapirol, Aatiram, Accel TMT, Accelerator T, Aceto TETD, Arasan, Atiram, Cyuram, Delsan, Ekagom TB, ENT-987, Falitiram, Fermide, Fernacol, Fernasan, Fernide, Thiuram, TMTD
Chemical Name: tetramethylthiuram disulphide; bis(dimethylthiocarbomoyl) disulfide
CAS Registry No: 137-26-8
Uses: fungicide and also as seed disinfectant.
Molecular Formula: $C_6H_{12}N_2S_4$
Molecular Weight: 240.432
Melting Point (°C):
155.6 (Lide 2003)
Boiling Point (°C):
129 (20 mmHg, Howard 1991)
310–315 (15 mmHg, Montgomery 1993)
Density (g/cm^3 at 20°C):
1.29 (Spencer 1982; Worthing & Hance 1991; Montgomery 1993; Tomlin 1994; Milne 1995)
Molar Volume (cm^3/mol):
256.6 (calculated-Le Bas method at normal boiling point)
186.4 (calculated-density,)
Dissociation Constant pK_a:
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
Entropy of Fusion, ΔS_{fus} (J/mol K):
Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F: 0.0523 (mp at 155.6°C)

Water Solubility (g/m^3 or mg/L at 25°C or as indicated):
17.4 (22°C, Spencer 1973, 1982)
30 (Martin & Worthing 1977; Worthing & Walker 1987, Worthing & Hance 1991)
30 (Hartley & Kidd 1987; Montgomery 1993; Milne 1995)
30 (20–25°C, selected, Wauchope et al. 1992; Hornsby et al. 1996)
18 (room temp., Tomlin 1994)

Vapor Pressure (Pa at 25°C or as indicated):
negligible (Hartley & Kidd 1987; Worthing & Hance 1991)
0.00133 (Halfon et al. 1996)
< 0.00133 (20–25°C, selected, Wauchope et al. 1992; Hornsby et al. 1996)
0.307 (Tomlin 1994)

Henry's Law Constant (Pa·m^3/mol at 25°C):
< 0.008 (calculated-P/C, Lyman et al. 1982)
0.0107 (calculated-P/C, this work)

Octanol/Water Partition Coefficient, log K_{OW}:
1.73 (Tomlin 1994)

Bioconcentration Factor, log BCF:
1.96 (calculated-S, Kenaga 1980)
1.96 (calculated-S, Lyman et al. 1982; quoted, Howard 1991)

Sorption Partition Coefficient, log K_{OC}:

2.83	(calculated-S, Kenaga 1980)
2.83	(calculated-S, Lyman et al. 1982; quoted, Howard 1991)
2.83	(20–25°C, selected, Wauchope et al. 1992; Hornsby et al. 1996)
2.82–3.39	(soil, Montgomery 1993)
2.83	(estimated-chemical structure, Lohninger 1994)

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

Volatilization:

Photolysis:

Oxidation: assuming an ambient hydroxyl radical concn. of 8.0×10^5 mol/cm^3, the photooxidation reaction $t_{½}$ ~ 26.6 d at 25°C (estimated, GEMS 1986; quoted, Howard 1991).

Hydrolysis: $t_{½}$ = 5.3 d was estimated based on exptl. rate k = 5.0×10^{-3} h^{-1} (Ellington et al. 1988; quoted, Howard 1991; Montgomery 1993);
$t_{½}$ = 128 d at pH 4, $t_{½}$ = 18 d at pH 7 and $t_{½}$ = 9 h at pH 9 (Tomlin 1994).

Biodegradation:

Biotransformation:

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

Half-Lives in the Environment:

Air: assuming an ambient hydroxyl radical concn. of 8.0×10^5 mol/cm^3, the photooxidation reaction $t_{½}$ ~ 26.6 d at 25°C (estimated, GEMS 1986; quoted, Howard 1991).

Surface water: calculated hydrolysis $t_{½}$ = 5.3 d at pH 7 (Ellington et al. 1988);
hydrolysis $t_{½}$ = 128 d, $t_{½}$ = 18 d and $t_{½}$ = 9 h at pH 4,7 and 9 (Tomlin 1994).

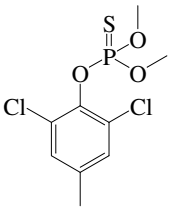
Groundwater:

Sediment:

Soil: $t_{½}$ = 15 d in soil (Halfon et al. 1996);
field $t_{½}$ = 15 d (20–25°C, selected, Wauchope et al. 1992; Hornsby et al. 1996);
degradation $t_{½}$ = 0.5 d in sandy soil at pH 6.7 (Tomlin 1994).

Biota:

19.1.36 TOLCLOFOS-METHYL



Common Name: Tolclofos-methyl
Synonym: Risolex, Rizolex, S-3349
Chemical Name: *O*-2,6-dichloro-*p*-tolyl *O,O*-dimethyl phosphorothioate; *O*-(2,6-dichloro-4-methylphenyl) *O,O*-dimethyl phosphorothioate
CAS Registry No: 57018-04-9
Uses: as fungicide for control of soil-borne diseases caused by *Rhizoctonia, Sclerotium* and *Typhula* spp.; also used as a seed, bulb or tuber treatment, soil drench, foliar spray, or by soil incorporation.
Molecular Formula: $C_9H_{11}Cl_2O_3PS$
Molecular Weight: 301.127
Melting Point (°C):
78–80 (Hartley & Kidd 1987; Worthing & Hance 1991; Tomlin 1994; Milne 1995)
Boiling Point (°C):
Density (g/cm^3 at 20°C):
Molar Volume (cm^3/mol):
Dissociation Constant pK_a:
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
Entropy of Fusion, ΔS_{fus} (J/mol K):
Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F:

Water Solubility (g/m^3 or mg/L at 25°C or as indicated):
0.3–0.4 (23°C, Hartley & Kidd 1987)
0.3–0.4 (23°C, Worthing & Hance 1991)
1.10 (Tomlin 1994)
0.30 (20–25°C, selected, Augustiijn-Beckers et al. 1994; Hornsby et al. 1996)

Vapor Pressure (Pa at 25°C or as indicated):
0.057 (20°C, Hartley & Kidd 1987)
0.057 (20°C, Worthing & Hance 1991; Tomlin 1995)
0.0573 (20–25°C, selected, Augustijn-Beckers et al. 1994; Hornsby et al. 1996)
5.25×10^{-3}; 6.61×10^{-3}, 0.0234 (gradient GC method; estimation using modified Watson method: Sugden's parachor, McGowan's parachor, Tsuzuki 2000)

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

Octanol/Water Partition Coefficient, log K_{OW}:
4.56 (Worthing & Hance 1991; Tomlin 1994)

Bioconcentration Factor, log BCF:

Sorption Partition Coefficient, log K_{OC}:
3.30 (soil, estimated, Augustijn-Beckers et al. 1994; Hornsby et al. 1996)

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

Photolysis: photodegradable with 8 h of sunlight: $t_{½}$ = 44 d in water, $t_{½}$ = 15–28 d in lake and river water, and $t_{½}$ < 2 d on soil surface (Hartley & Kidd 1987; Tomlin 1994).

