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# 17 Herbicides

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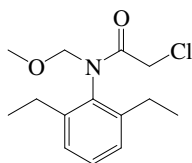
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	Dinitramine	3542
	Fluchloralin	3564
	Isopropalin	3575
	Nitralin	3610
	Oryzalin	3616
	Pendimethalin	3620
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	Bifenox	3484
	Fluorodifen	3568
	Nitrofen	3612
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	Dinoseb	3544
	PCP (Pentachlorophenol) (See <a href="#">Chapter 14</a> . Phenolic Compounds and <a href="#">Chapter 18</a> . Insecticides)	
	Phenoxyalkanoic acids:	
	2,4-D	3517
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	Fenoprop	3560
	MCPA	3584
	MCPB	3587
	Mecoprop	3589
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## 17.1 LIST OF CHEMICALS AND DATA COMPILATIONS (By Functional Group)

### 17.1.1 HERBICIDES

#### 17.1.1.1 Alachlor



Common Name: Alachlor

Synonym: alachlore, alochlor, Alanex, Bronco, Bullet, Cannon, Lasso, Lazo, metachlor, Pillarzo

Chemical Name: 2-chloro-2,6-diethyl-*N*-methoxymethylacetanilide; 2-chloro-*N*-(2,6-diethylphenyl)-*N*-(methoxymethyl)acetamide

Uses: pre-emergence, early post-emergence or soil-incorporated herbicide to control most annual grasses and many annual broadleaf weeds in beans, corn, cotton, milo, peanuts, peas, soybeans, sunflower, and certain woody ornamentals.

CAS Registry No: 15972-60-8

Molecular Formula:  $C_{14}H_{20}ClNO_2$

Molecular Weight: 269.768

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

40 (Lide 2003)

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

100 (at 0.02 mmHg, Ashton & Crafts 1981; Herbicide Handbook 1989; Worthing & Hance 1991; Montgomery 1993; Tomlin 1994; Milne 1995)

135 (at 0.30 mmHg, Herbicide Handbook 1989; Milne 1995)

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

1.133 ( $25^{\circ}C$ , Hartley & Kidd 1987; Montgomery 1993; Tomlin 1994)

Molar Volume ( $cm^3/mol$ ):

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

Dissociation Constant  $pK_a$ :

Enthalpy of Fusion,  $\Delta H_{fus}$  (kJ/mol):

29.288 (DSC method, Plato 1972)

Entropy of Fusion,  $\Delta S_{fus}$  (J/mol K):

Fugacity Ratio at  $25^{\circ}C$  (assuming  $\Delta S_{fus} = 56$  J/mol K), F: 0.713 (mp at  $40^{\circ}C$ )

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

242 ( $20^{\circ}C$ , Weber 1972; Weber et al. 1980)

200 (Bailey & White 1965)

242 (Herbicide Handbook 1974, 1978, 1983, 1989; Martin & Worthing 1977)

240 (Hartley & Graham-Bryce 1980; Beste & Humburg 1983)

148 (Khan 1980)

242 (Ashton & Crafts 1981; Worthing & Walker 1987, Worthing & Hance 1991)

242 (Hartley & Kidd 1983, 1987; Tomlin 1994)

130 ( $20^{\circ}C$ , selected, Suntio et al. 1988; quoted, Majewski & Capel 1995)

148, 242 (literature data variability, Heller et al. 1989)

140 ( $23^{\circ}C$ , Budavari 1989)

240 (Wauchope 1989)

240 ( $20$ – $25^{\circ}C$ , selected, Wauchope et al. 1992; Hornsby et al. 1996)

23.5 (calculated-group contribution fragmentation method, Kühne et al. 1995)

140 ( $23^{\circ}C$ , Milne 1995)

512 (predicted-AQUAFAC, Lee et al. 1996)

532, 785 (supercooled liquid  $S_L$ : literature derived value LDV, final adjust value FAV, Muir et al. 2004)