Half-Lives in the Environment:

Air:

Surface water: photodegradable with 8 hours of sunlight in water with $t_{½}$ = 44 d, $t_{½}$ = 15–28 d in lake and river water, and $t_{½}$ < 2 d on soil surface (Hartley & Kidd 1987);
Photodegration $t_{½}$ = 44 d in water, $t_{½}$ = 15–28 d in lake (Tomlin 1994).

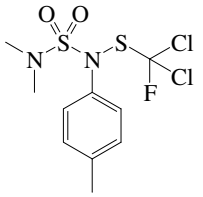
Groundwater:

Sediment:

Soil: $t_{½}$ < 2 d from soil surface by photodegradation (Tomlin 1994);
field $t_{½}$ = 30 d (20–25°C, Augustijn-Beckers et al. 1994; Hornsby et al. 1996)

Biota:

19.1.37 TOLYLFLUANID



Common Name: Tolylfluanid
Synonym: Tolylfluanide
Chemical Name: *N*-dichlorofluoromethylthio-*N′N′*-dimethyl-*N*-*p*-tolylsulphamide; 1,1-dichloro-*N*-[(dimethylamino)-sulfonyl]-1-fluoro-*N*-(4-methylphenyl)methane-sulfenamide
Uses: fungicide/acaricide; to control scab on apples and pears; *Botrytis* on strawberries, raspberries, blackberries, currants, grapes, ornamentals, etc.
CAS Registry No: 731-27-1
Molecular Formula: $C_{10}H_{13}Cl_2FN_2O_2S_2$
Molecular Weight: 347.257
Melting Point (°C):
95–97 (Hartley & Kidd 1987; Worthing & Hance 1991; Milne 1995)
96 (Tomlin 1994)
Boiling Point (°C): dec. on distillation (Tomlin 1994)
Density (g/cm^3 at 20°C): 1.52 (Tomlin 1994)
Molar Volume (cm^3/mol):
326.0 (calculated-Le Bas method at normal boiling point)
Dissociation Constant pK_a:
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
Entropy of Fusion, ΔS_{fus} (J/mol K):
Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F: 0.201 (mp at 96°C)

Water Solubility (g/m^3 or mg/L at 25°C or as indicated):
4000 (Martin & Worthing 1977; quoted, Kenaga 1980)
4000 (room temp., Hartley & Kidd 1987; Worthing & Hance 1991)
0.90 (room temp., Tomlin 1994)

Vapor Pressure (Pa at 25°C or as indicated):
< 0.001 (20°C, Hartley & Kidd 1987)
1.3×10^{-5} (45°C, Worthing & Hance 1991)
1.6×10^{-5} (20°C, Tomlin 1994)

Henry's Law Constant (Pa·m^3/mol):

Octanol/Water Partition Coefficient, log K_{OW}:
3.95 (20°C, Worthing & Hance 1991)
3.90 (Tomlin 1994)
3.95 (selected, Hansch et al. 1995)
4.36 (RP-HPLC-RT correlation, Nakamura et al. 2001)

Bioconcentration Factor, log BCF:
0.778 (calculated, Kenaga 1980)

Sorption Partition Coefficient, log K_{OC}:
1.66 (soil, calculated-S, Kenaga 1980)

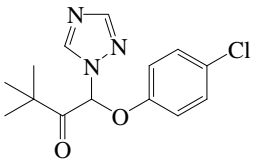
Environmental Fate Rate Constants, k, or Half-Lives, $t_{½}$:

Hydrolysis: $t_{½}$ = 12 d at 22°C and pH 4, $t_{½}$ = 29 h at pH 7 and $t_{½}$ < 10 min at pH 9 (Worthing & Hance 1991; Tomlin 1994).

Half-Lives in the Environment:

Soil: half-life of a few days (Tomlin 1994).

19.1.38 TRIADIMEFON



Common Name: Triadimefon
Synonym: Amiral, Bayleton, MEB 6447, Triadimefone
Chemical Name: 1-(4-chlorophenoxy)-3,3-dimethyl-1-(1*H*-1,2,4-triazol-1-yl)butanone; 1-(4-chlorophenoxy)-3,3-dimethyl-1-(1*H*-1,2,4-triazol-1-yl)-2-butanone
CAS Registry No: 43121-43-3
Uses: as fungicide for control of powdery mildews, rusts in cereals and *Rhynchosporium* in cereals and control of bunt, smuts, *Typhula* spp., seedling blight, leaf stripe, net blotch, and other cereal diseases when used for seed treatment, etc.
Molecular Formula: $C_{14}H_{16}ClN_3O_2$
Molecular Weight: 293.749
Melting Point (°C):
82 (Lide 2003)
Boiling Point (°C):
Density (g/cm^3 at 20°C):
1.22 (Hartley & Kidd 1987; Tomlin 1994; Milne 1995)
Molar Volume (cm^3/mol):
321 (calculated-Le Bas method at normal boiling point)
240.8 (calculated-density)
Dissociation Constant pK_a:
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
Entropy of Fusion, ΔS_{fus} (J/mol K):
Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F: 0.276 (mp at 82°C)

Water Solubility (g/m^3 or mg/L at 25°C or as indicated):
260 (Martin & Worthing 1977)
260 (20°C, Hartley & Kidd 1987; Worthing & Hance 1991; Milne 1995)
71.5 (20–25°C, selected, Wauchope et al. 1992; Hornsby et al. 1996)
71.5 (selected, Lohninger 1994)
64 (20°C, Tomlin 1994)
69; 72 (calculated-group contribution fragmentation method; quoted exptl., Kühne et al. 1995)

Vapor Pressure (Pa at 25°C or as indicated):
$< 1.0 \times 10^{-4}$ (20°C, Hartley & Kidd 1987; Worthing & Hance 1991)
2.00×10^{-6} (20–25°C, selected, Wauchope et al. 1992; Hornsby et al. 1996)
2.00×10^{-5}, 6.0×10^{-5} (20, 25°C, Tomlin 1994)

Henry's Law Constant (Pa·m^3/mol):

Octanol/Water Partition Coefficient, log K_{OW}:
1.80 (shake flask-UV at pH 5, Barak et al. 1983)
3.26 (shake flask, Hansch & Leo 1987)
2.77 (shake flask-LC, Patil et al. 1988)
3.18 (Worthing & Hance 1991; Milne 1995)
2.90 (shake flask at pH 7, Baker et al. 1992)
3.26 (recommended, Sangster 1993)
2.77 (recommended, Hansch et al. 1995)

3.03 (Pomona-database, Müller & Kördel 1996)
3.12 (RP-HPLC-RT correlation using short ODP column, Donovan & Pescatore 2002)

Bioconcentration Factor, log BCF:

1.43 (calculated, Kenaga 1980)

Sorption Partition Coefficient, log K_{OC}:

2.41 (soil, calculated-S, Kenaga 1980)
2.48 (20–25°C, selected, Wauchope et al. 1992; Hornsby et al. 1996)
2.57 (HPLC-screening method, Kördel et al. 1993)
2.48 (estimated-chemical structure, Lohninger 1994)
2.48 (soil, Tomlin 1994)
2.71 (soil, calculated-MCI $^{1}\chi$, Sabljic et al. 1995)
2.57; 3.72 (HPLC-screening method; calculated-PCKOC fragment method, Müller & Kördel 1996)
3.19, 2.277, 2.536, 2.39, 2.96 (first generation Eurosoils ES-1, ES-2, ES-3, ES-4, ES-5, shake flask/batch equilibrium-HPLC/UV, Gawlik et al. 1998, 1999)
2.826, 2.56, 2.512, 2.381, 3.046 (second generation Eurosoils ES-1, ES-2, ES-3, ES-4, ES-5, shake flask/batch equilibrium-HPLC/UV Gawlik et al. 1999)
2.826, 2.560, 2.512, 2.381, 3.046 (second generation Eurosoils ES-1, ES-2, ES-3, ES-4, ES-5, shake flask/batch equilibrium-HPLC/UV and HPLC-k′ correlation, Gawlik et al. 2000)
2.71; 2.43 (soil, quoted obs.; estimated-general model using molecular descriptors, Gramatica et al. 2000)

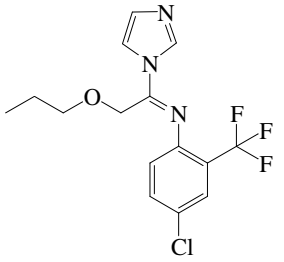
Environmental Fate Rate Constants, k, or Half-Lives, $t_{½}$:

Hydrolysis: $t_{½}$ > 1 yr at 22°C and pH 3, 6, and 9 (Worthing & Hance 1991; Tomlin 1994).

Half-Lives in the Environment:

Soil: field $t_{½}$ = 26 d (20–25°C, selected, Wauchope et al. 1992; Hornsby et al. 1996).

19.1.39 TRIFLUMIZOLE



Common Name: Triflumizole
Synonym: NF-114, Triflumizol, Trifmine
Chemical Name: (*E*)-4-chloro-α,α,α,-trifluoro-*N*-(1-imidazol-1-yl-2-propoxyethylidene)-*o*-tolui-dine; 1-[1-[[4-chloro-2-(trifluoromethyl)phenyl]imino]-2-propoxyethyl]-1*H*-imidazole
CAS Registry No: 68694-11-1
Uses: as fungicide for control of powdery mildews in fruit, vines, and vegetables; scab and rust in apples and pears; also used as seed treatment for barley, etc.
Molecular Formula: $C_{15}H_{15}ClF_3N_3O$
Molecular Weight: 345.574
Melting Point (°C):
63.5 (Hartley & Kidd 1987; Worthing & Hance 1991; Tomlin 1994; Milne 1995; Lide 2003)
Boiling Point (°C):
Density (g/cm^3 at 20°C):
Molar Volume (cm^3/mol):
359.5 (calculated-Le Bas method at normal boiling point)
Dissociation Constant pK_a:
3.70 (Augustijn-Beckers et al. 1994; Tomlin 1994; Hornsby et al. 1996)
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
Entropy of Fusion, ΔS_{fus} (J/mol K):
Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F: 0.419 (mp at 63.5°C)

Water Solubility (g/m^3 or mg/L at 25°C or as indicated):
12500 (20°C, Hartley & Kidd 1987; Worthing & Hance 1991; Tomlin 1994; Milne 1995)
12500 (20–25°C, selected, Augustijn-Beckers et al. 1994; Hornsby et al. 1996)

Vapor Pressure (Pa at 25°C or as indicated):
1.40×10^{-6} (Worthing & Hance 1991)
1.47×10^{-6} (20–25°C, selected, Augustijn-Beckers et al. 1992; Hornsby et al. 1996)
1.86×10^{-4} (Tomlin 1994)

Henry's Law Constant (Pa·m^3/mol at 25°C or as indicated):
4.07×10^{-8} (20–25°C, calculated-P/C, this work)

Octanol/Water Partition Coefficient, log K_{OW}:
1.40 (Worthing & Hance 1991; Milne 1995; Tomlin 1994)
1.40 (selected, Hansch et al. 1995)

Bioconcentration Factor, log BCF:

Sorption Partition Coefficient, log K_{OC}:
3.03–3.22 (Tomlin 1994)
1.60 (20–25°C, estimated, Augustijn-Beckers et al. 1994; Hornsby et al. 1996)

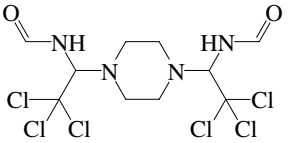
Environmental Fate Rate Constants, k, or Half-Lives, $t_{½}$:

Photolysis: aqueous solutions degraded by sunlight with $t_{½}$ = 29 h (Worthing & Hance 1991; Tomlin 1994).

Half-Lives in the Environment:

Soil: $t_{½}$ = 14 d on clay (Worthing & Hance 1991);
field $t_{½}$ = 14 d (20–25°C, selected, Augustijn-Beckers et al. 1994; Hornsby et al. 1996).

19.1.40 TRIFORINE



Common Name: Triforine
Synonym: Biformychloazin, Cela W524, Compound W, Denarin, FMC, Funginex, Saprol, W 524
Chemical Name: 1.1′-piperazine-1,4-diyldi-[*N*-(2,2,2-trichloroethyl)formamide]; 1,4-bis(2,2,2-trichloro-1-formamidoethyl) piperazine; *N,N′*-[1,4-piperazinediylbis(2,2,2-trichloro-ethylidene)]bisformamide
Uses: systemic fungicide to control powdery mildews on cereals, fruit, vines, hops, cucurbits, vegetables, and ornamentals, etc.; also used to suppress spider mite activity.
CAS Registry No: 26644-46-2
Molecular Formula: $C_{10}H_{14}Cl_6N_4O_2$
Molecular Weight: 434.962
Melting Point (°C):
155 (dec., Hartley & Kidd 1987; Worthing & Hance 1991; Tomlin 1994; Milne 1995; Lide 2003)
Boiling Point (°C):
Density (g/cm^3 at 20°C): 1.554 (Tomlin 1994)
Molar Volume (cm^3/mol):
389.2 (calculated-Le Bas method at normal boiling point)
279.9 (calculated-density)
Dissociation Constant pK_a:
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
Entropy of Fusion, ΔS_{fus} (J/mol K):
Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F: 0.053 (mp at 155°C)

Water Solubility (g/m^3 or mg/L at 25°C or as indicated):
30 (rm. temp., Hartley & Kidd 1987; Worthing & Hance 1991)
6.0 (rm. temp., Worthing & Hance 1991; Milne 1995)
30 (20–25°C, selected, Wauchope et al. 1992; Hornsby et al. 1996)
30 (selected, Lohninger 1994)
9.0 (20°C, Tomlin 1994)

Vapor Pressure (Pa at 25°C or as indicated):
2.6×10^{-5} (Hartley & Kidd 1987)
2.7×10^{-5} (Worthing & Hance 1991; Tomlin 1994)
2.7×10^{-5} (20–25°C, selected, Wauchope et al. 1992; Hornsby et al. 1996)

Henry's Law Constant (Pa·m^3/mol):

Octanol/Water Partition Coefficient, log K_{OW}:
2.20 (Worthing & Hance 1991; Tomlin 1994; Milne 1995)

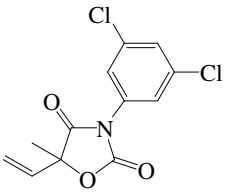
Bioconcentration Factor, log BCF:

Sorption Partition Coefficient, log K_{OC}:
2.73 (20–25°C, estimated, Wauchope et al. 1992; Hornsby et al. 1996)
2.30 (estimated-chemical structure, Lohninger 1994)

Environmental Fate Rate Constants, k, or Half-Lives, $t_{½}$:
Hydrolysis: $t_{½}$ = 3.5 d at pH 5, 25°C in aqueous solutions (Tomlin 1994).