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

0.00293	(20°C, Weber 1972; Worthing & Walker 1987, Worthing & Hance 1991)
0.00293	(Herbicide Handbook 1974, 1983, 1989)
0.00293	(20–25°C, Weber et al. 1980)
0.00293	(Ashton & Crafts 1981; Schnoor & McAvoy 1981; Schnoor 1992)
0.00290	(Beste & Humburg 1983)
0.00290	(Hartley & Kidd 1987; Worthing & Hance 1991; Tomlin 1994)
0.00300	(20°C, selected, Suntio et al. 1988; quoted, Majewski & Capel 1995)
0.00187	(20–25°C, selected, Wauchope et al. 1992; Hornsby et al. 1996)
0.00413	(Montgomery 1993)
0.0064. 0.0044	(supercooled liquid $P_L$ : literature derived value LDV, final adjust value FAV, Muir et al. 2004)

Henry's Law Constant (Pa·m<sup>3</sup>/mol at 25°C or as indicated. Additional data at other temperatures designated \* are compiled at the end of this section):

$6.20 \times 10^{-3}$	(20°C, calculated-P/C, Suntio et al. 1988)
$8.43 \times 10^{-4}$	(wetted-wall-GC/ECD, Fendinger & Glotfelty 1988)
$3.26 \times 10^{-3}$	(calculated-P/C, Taylor & Glotfelty 1988)
$1.12 \times 10^{-3}$	(fog chamber-GC/ECD, Fendinger et al. 1989)
$8.38 \times 10^{-4}$	(23°C, known LWAPC of Fendinger et al. 1989, Meylan & Howard 1991)
$1.21 \times 10^{-5}$	(bond-estimated LWAPC, Meylan & Howard 1991)
$3.26 \times 10^{-3}$	(20°C, calculated-P/C, Muir 1991)
$6.20 \times 10^{-3}$	(calculated-P/C, Montgomery 1993)
$3.22 \times 10^{-3}$	(Gish et al. 1995)
$7.24 \times 10^{-3}$ *	(Gas stripping-GC/MS, measured range 10–25°C, Gautier et al. 2003)
$\ln [H'/(M \text{ atm}^{-1})] = -20.946 + 9200/(T/K)$ ; temp range 2830298 K (gas stripping-GC/MS, Gautier et al. 2003)	
0.00101. 1.49	(literature derived value LDV, final adjust value FAV, Muir et al. 2004)

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

2.92	(Leo et al. 1971)
2.30	(Kenaga 1980)
2.64	(Rao & Davidson 1980)
3.087	(shake flask, Dubelman & Bremer 1983)
3.52	(shake flask, Log P Database, Hansch & Leo 1987)
3.27	(RP-HPLC-RT correlation, Sicbaldi & Finizio 1993)
3.52	(recommended, Sangster 1993)
3.52	(recommended, Hansch et al. 1995)
3.27	(RP-HPLC-RT correlation, Finizio et al. 1997)
3.09	(literature derived value LDV, Muir et al. 2004)

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

9.31	(final adjust value FAV, Muir et al. 2004)
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## Bioconcentration Factor, log BCF:

1.45	(calculated-solubility, Kenaga 1980)
0.954	(calculated- $K_{OC}$ , Kenaga 1980)
1.88	(Schnoor & McAvoy 1981, Schnoor 1992)
0.778	(freshwater fish, Call et al. 1984)
1.70	(Pait et al. 1992)

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

2.28	(soil, Beestman & Demming 1976)
2.32	(soil, calculated, Kenaga & Goring 1980)
2.30	(soil, Kenaga 1980)
1.70	(sediment/water, Schnoor & McAvoy 1981)

- 1.91 (soil, average for soils 2–7, Weber & Peter 1982)  
 2.08 (soil, screening model calculations, Jury et al. 1987b)  
 2.28 (Carsel 1989)  
 2.18, 2.23, 2.28, 2.53 (soil, lit. values, Bottoni & Funari 1992)  
 2.23 (soil, 20–25°C, selected, Wauchope et al. 1992; Hornsby et al. 1996)  
 1.63–2.28 (quoted values, Montgomery 1993)  
 2.21 (selected, Wienhold & Gish 1994)  
 2.28 (soil, calculated-MCI  $^1\chi$ , Sabljic et al. 1995)  
 2.28; 2.53 (soil, quoted exptl.; estimated-general model using molecular descriptors, Gramatica et al. 2000)  
 2.22, 2.22, 2.20 (soils: organic carbon OC  $\geq 0.1\%$ , OC  $\geq 0.5\%$ ,  $0.1 \leq \text{OC} < 0.5\%$ , average, Delle Site 2001)