Half-Lives in the Environment:
Soil: $t_{½}$ ~ 3 wk in soil (Hartley & Kidd 1987; Tomlin 1994);
field $t_{½}$ = 21 d (20–25°C, estimated, Wauchope et al. 1992; Hornsby et al. 1996).

19.1.41 VINCLOZOLIN



Common Name: Vinclozolin
Synonym: BAS 352F, Ronilan, Vorlan
Chemical Name: (*RS*)-3-(3,5-dichlorophenyl)-5-vinyl-1,3-oxazolidine-2,4-dione; 3-(3,5-dichlorophenyl)-5-ethenyl-5-methyl-2,4-oxazolidinedione
CAS Registry No: 50471-44-8
Uses: fungicide to control *Botrytis/Sclerotinie* spp. in vines, oilseed rape, vegetables, fruit, and ornamentals, etc.
Molecular Formula: $C_{12}H_9Cl_2NO_3$
Molecular Weight: 286.110
Melting Point (°C):
108 (Hartley & Kidd 1987; Worthing & Hance 1991; Tomlin 1994; Milne 1995: Lide 2003)
Boiling Point (°C):
131 (at 0.05 mmHg, Hartley & Kidd 1987; Tomlin 1994; Milne 1995)
Density (g/cm^3 at 20°C):
1.51 (Worthing & Hance 1991; Tomlin 1994; Milne 1995)
Molar Volume (cm^3/mol):
266.3 (calculated-Le Bas method at normal boiling point, this work)
189.5 (calculated-density, this work)
Dissociation Constant pK_a:
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
Entropy of Fusion, ΔS_{fus} (J/mol K):
Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F: 0.153 (mp at 108°C)

Water Solubility (g/m^3 or mg/L at 25°C or as indicated):
1000 (Martin & Worthing 1977)
1000 (20°C, Hartley & Kidd 1987)
3.40 (20°C, Worthing & Hance 1991; Tomlin 1994; Milne 1995)
1000 (20–25°C, estimated, Augustijn-Beckers et al. 1994; Hornsby et al. 1996)

Vapor Pressure (Pa at 25°C or as indicated):
< 0.010 (20°C, Hartley & Kidd 1987)
1.6×10^{-5} (20°C, Worthing & Hance 1991; Tomlin 1994)
1.6×10^{-5} (20–25°C, selected, Augustijn-Beckers et al. 1994; Hornsby et al. 1996)
1.3×10^{-4} (20°C, Siebers et al. 1994)

Henry's Law Constant (Pa·^{3}/mol at 25°C or as indicated):
0.011 (20°C, quoted, Siebers et al. 1994)

Octanol/Water Partition Coefficient, log K_{OW}:
3.00 (Stevens et al. 1988)
3.00 (pH 7, Worthing & Hance 1991; Tomlin 1994; Milne 1995)
2.47 (shake flask-HPLC at pH 6, Nielsen et al. 1992)
3.00, 2.47 (Sangster 1993)
3.10 (recommended, Hansch et al. 1995)

Bioconcentration Factor, log BCF:
1.26 (calculated, Kenaga 1980)

Sorption Partition Coefficient, log K_{OC}:

1.99	(soil, calculated-S, Kenaga 1980)
2.0–2.87	(soil, Tomlin 1994)
2.0	(soil, 20–25°C, estimated, Augustijn-Beckers et al. 1994; Hornsby et al. 1996)

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

Volatilization:

Photolysis: when irradiation with UV light, $\lambda \geq 290$ nm, for vinclozolin aqueous solution (1 ppm): 10% and 11% photodegraded in 1 h, in the presence of 1 ppm humic acid and 1 ppm fulvic acid, respectively; irradiation of vinclozolin (2 ppm) in water with $t_{½}$ = 7 min and 92 min in the presence of TiO_2 (20 ppm), and Fe_2O_3 (100 ppm), respectively. (Hustert & Moza 1997)

Oxidation:

Hydrolysis: stable in neutral and weakly acidic media, in 0.1 N NaOH, 50% hydrolysis occurs in 3.8 h (Hartley & Kidd 1987; Tomlin 1994).

Biodegradation:

Biotransformation:

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

Half-Lives in the Environment:

Air:

Surface water: photodegradation of vinclozolin aqueous solution (2 ppm), $t_{½}$ = 7 min and 92 min in the presence of TiO_2 (20 ppm), and Fe_2O_3 (100 ppm), respectively, when irradiated with UV light (Hustert & Moza 1997)

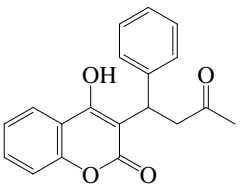
Groundwater:

Sediment:

Soil: field $t_{½}$ = 20 d (20–25°C, selected, Augustijn-Beckers et al. 1994; Hornsby et al. 1996).

Biota:

19.1.42 WARFARIN



Common Name: Warfarin
Synonym: Coumafen, Zoocoumarin
Chemical Name: 3-(α-acetonylbenzyl)-4-hydroxycoumarin
CAS Registry No: 81-81-2
Use: rodenticide
Molecular Formula: $C_{19}H_{16}O_4$
Molecular Weight: 308.328
Melting Point (°C):
161 (Lide 2003)
Boiling Point (°C): dec. (Montgomery 1993)
Density (g/cm^3 at 20°C):
Molar Volume (cm^3/mol):
Dissociation Constant pK_a:
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
Entropy of Fusion, ΔS_{fus} (J/mol K):
Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F: 0.0463 (mp at 161°C)

Water Solubility (g/m^3 or mg/L at 25°C or as indicated):
40 (shake flask, Coon et al. 1954)
17 (20°C, Hartley & Kidd 1987; Worthing & Walker 1987)
17 (20°C, Montgomery 1993; Tomlin 1994)

Vapor Pressure (Pa at 25°C or as indicated):
1.55×10^{-4} (21.5°C, Hartley & Kidd 1987)
9.0 (21.5°C, Worthing & Walker 1987; Tomlin 1994)

Henry's Law Constant (Pa·m^3/mol at 25°C):
2.86×10^{-4} (calculated-P/C, Howard 1991)

Octanol/Water Partition Coefficient, log K_{OW}:
2.52 (at pH 3, Howard 1991)
3.20 (calculated, Montgomery 1993)
3.12 (RP-HPLC-RT correlation using short ODP column, Donovan & Pescatore 2002)

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

Bioconcentration Factor, log BCF:
1.68 (calculated, Howard 1991)

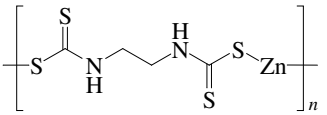
Sorption Partition Coefficient, log K_{OC}:
2.75 (estimated, Howard 1991)
2.96 (calculated, Montgomery 1993)