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

- Volatilization:  $k(\text{measured}) = 9000 \text{ d}^{-1}$  and  $k(\text{estimated}) = 49000 \text{ d}^{-1}$  (Glottfelty et al. 1989);  
 estimated  $t_{1/2} = 2444 \text{ d}$  from 1-m depth of water at 20°C (Muir 1991)  
 Volatilization rate  $k = 4.4 \times 10^{-4} \text{ d}^{-1}$ ,  $2.8 \times 10^{-3} \text{ d}^{-1}$ ,  $4.3 \times 10^{-3} \text{ d}^{-1}$  at 15, 25, 35°C, respectively, for commercial formulation;  $k = 5.8 \times 10^{-5} \text{ d}^{-1}$ ,  $8.7 \times 10^{-3} \text{ d}^{-1}$ ,  $1.4 \times 10^{-2} \text{ d}^{-1}$  at 15, 25, 35°C, respectively, for starch encapsulated formulation after application (Weinhold et al. 1993)  
 Photolysis:  $t_{1/2} = 2.25 \text{ h}$  in distilled water (Tanaka et al. 1981; quoted, Cessna & Muir 1991); 640 ppb contaminated water in the presence of  $\text{TiO}_2$  and  $\text{H}_2\text{O}_2$  photodegraded to 3.5 ppb by 15 h solar irradiation with complete degradation after 75 h (Muszkat et al. 1992).  
 Oxidation: rate constant k, for gas-phase second order rate constants,  $k_{\text{OH}}$  for reaction with OH radical,  $k_{\text{NO}_3}$  with  $\text{NO}_3$  radical and  $k_{\text{O}_3}$  with  $\text{O}_3$  or as indicated, \*data at other temperatures see reference:  
 $k(\text{aq.}) = (3.8 \pm 0.4) \text{ M}^{-1} \text{ s}^{-1}$  for direct reaction with ozone in water at pH 2–6.0 and 21°C, with a half-life of 2.4 h at pH 7 (Yao & Haag 1991).  
 $k(\text{calc}) = 7 \times 10^9 \text{ M}^{-1} \text{ s}^{-1}$  for the reaction with hydroxyl radical in aqueous solutions at  $24 \pm 1^\circ\text{C}$  (Haag & Yao 1992)  $k_{\text{OH}} = 2.3 \times 10^{-11} \text{ cm}^3 \cdot \text{molecule}^{-1} \text{ s}^{-1}$  with calculated tropospheric lifetime about 0.5 d at 298 K assuming an average OH concn of  $1 \times 10^6 \text{ molecule/cm}^3$  (Gautier et al. 2003)  
 Hydrolysis: alkaline chemical hydrolysis  $t_{1/2} > 365 \text{ d}$  (Schnoor & McAvoy 1981; quoted, Schnoor 1992).  
 Biodegradation:  $t_{1/2} < 6$  months for 0.07  $\mu\text{g/mL}$  to biodegrade in ground water,  $t_{1/2} > 15$  months for 10.0  $\mu\text{g/mL}$  to biodegrade in groundwater both at 25°C and  $t_{1/2} < 12 \text{ wk}$  for 3.2  $\mu\text{g/mL}$  to biodegrade in soil-water suspension at 35°C (Weidner 1974; quoted, Muir 1991);  
 $t_{1/2} = 23 \text{ d}$  for 0.244  $\mu\text{g/mL}$  to biodegrade in river water at 23°C with biodegradation rate  $k = 0.030 \text{ d}^{-1}$  (Schnoor et al. 1982; quoted, Muir 1991);  
 $t_{1/2} = 18 \text{ d}$  from screening model calculations (Jury et al. 1987b);  
 $t_{1/2} > 6 \text{ wk}$  for 0.01–1.0  $\mu\text{g/mL}$  to biodegrade in sewage effluent lake water at 28°C (Novick & Alexander 1985; quoted, Muir 1991);  
 overall degradation rate constant  $k = 0.0403 \text{ h}^{-1}$  with  $t_{1/2} = 17.2 \text{ h}$  in sewage sludge and rate constant  $k = 0.1601 \text{ d}^{-1}$  with  $t_{1/2} = 4.3 \text{ d}$  in garden soil (Müller & Buser 1995).