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

Oxidation: Photooxidation $t_{½}$ = 0.254–1.87 h was estimated based on rate constants for reaction with hydroxyl radicals and ozone in air (Howard et al. 1991).
Hydrolysis: very slow with a $t_{½}$ = 16 yr at pH 7; the chemical hydrolysis rate constants, $k = 1.4 \times 10^{-4}$ M^{-1} h^{-1} for acid, neutral-$k = 4.9 \times 10^{-6}$ M^{-1} h^{-1} and $k = 0.026$ M^{-1} h^{-1} for base (Ellington et al. 1988; quoted, Howard 1991).
Biodegradation: aqueous aerobic $t_{½}$ = 168–672 h, anaerobic $t_{½}$ = 672–2688 h were estimated based on aqueous aerobic biodegradation (Howard et al. 1991).
Biotransformation:
Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants:

Half-Lives in the Environment:
Air: estimated $t_{½}$ = 11.6 min due to reaction with photochemically produced hydroxyl radicals and ozone in the vapor phase (Howard 1991);
$t_{½}$ = 0.254–1.87 h based on estimated photooxidation in air (Howard et al. 1991).
Surface water: $t_{½}$ = 168–672 h based on estimated unacclimated aqueous aerobic biodegradation (Howard et al. 1991);
slow hydrolysis $t_{½}$ = 15 yr at pH 7 (Howard 1991).
Groundwater: $t_{½}$ = 336–1344 h based on estimated aqueous aerobic biodegradation (Howard et al. 1991).
Sediment:
Soil: $t_{½}$ = 168–672 h based on estimated unacclimated aqueous aerobic biodegradation (Howard et al. 1991).
Biota:

19.1.43 ZINEB



Common Name: Zineb
Synonym: Dithane Z-78, Parzate Zineb, Lonaol, Aspor
Chemical Name: zinc ethylene-1,2-bisdithiocarbamate
CAS Registry No: 12122-67-7
Uses: fungicide
Molecular Formula: $(C_4H_6N_2S_4Zn)_x$
Molecular Weight: $(275.773)_x$
Melting Point (°C):
decomposes without melting (Worthing & Walker 1983)
157 (dec., Tomlin 1994; Lide 2003)
Boiling Point (°C):
Density (g/cm^3 at 20°C):
Molar Volume (cm^3/mol):
Dissociation Constant pK_a:
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
Entropy of Fusion, ΔS_{fus} (J/mol K):
Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F: 0.0507 (mp at 157°C)

Water Solubility (g/m^3 or mg/L at 25°C or as indicated):

1	(Melnikov 1971)
10	(Spencer 1982)
≈10	(Worthing & Walker 1983, 1987; quoted, Howard 1991)
10	(room temp., Tomlin 1994)
10	(20–25°C, selected, Augustijn-Beckers et al. 1994; Hornsby et al. 1996)

Vapor Pressure (Pa at 25°C or as indicated):

negligible at rm. temp. (Worthing & Walker 1983)	
1.07×10^{-5}	(20°C, quoted, Howard 1991)
$< 1 \times 10^{-5}$	(20°C, Hartley & Kidd 1987; Tomlin 1994)
1.0×10^{-5}	(10–25°C, estimated, Augustijn-Beckers et al. 1994; Hornsby et al. 1996)

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

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

≤ 1.30	(Tomlin 1994)

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

Bioconcentration Factor, log BCF:

2.11, 2.23, < 1.0,	(activated sludge, algae, Golden ide, Freitag et al. 1985)
2.28	(calculated-S, Kenaga 1980b; quoted, Howard 1991)

Sorption Partition Coefficient, log K_{OC}:

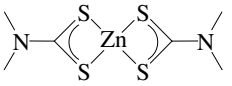
3.08	(soil, calculated-S, Kenaga 1980b; quoted, Howard 1991)
3.0	(soil, selected, Augustijn-Beckers et al. 1994; Hornsby et al. 1996)

Environmental Fate Rate Constants, k, or Half-Lives, $t_{½}$:
Photolysis: unstable to light, moisture and heat on prolonged storage (Tomlin 1994).

Half-Lives in the Environment:

Air: $t_{½}$ = 11–14 d in greenhouse experiment, microagroecosystem chambers (Nash & Beall 1980);
$t_{½}$ = 11–14 d by gravitational settling and degradation (Howard 1991).
Surface water:
Groundwater:
Sediment:
Soil: $t_{½}$ = 23 d in 1-cm surface soil (sandy loam with pH 6.7), greenhouse experiment in microagroecosystem chambers (Nash & Beall 1980);
$t_{½}$ = 16–23 d upper layer of soil (Howard 1991);
field $t_{½}$ ~ 30 d (estimated, Augustijn-Beckers et al. 1994; Hornsby et al. 1996).
Biota: $t_{½}$ = 14 d on tomato leaves, green house experiment, microagroecosystem chambers (Nash & Beall 1980);
$t_{½}$ = 7 d for tomato fruit in the field, $t_{½}$ = 3.4 d for soybean leaves and $t_{½}$ = 9 d for tomatoes (Nash 1983);
$t_{½}$ = 14 d for tomato leaves, $t_{½}$ = 7 d for tomatoes, $t_{½}$ = 11 d for lettuce and $t_{½}$ = 35 d for grapes (Howard 1991).

19.1.44 ZIRAM



Common Name: Ziram
Synonym: Aaprotect, Fuklasin, Zerlate, zirmane
Chemical Name: zinc bis(dimethyldithiocarbamate)
CAS Registry No: 137-30-4
Uses: fungicide, bird and rodent repellent
Molecular Formula: $C_6H_{12}N_2S_4Zn$
Molecular Weight: 305.841
Melting Point (°C):
250 (Howard 1991; Lide 2003)
Boiling Point (°C):
Density (g/cm^3 at 20°C):
2.00 (Spencer 1982)
1.66 (25°C, Hartley & Kidd 1987; Tomlin 1994; Milne 1995)
Molar Volume (cm^3/mol):
Dissociation Constant pK_a:
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
Entropy of Fusion, ΔS_{fus} (J/mol K):
Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F: 0.0062 (mp at 250°C)

Water Solubility (g/m^3 or mg/L at 25°C or as indicated):
65 (Melnikov 1971)
65 (Martin & Worthing 1977; Worthing & Walker 1983, 1987)
4.0 (20°C, Spencer 1982)
65 (Hartley & Kidd 1987)
0.03 (20°C, Tomlin 1994)
65 (20–25°C, selected, Augustijn-Beckers et al. 1994; Hornsby et al. 1996)
65 (Milne 1995)

Vapor Pressure (Pa at 25°C or as indicated):
negligible (Worthing & Walker 1983, 1987; quoted, Howard 1991)
1.33×10^{-5} (20–25°C, Augustijn-Beckers et al. 1994; Hornsby et al. 1996)
$< 1 \times 10^{-6}$ (extrapolated, Tomlin 1994)

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

Octanol/Water Partition Coefficient, log K_{OW}:
1.086 (Tomlin 1994)

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

Bioconcentration Factor, log BCF:
1.77 (calculated-S, Kenaga 1980b; quoted, Howard 1991)

Sorption Partition Coefficient, log K_{OC}:
2.64 (soil, calculated-solubility, Kenaga 1980b; quoted, Howard 1991)
2.60 (soil, estimated, Augustijn-Beckers et al. 1994; Hornsby et al. 1996)

Environmental Fate Rate Constants, k, or Half-Lives, $t_{½}$:
Hydrolysis: decomposed in acidic media (Tomlin 1994).

Half-Lives in the Environment:

Air:
Surface water: decomposed in acidic media, and by UV irradiation (Tomlin 1994).
Groundwater:
Sediment:
Soil: field $t_{½}$ ~ 30 d (estimated, Augustijn-Beckers et al. 1992; Hornsby et al. 1996).
Biota: for orally administered to rate was mostly eliminated within 1–2 d (Tomlin 1994).

TABLE 19.2.1
Common names, chemical names and physical properties of fungicides

Name	Synonym	Chemical name	Molecular formula	Molecular weight, MW g/mol	m.p. °C	Fugacity ratio, F at 25°C*	pK_a
Anilazine [101-05-3]	Botrysan, Direz, Dyren	2-chloro-*N*-(4,6-dichloro-1,3,5-triazin-2-yl)aniline	$C_9H_5Cl_3N_4$	275.522	160	0.0474	
Benalaxyl [71626-11-4]	Galben	methyl *N*-phenylacetyl-*N*-2,6-xylyl-*DL*-alaninate	$C_{20}H_{23}NO_3$	325.402	79	0.295	
Benodanil [15310-01-8]	Calirux	2-iodo-*N*-phenylbenzamide	$C_{13}H_{10}INO$	323.129	137	0.0796	
Benomyl [17804-35-2]	Benlate	methyl 1-(butylcarbamoyl)benz-imidazol-2-ylcarbamate	$C_{14}H_{18}N_4O_3$	290.318	140	0.0744	
Bitertanol [70585-36-3]	Baycor, Baymat, Biloxa, Siibutol	1-(biphenyl-4-yloxy)-3,3-dimethyl-1-1*H*-1,2,4-triazol-1-yl)butan-2-ol	$C_{20}H_{23}N_3O_2$	337.415	118 eutectic	0.122	
diastereoisomer A [70585–38–5]			337.415	136.7	0.0802		
diastereoisomer B [55179–31–2]			337.415	145.2	0.0662		
Buprirmate [41483-43-6]	Nimrod, Nimrod T	5-butyl-2-ethylamino-6-methyl-pyrimidinyl dimethylsulfamate	$C_{13}H_{24}N_4O_3S$	316.419	50–51	0.562	
Captan [133-06-2]	Aacaptan, Amercide, Captab, orthocide	*N*-trichloromethylthio-4-cyclohexene-1,2-dic arboximide	$C_9H_8Cl_3NO_2S$	300.590	172.5	0.0357	
Carbendazim [10605-21-7]	Bavistin, BCM, Carbendazol	carbamic acid, methyl-1*H*-benzimidazol-2-yl	$C_9H_9N_3O_2$	191.186	300 dec	0.0020	4.48 4.2
Carboxin [5234-68-4]	Vitavax, carbathiin	5,6-dihydro-2-methy-1,4-oxathi-ine-3-carbo xanilide	$C_{12}H_{13}NO_2S$	235.302	94	0.210	
Chloroneb [2675-77-6]	Tersan SP	1,4-dichloro-2,5-dimethoxybenzene	$C_8H_8Cl_2O_2$	207.055	134	0.0852	
Chloropicrin [76-06-2]	Nitrochloroform	trichloronitromethane	CCl_3NO_2	164.376	–64	1	
Chlorothalonil [1897-45-6]	Bravo, Daconil	2,4,6-tetrachloro-1,3-benzene-dicarbonitrile	$C_8Cl_4N_2$	265.911	250	0.0062	
Dazomet (Fum.) [533-74-4]	Salvo, Mylone, Basamid	3,5-dimethyl-1,3,5-thiadiazinane-2-thione	$C_5H_{10}N_2S_2$	162.276	106	0.16	
Dichlofluanid [1085-98-9]	Euaren, Elvaron	*N*-dichlorofluoromethylthio-*N,N'*-dimethyl-*N*-phenylsuphamide	$C_9H_{11}Cl_2FN_2O_2S_2$	333.229	105.3	0.163	
Dichlone [117–80–6]	Phygon	2,3-dichloro-1,4-naphthoquinone	$C_{10}H_4Cl_2O_2$	227.044	195	0.0215	
Dicofol [115–32–2]	Kelthan	2,2,2-trichloro-1,1-bis(4-chlorophenyl) ethenol	$C_{14}H_9Cl_5O$	370.485	77.5	0.305	
Dithianon [3347-22-6]	Delan	5,10-dihydro-5,10-dioxonaphtho[2,3-*b*-]-1,4-dithi-in-2,3-dicarbonitrile	$C_{13}H_4N_2O_2S_2$	296.324	220	0.0122	