#### Biotransformation:

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

#### Half-Lives in the Environment:

- Air: tropospheric lifetime of 0.5 d for gas phase reaction with OH radicals; wet deposition lifetime estimated to be 2.8 d in the atmosphere by rainfall (Gautier et al. 2003)  
 Surface water:  $t_{1/2} = 23 \text{ d}$  for 0.244  $\mu\text{g/mL}$  to biodegrade in river water at 23°C with biodegradation rate  $k = 0.030 \text{ d}^{-1}$  (Schnoor et al. 1982; quoted, Muir 1991);  
 $t_{1/2} > 6 \text{ wk}$  for 0.01–1.0  $\mu\text{g/mL}$  to biodegrade in sewage effluent lake water at 28°C (Novick & Alexander 1985; quoted, Muir 1991);  
 $k(\text{measured}) = (3.8 \pm 0.4) \text{ M}^{-1} \text{ s}^{-1}$  for direct reaction with ozone in water at pH 2–6 and 21°C, with  $t_{1/2} = 2.4 \text{ h}$  at pH 7 (Yao & Haag 1991).  
 Ground water:  $t_{1/2} < 6$  months for 0.07  $\mu\text{g/mL}$  to biodegrade in groundwater, and  $t_{1/2} > 15$  months for 10.0  $\mu\text{g/mL}$  to biodegrade in groundwater both at 25°C (Weidner 1974; quoted, Muir 1991) reported  $t_{1/2} = 7, 4\text{--}21$  and 38 d (Bottoni & Funari 1992)  
 Sediment:

Soil: dissipation  $t_{1/2} = 7.8$  d in soil (Beestman & Demming 1974); measured dissipation rate  $k = 0.077$  d<sup>-1</sup> (Zimdahl & Clark 1982);  
 $t_{1/2} = 23$  and  $5.7$  d in soil containing 6 and 15% moisture, respectively (Walker & Brown 1985);  
 $t_{1/2} = 18$  d from screening model calculations (Jury et al. 1987b);  
estimated dissipation rate  $k = 0.020$  and  $0.036$  d<sup>-1</sup> (Nash 1988);  
field  $t_{1/2} < 1.5$  wk by using field lysimeters (Bowman 1990);  
degradation rate constant  $k = (4.52 \pm 0.192) \times 10^{-2}$  d<sup>-1</sup> with  $t_{1/2} = 15.3$  d in control soil and  $k = (7.27 \pm 0.772) \times 10^{-2}$  d<sup>-1</sup> with  $t_{1/2} = 9.53$  d in pretreated soil in the field;  $k = (2.77 \pm 0.226) \times 10^{-2}$  d<sup>-1</sup> with  $t_{1/2} = 25$  d in control soil and  $k = (14.1 \pm 1.75) \times 10^{-2}$  d<sup>-1</sup> with  $t_{1/2} = 4.93$  d in pretreated soil once only in the laboratory (Walker & Welch 1991);  
selected field  $t_{1/2} = 15$  d (Wauchope et al. 1992; Hornsby et al. 1996; quoted, Richards & Baker 1993);  
soil  $t_{1/2} = 30$  d (quoted, Pait et al. 1992);  
reported  $t_{1/2} = 7, 4\text{--}21$  and  $38$  d (Bottoni & Funari 1992);  
soil  $t_{1/2} = 14\text{--}28$  d (Di Guardo et al. 1994);  
dissipation  $t_{1/2} = 42$  d from soil surface (Gish et al. 1995);  
degradation  $t_{1/2} = 4.3$  d in garden soil (Müller & Buser 1995);  
 $t_{1/2} = 15$  d (selected, Halfon et al. 1996);  
dissipation  $t_{1/2}(\text{calc}) = 5$  and  $5.3$  d in soil in model ecosystem,  $t_{1/2} = 3.3$  and  $3.4$  d in water in model ecosystem (Ramesh & Maheswari 2004).