Edifenphos [17109-49-8]	EDDP, Hinosan	*O*-ethyl *S,S*-diphenyl-phosphoradithioate	$C_{14}H_{15}O_2PS_2$	310.371	–25	1	
Ethirimol [23947-60-6]		5-butyl-2-ethylamino-6-methyl-pyrimidim-4-ol	$C_{11}H_{19}N_3O$	209.288	160	0.0474	
Etridiazole [2593-15-9]	ethazol, ethazole, Terazole	ethyl 3-trichloromethyl-1,2,4-thiadiazolyl ether	$C_5H_5Cl_3N_2OS$	247.530	19.9	1	2.27
Fenarimol [60168-88-9]	Bloc, Rimidin, Rubigan	(±)-2,4-dichloro-α-(pyrimidin-5-yl) benzhydryl alcohol	$C_{17}H_{12}Cl_2N_2O$	331.195	118	0.122	
Fenfuram [24691-80-3]	fenfurame	2-methyl-3-fruanilide	$C_{12}H_{11}NO_2$	201.221	109–110	0.148	
Fenpropimorph [67564-91-4]	Corbel, Mistral	(±)-*cis*-4-[3-(4-*tert*-butylphenyl)-2-methylpropyl]-2,6-dimethylmorpholine	$C_{20}H_{33}NO$	303.482	oil	1	6.98
Folpet [133-07-3]	Foltan, Folpan, Folpel, Spolacid	*N*-(trichloromethylthio)phthalimide	$C_9H_4Cl_3NO_2S$	296.558	177	0.0323	
Formaldehyde [50–00–0]	Formalin, methanal	formaldehyde	HCHO	30.026	–92	1	
Furalaxyl [57646-30-7]	Fongarid	methyl-*N*-(2-furoyl)-*N*-(2,6-xylyl)-*DL*-alaninate	$C_{17}H_{19}NO_4$	301.337	70	0.362	
Hexachlorobenzene [118–74-1]	HCB	hexachlorobenzene	C_6Cl_6	284.782	228.83	0.010	
Imazalil [35554-44-0]	Bromazil, Deccozil	(±)-1-(β-allyloxy-2,4-dichlorophenyl-ethyl)imidazole	$C_{14}H_{14}Cl_2N_2O$	297.179	50	0.568	
Iprobenfos [26087-47-8]	Kitazin	*S*-benzy *O,O*-di-isopropyl phosphoro-thioate	$C_{13}H_{21}O_3PS$	288.342	oil	1	
Mancozeb [8018–01–7]	Dithane ultra, Dithane M45				192–194 dec		
Maneb [12427–38–2]	MEB, Dithane, Bravo	manganese ethylenebis(dithiocarbamate)	$(C_4H_6MnN_2S_4)_x$	$(265.302)_x$	dec 200		
Metalaxyl [57837-19-1]	Ridomil, Apron Fubol	methyl *N*-(2-methoxyacetyl)-2,6-xylyl)-*DL*-alaninate	$C_{15}H_{21}NO_4$	279.333	71	0.354	<< 0
Metiram [9006-42-4]	Carbatene, Polyram	zinc ammoniate ethylenebisdithio-carbamate-poly(ethylenethiurmdisulfide)					
Nitrapyrin [1929–82–4]	N-Serve	2-chloro-6-(trichloromethyl)pyridine	$C_6H_3C_{14}N$	230.907	63	0.424	
Oxycarboxin [5259-88-1]	Plantvax	5,6-dihydro-2-methyl-1,4-oxathi-ine-3- carboxanilide 4,4-dioxide	$C_{12}H_{13}NO_4S$	267.301	129	0.0954	
Penconazole [66246-88-6]	Topas, Topaz, Topaze	1-(2,4-dichloro-β-propylphenyl-ethyl)-1*H*-1,2,4-trizaole	$C_{13}H_{15}Cl_2N_3$	284.184	60	0.454	1.51
Procymidone [32809-16-8]	Sumisclex, Sumilex	*N*-(3,5-dichlorophenyl)-1,2-dimethyl-cyclopropane-1,2-dicarboximide	$C_{13}H_{11}Cl_2NO_2$	284.138	166	0.0414	
Propargite [2312–35–8]	Comite, Omite	2-[4-(1,1-dimethylethyl)phenoxy]cyclohexyl 2-propynyl sulfite	$C_{16}H_{26}O_4S$	360.472	liquid	1	
Propiconazole [60207-90-1]		(±)-1-[2,4-(dichlorophenyl)-4-propyl-1,3-dioxolan-2-methyl]-	$C_{15}H_{17}Cl_2N_3O_2$	342.221	liquid	1	1.09

(*Continued*)

TABLE 19.2.1 (*Continued*)

Name	Synonym	Chemical name	Molecular formula	Molecular weight, MW g/mol	m.p. °C	Fugacity ratio, F at 25°C*	pK_a
Quintozene [82-68-8]	Tritisan, Botrilex, Terrachlor	pentachloronitrobenzene	$C_6Cl_5NO_2$	295.335	144	0.0680	
Tecnazene [117-18-0]	Folosan, Fusarex	1,2,4,5-tetrachloro-3-nitrobenzene	$C_6HCl_4NO_2$	260.890	99.5	0.186	
Thiabendazole [148-79-8]	Mertect, Storite	2-(thiazol-4-yl)benzimidazole	$C_{10}H_7N_3S$	201.248	304–305	0.00181	
Thiophanate-methyl [23564-05-8]	Topsin M, Mildothane	dimethyl 4,4'-(*o*-phenylene)bis(3-thioallphanate)	$C_{12}H_{14}N_4O_4S_2$	342.394	172 dec	0.0361	7.28
Thiram [137-26-8]	Arasan, Tersan, Fernasan	tetramethylthiuram disulphide	$C_6H_{12}N_2S_4$	240.432	155.6	0.0523	
Tolclofos-methyl [57018-04-9]	Rizolex	*O*-2,6-dichloro-*p*-tolyl *O,O*-dimethyl phosphorothioate	$C_9H_{11}Cl_2O_3PS$	301.127	78-80	0.295	
Tolylfluanid [731-27-1]	Euparen M	*N*-dichlorofluoromethylthio-*N,N*'-dimethyl-*N*-*p*-tolysulphamide	$C_{10}H_{13}Cl_2FN_2O_2S_2$	347.257	96	0.201	
Triadimefon [43121-43-3]	Amiral, Bayeton	1-(-chlorophenoxy)-3,3-dimethyl-1-1*H*-1,2,4 -triazol-1-yl)butanone	$C_{14}H_{16}ClN_3O_2$	293.749	82	0.276	
Triadimenol [55219-65-3]	Baytan	1-(4-chlorophenoxy)-3,3-dimethyl-1-(1*H*-1,2,4-triazol-1-yl)butan-2-ol	$C_{14}H_{18}ClN_3O_2$	295.764	121–127		
Tricyclazole [41814-78-2]	Beam, Bim, Blascide	5-methyl-1,2,4-triazolo[3,4-*b*]-benzothiazole	$C_9H_7N_3S$	189.237	187	0.0257	
Triflumizole [99387–89–0]	Trifmine	(*E*)-4-chloro-α,α,α-trifluoro-*N*-(1-imidazol-1-yl-propoxyethylidene)-*o*-toluidine	$C_{15}H_{15}ClF_3N_3O$	345.747	63.5	0.419	3.70
Triforine [26644-46-2]		1,4-bis(2,2,2-trichloro-1-formamido-ethyl) piperazine	$C_{10}H_{14}Cl_6N_4O_2$	434.962	155 dec	0.0530	
Vinclozolin [50471-44-8]	Ronilan	(*RS*)-3-(3,5-dichlorophenyl)-5-methyl-5-vinyl-1,3-oxazolidine-2,4-dione	$C_{12}H_9Cl_2NO_3$	286.110	108	0.153	
Warfarin (R.) [81-81-2]	Coumarin Dethmor	4-hydroxy-3-(3-*oxo*-1-phenylbutyl)-2*H*-1-benzopyran-2-one	$C_{19}H_{16}O_4$	308.328	161	0.0463	
Zineb [12122-67-7]	Zinebe	zine ethylenebis(dithiocarbamate)	$C_4H_6N_2S_4Zn$	275.773	157 dec	0.0507	
Ziram [137-30-4]	Zirame	zinc bis(dimethyldithiocarbamate)	$C_6H_{12}N_2S_4Zn$	305.841	250	0.0062	

Note: Fum.—fumigant, I—insecticide, R.—rodenticide

* Assuming ΔS_{fus} = 56 J/mol K

TABLE 19.2.2
Summary of selected physical-chemical properties of fungicides at 25°C