Biota: biochemical  $t_{1/2} = 18$  d from screening model calculations (Jury et al. 1987b).

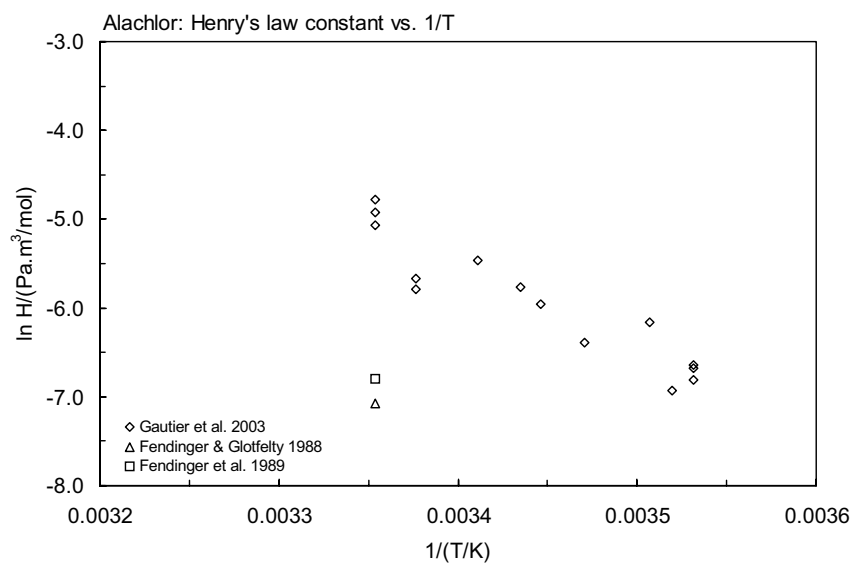
**TABLE 17.1.1.1.1**  
**Reported Henry's law constants of alachlor at various temperatures**

Gautier et al. 2003

gas stripping-GC/MS

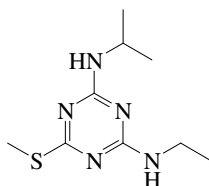
$t/^{\circ}\text{C}$	$H/(\text{Pa m}^3/\text{mol})$	$t/^{\circ}\text{C}$	$H/(\text{Pa m}^3/\text{mol})$
10	$1.097 \times 10^{+3}$	23	$3.46 \times 10^{+3}$
10	$1.26 \times 10^{+3}$	25	$6.33 \times 10^{+3}$
10	$1.30 \times 10^{+3}$	25	$8.44 \times 10^{+3}$
11	$9.76 \times 10^{+4}$	25.0	$7.24 \times 10^{+3}$
12	$2.115 \times 10^{+3}$		
15	$1.68 \times 10^{+3}$	Arrhenius expression:	
17	$2.58 \times 10^{+3}$	$\ln H'/(M \text{ atm}^{+1}) = -A + B/(T/K)$	
18	$3.13 \times 10^{+3}$	A	20.946
20	$4.24 \times 10^{+3}$	B	9200
23	$3.07 \times 10^{+3}$		





**FIGURE 17.1.1.1.1** Logarithm of Henry's law constant versus reciprocal temperature for alachlor.

## 17.1.1.2 Ametryn



Common Name: Ametryn

Synonym: Amephyt, Ametrex, Evik, Gesapax

Chemical Name: 6-methylthio-2-(ethylamino)-4-(isopropylamino)-1,3,5-triazine; N-ethyl-N'-(1-methylethyl)-6-(methyl-thio)-1,3,5-triazine-2,4-diamine

Uses: herbicide to control broadleaf and grass weeds in corn, sugarcane, some citrus fruits, and in noncropland; also used as pre-harvest and post-harvest dessicant in potatoes to control crop and weeds.

CAS Registry No: 834-12-8

Molecular Formula:  $C_9H_{17}N_5S$

Molecular Weight: 227.330

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

88 (Lide 2003)

Boiling Point ( $^{\circ}C$ ): 328.78 (Rordorf 1989)

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

1.19 (Hartley & Kidd 1987; Worthing & Hance 1991; Montgomery 1993; Tomlin 1994)

Molar Volume ( $cm^3/mol$ ):

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

Dissociation Constant:

4.00 ( $pK_a$ , Weber 1970; quoted, Bintein & Devillers 1994)

4.10 ( $pK_a$ , Worthing & Hance 1991; Montgomery 1993)

10.07 ( $pK_b$ , Wauchope et al. 1992; Hornsby et al. 1996)

9.90 ( $pK_b$ , Tomlin 1994)

Enthalpy of Vaporization,  $\Delta H_v$  (kJ/mol):

91.96 (Rordorf 1989)

Enthalpy of Fusion,  $\Delta H_{fus}$  (kJ/mol):

19.8 (Rordorf 1989)

Entropy of Fusion,  $\Delta S_{fus}$  (J/mol K):

55 (Rordorf 1989)

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

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

700 (Woodford & Evans 1963)

405, 195, 192 ( $26^{\circ}C$ , shake flask-UV at pH 3.0, 7.0, 10.0, Ward & Weber 1968)

185 (Martin & Worthing 1977; Herbicide Handbook 1978)

185 ( $20^{\circ}C$ , Khan 1980; Ashton & Crafts 1981; Verschueren 1983)

194 (Weber et al. 1980)

185 ( $20^{\circ}C$ , Hartley & Kidd 1987; Herbicide Handbook 1989; Worthing & Hance 1991; Montgomery 1993; Milne 1995)

185 ( $20$ – $25^{\circ}C$ , selected, Wauchope et al. 1992; Hornsby et al. 1996)

200 (Tomlin 1994)

134 (calculated-group contribution fragmentation method, Kühne et al. 1995)

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

$1.12 \times 10^{-4}$  ( $20^{\circ}C$ , extrapolated-Antoine eq. from gas saturation-GC measurements, measured range  $50$ – $130^{\circ}C$ , Friedrich & Stambach 1964) (See figure at the end of this section.)

$\log(P/mmHg) = 11.911 - 4933/(T/K)$ , temp range  $50$ – $130^{\circ}C$  (gas saturation-GC, data presented in Antoine eq., Friedrich & Stambach 1964) (See figure at the end of this section.)

- $1.12 \times 10^{-4}$  (20°C, Khan 1980; Ashton & Crafts 1981; Verschueren 1983)
- $1.12 \times 10^{-4}$  (20°C, Hartley & Kidd 1987; Worthing & Hance 1991; Montgomery 1993)
- $\log(P_g/kPa) = 11.036 - 5270/(T/K)$ , temp range 323–403 K, (solid, Antoine eq., Stephenson & Malanowski 1987)
- $1.00 \times 10^{-4}$  (20°C, selected, Suntio et al. 1988)
- $1.12 \times 10^{-4}$ ,  $4.40 \times 10^{-4}$  (20°C, 30°C, Herbicide Handbook 1989)
- $3.74 \times 10^{-4}$ ,  $1.40 \times 10^{-2}$ , 0.30, 4.40, 46 (25, 50, 70, 100, 125°C, gas saturation-GC, Rordorf 1989)
- $\log(P_g/Pa) = 16.85 - 6048.6/(T/K)$ ; measured range 49.5–85°C (gas saturation-GC, Rordorf 1989)
- $\log(P_L/Pa) = 13.396 - 4803.6/(T/K)$ ; measured range 49.5–140°C (gas saturation-GC, Rordorf 1989)
- $3.65 \times 10^{-4}$  (20–25°C, selected, Wauchope et al. 1992; Hornsby et al. 1996)
- $3.65 \times 10^{-4}$  (Tomlin 1994)

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

- $1.20 \times 10^{-4}$  (20°C, calculated, Suntio et al. 1988)
- $1.38 \times 10^{-4}$  (calculated-P/C, Montgomery 1993)
- $1.23 \times 10^{-4}$  (calculated-P/C, this work)