	Selected properties							
	Vapor pressure		Solubility				Henry's law constant H/(Pa·m³/mol)	log K_{OC}
Compound	P^S/Pa	P_L/Pa	S/(g/m³)	C^S/(mol/m³)	C_L/(mol/m³)	log K_{OW}	calcd P/C	reported
Anilazine	8.20×10^{-7}	1.77×10^{-5}	8	0.0290	0.628	3.80	2.82×10^{-5}	3.0
Benalaxyl	0.00133	4.65×10^{-3}	37	0.1137	0.398	3.40	0.012	3.44–3.86
Benodanil	1.00×10^{-8}	1.28×10^{-7}	2	0.0062	0.0793		1.62×10^{-6}	2.85
Benomyl	1.33×10^{-8}*	1.82×10^{-7}	2.0*	0.0069	0.0945	2.30	1.93×10^{-6}	3.28
Bitertanol	1.00×10^{-6}	8.31×10^{-6}	5	0.0118	0.0984		8.45×10^{-5}	
diastereoisomer A	2.20×10^{-9}	2.80×10^{-8}	2.9	0.0069	0.0874	4.10	3.20×10^{-7}	
diastereoisomer B	2.50×10^{-9}	3.86×10^{-8}	1.6	0.0038	0.0585	4.40	6.60×10^{-7}	
Buprirmate	0.00067	1.21×10^{-3}	22	0.0695	0.126	3.90	9.64×10^{-3}	2.9
Captan	1.10×10^{-5}	4.23×10^{-4}	5.1	0.0170	0.653	2.30	6.48×10^{-4}	2.29
Carbendazim	6.50×10^{-8}	3.82×10^{-5}	8	0.0418	24.60	1.52	1.55×10^{-6}	2.35
Carboxin	1.30×10^{-5}	5.98×10^{-5}	195	0.829	3.811	2.17	1.57×10^{-5}	2.41
Chloroneb	0.40	4.788	8	0.0386	0.462		173.8	3.06
Chloropicrin (I,Fum.)	2400	2400	2270	13.81	13.81	2.07	197.3	1.79
Chlorothalonil	0.133*	22.86	0.6	0.0023	0.388	2.64	58.94	3.2
Dazomet (Fum.)	4.0×10^{-4}	2.47×10^{-3}	3000	18.48	114.3	0.15	2.16×10^{-5}	0.48
Dichlofluanid	2.10×10^{-5}	1.32×10^{-4}	1.3	0.0039	0.0245	3.70	5.38×10^{-3}	
Dithianon	6.60×10^{-5}	6.28×10^{-4}	0.5	0.0017	0.1605	3.20	0.0391	
Edifenphos	0.013	0.013	56	0.180	0.180	3.48	0.072	
Ethirimol	2.67×10^{-4}	5.78×10^{-3}	200	0.956	20.68	2.3	2.79×10^{-4}	
Etridiazole	0.013	0.013	50	0.202	0.202	3.37	0.0644	
Fenarimol	2.93×10^{-5}	2.44×10^{-4}	14	0.0423	0.351	3.69	6.93×10^{-4}	2.78
Fenfuram	2.0×10^{-5}	1.39×10^{-4}	100	0.497	3.444		4.02×10^{-5}	2.48
Fenpropimorph	0.0023	2.30×10^{-3}	4.3	0.0142	0.014		0.162	2.94–3.65
Folpet	0.0013	0.0414	1	0.0034	0.107	3.63	0.386	3.27
Formaldehyde	> 1 atm		miscible			0.35		
Furalaxyl			230	0.763	2.127	2.61		
Imazalil	9.30×10^{-6}	1.75×10^{-5}	1400	4.71	8.853	3.82	1.97×10^{-6}	3.60
Metalaxyl	7.47×10^{-4}	2.18×10^{-3}	8400	30.08	87.71	1.75	2.48×10^{-5}	1.7
Metiram	< 0.00001		0.1			0.30		5.7
Oxycarboxin	0.00133	0.0139	1000	3.741	39.06	0.74	3.56×10^{-4}	1.98
Penconazole	0.00021	4.66×10^{-4}	73	0.257	0.570	3.72	8.18×10^{-4}	2.62

(Continued)

TABLE 19.2.2 (*Continued*)

	Selected properties							
	Vapor pressure		Solubility				Henry's law constant H/(Pa·m³/mol)	log K_{OC}
Compound	P^S/Pa	P_L/Pa	S/(g/m³)	C^S/(mol/m³)	C_L/(mol/m³)	log K_{OW}	calcd P/C	reported
Procymidone	0.0187	0.4534	4.5	0.0158	0.384	3.14	1.181	3.18
Propiconazole	5.60×10^{-5}	5.60×10^{-5}	110	0.321	0.321	3.72	1.74×10^{-4}	2.82
Quintozene	0.0066	0.104	0.44	0.0015	0.023	4.64	4.430	4.3, 3.38
Tecnazene			0.44	0.0017	0.0091			
Thiabendazole	5.33×10^{-7}	3.13×10^{-4}	50	0.249	146.1	2.69	2.14×10^{-6}	3.4
Thiophanate-methyl	1.30×10^{-5}	3.70×10^{-4}	3.5	0.0102	0.291	1.50	1.27×10^{-3}	3.26
Thiram	0.00133	0.0209	30	0.125	1.963	1.73	0.0107	2.83
Tolclofos-methyl	0.0573	0.196	0.3	0.001	0.0034	4.56	57.51	3.3
Tolylfluanid	1.6×10^{-5}	8.06×10^{-5}	0.9	0.0026	0.0131	3.90	6.17×10^{-3}	1.66
Triadimefon	2.0×10^{-6}	7.37×10^{-6}	71.5	0.243	0.897	3.26	8.22×10^{-6}	
Triadimenol	4.13×10^{-8}	4.03×10^{-7}	47	0.159	1.549	3.08	2.60×10^{-7}	3.00
diastereoisomer A	< 0.001		62	0.210	2.761	3.08		
diastereoisomer B	4.10×10^{-8}	4.85×10^{-7}	32	0.108	1.280	3.28		
Tricyclazole	2.67×10^{-5}	1.09×10^{-3}	1600	8.46	346.2	1.40	3.16×10^{-6}	3.00
Triflumizole	1.47×10^{-6}	3.53×10^{-6}	12500	36.16	86.90		4.07×10^{-8}	
Triforine	2.67×10^{-5}	5.16×10^{-4}	30	0.069	1.332	2.20	3.87×10^{-4}	2.3
Vinclozolin	1.33×10^{-5}	8.81×10^{-5}	1000	3.495	23.14	3.00	3.81×10^{-6}	2.6
Warfarin (R.)	1.55×10^{-4}	3.43×10^{-3}	17	0.0551	1.221	3.20	2.81×10^{-3}	2.96
Zineb	1.33×10^{-5}		10	0.0363		1.30	3.67×10^{-4}	3.00
Ziram	1.0×10^{-6}	1.53×10^{-4}	65	0.213	32.61	1.086	4.70×10^{-6}	2.60

Note: * The reported values for this quantity vary considerably, whereas this selected value represents the best judgment of the authors. The reader is cautioned that it may be subject to a large error.

TABLE 19.2.3
Suggested half-life classes of fungicides in various environmental compartments at 25°C

Compound	Air class	Water class	Soil class	Sediment class
Benomyl	1	4	6	7
Captan	2	2	5	5
Chloropicrin	4	3	3	4
Chlorothalonil	4	4	5	6
Thiram	4	4	5	6

Class	Mean half-life (hours)	Range (hours)
1	5	< 10
2	17 (~ 1 day)	10–30
3	55 (~ 2 days)	30–100
4	170 (~ 1 week)	100–300
5	550 (~ 3 weeks)	300–1,000
6	1700 (~ 2 months)	1,000–3,000
7	5500 (~ 8 months)	3,000–10,000
8	17000 (~ 2 years)	10,000–30,000
9	55000 (~ 6 years)	> 30,000

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