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

- 2.69 (Kenaga & Goring 1980)
- 2.58 (Gerstl & Helling 1987)
- 2.98 (shake flask, Log P Database, Hansch & Leo 1987)
- 2.82 (Worthing & Hance 1991)
- 2.98 (shake flask, Biagi et al. 1991)
- 3.07 (RP-HPLC-RT correlation, Finizio et al. 1991)
- 2.88 (RP-HPLC-RT correlation, Sicbaldi & Finizio 1993)
- 2.98 (recommended, Sangster 1993)
- 2.63 (Tomlin 1994)
- 2.61 (shake flask-UV, Liu & Qian 1995)
- 2.58 (calculated-RP-HPLC- $k'$  correlation, Liu & Qian 1995)
- 2.83 (Milne 1995)
- 2.98 (recommended, Hansch et al. 1995)
- 2.88 (RP-HPLC-RT correlation, Finizio et al. 1997)

Bioconcentration Factor,  $\log BCF$ :

- 1.52 (calculated-S, Kenaga 1980)
- 1.32 (calculated- $K_{oc}$ , Kenaga 1980)

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

- 2.59 (soil, Hamaker & Thompson 1972;)
- 2.40 (soil, calculated, Kenaga & Goring 1980)
- 2.59 (soil, Kenaga & Goring 1980)
- 2.59 (Rao & Davidson 1980)
- 2.59, 2.86 (quoted, calculated-MCI  $\chi$ , Gerstl & Helling 1987)
- 2.59, 2.51 (reported as  $\log K_{OM}$ , estimated as  $\log K_{OM}$ , Magee 1991)
- 2.40–2.59, 2.58 (soil, quoted values, Bottoni & Funari 1992)
- 2.48 (soil, 20–25°C, selected, Wauchope et al. 1992; Hornsby et al. 1996)
- 2.23–2.44 (Montgomery 1993)
- 2.48 (Tomlin 1994)
- 2.42 (calculated- $K_{ow}$ , Liu & Qian 1995)
- 2.59 (soil, calculated-MCI  $^1\chi$ , Sabljic et al. 1995)
- 2.70, 2.59 (soil, estimated-class-specific model, estimated-general model using molecular descriptors, Gramatica et al. 2000)
- 2.52, 2.63, 2.60, 2.35 (soils with organic carbon  $OC \geq 0.5\%$  at: pH 4.5–9.0, pH 4.5–5.4, pH 5.5–6.0, pH-6.1, average, Delle Site 2001)
- 1.84, 2.23 (Kishon river sediments, sorption isotherm, Chefetz et al. 2004)

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

## Volatilization:

Photolysis:  $t_{1/2} = 10$  h for  $10 \mu\text{g mL}^{-1}$  to degrade in distilled water under  $> 290$  nm light and  $t_{1/2} = 3.3$  h in 1% acetone solution (Burkhard & Guth 1976; quoted, Cessna & Muir 1991);

$t_{1/2} = 2.25$  h for 17% of  $33 \mu\text{g mL}^{-1}$  to degrade in 0.2% aqueous solutions of the surfactant Triton X-100 and for 8% of  $33 \mu\text{g/mL}$  to degrade in distilled water both under 300 nm light (Tanaka et al. 1981; quoted, Cessna & Muir 1991).

## Oxidation:

Hydrolysis:  $t_{1/2} = 32$  d at pH 1 and  $t_{1/2} > 200$  d at pH 13 (Montgomery 1993).

## Biodegradation:

## Biotransformation:

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

## Half-Lives in the Environment:

## Air:

## Surface water:

Groundwater: reported half-lives or persistence,  $t_{1/2} = 7$ –120 d (Bottoni & Funari 1992)

## Sediment:

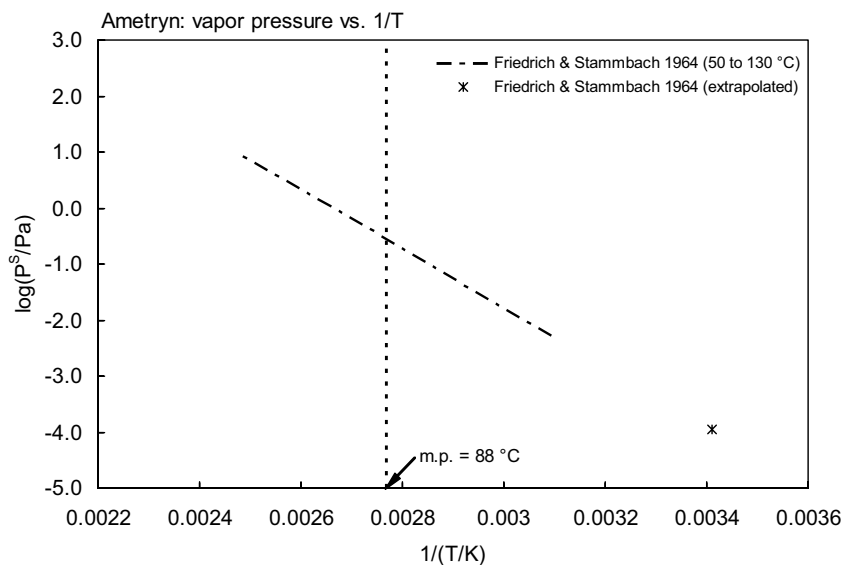
Soil:  $t_{1/2} = 6.0$  months at  $15^\circ\text{C}$  and  $t_{1/2} = 4.5$  months at  $30^\circ\text{C}$  in soils (Freed & Haque 1973);

$t_{1/2} = 70$ –120 d (Bottoni & Funari 1992);

selected  $t_{1/2} = 60$  d (Wauchope et al. 1992; Hornsby et al. 1996);

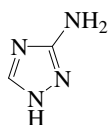
$t_{1/2} = 70$ –129 d in soil (Tomlin 1994).

## Biota:



**FIGURE 17.1.1.2.1** Logarithm of vapor pressure versus reciprocal temperature for ametryn.

## 17.1.1.3 Amitrole



Common Name: Amitrole

Synonym: Amazole, Amitrol, Amizole, aminotriazole, Azolan, Azole, cytrol, Diurol

Chemical Name: 3-amino-1,2,4-triazole; 3-amino-*s*-triazole; 1H-1,2,4-triazol-3-amine

Uses: nonselective, foliage-applied herbicide in uncropped land and orchards to control perennial weeds in certain grasses.

CAS Registry No: 61-82-5

Molecular Formula:  $C_2H_4N_4$

Molecular Weight: 84.080

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

159 (Khan 1980; Herbicide Handbook 1989; Lide 2003)

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

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

1.138 (Hartley & Kidd 1987; Herbicide Handbook 1989; Montgomery 1993; Tomlin 1994)

Molar Volume ( $cm^3/mol$ ):

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

Dissociation Constant:

9.83 ( $pK_b$ , Wauchope et al. 1992; Hornsby et al. 1996)

Enthalpy of Fusion,  $\Delta H_{fus}$  ( $kJ/mol$ ):

24.69 (DSC method, Plato 1972)

Entropy of Fusion,  $\Delta S_{fus}$  ( $J/mol K$ ):

Fugacity Ratio at  $25^{\circ}C$  (assuming  $\Delta S_{fus} = 56 J/mol K$ ), F: 0.0484 (mp at  $159^{\circ}C$ )

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

252000 (Freed & Burschel 1957)

280000 (Martin 1961; Spencer 1981)

280000 (Bailey & White 1965; Khan 1980; Weber et al. 1980; Ashton & Crafts 1981; Willis & McDowell 1982)

soluble (Wauchope 1978)

280000 (Worthing 1983, Worthing & Hance 1991)

280000 (Hartley & Kidd 1987; Herbicide Handbook 1989; Reinert 1989)

360000 ( $20-25^{\circ}C$ , selected, Wauchope et al. 1992; Lohninger 1994; Hornsby et al. 1996)

280000 ( $20^{\circ}C$  at pH 7, quoted, Montgomery 1993)

280000 ( $23^{\circ}C$ , Tomlin 1994)

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

$< 0.001$  (Agrochemicals Handbook 1983; quoted, Howard 1991)

$< 0.001$  (Hartley & Kidd 1987)

$5.50 \times 10^{-8}$  ( $20^{\circ}C$ , Worthing & Hance 1991; Tomlin 1994)

$5.87 \times 10^{-5}$  ( $20-25^{\circ}C$ , selected, Wauchope et al. 1992; Hornsby et al. 1996)

$5.51 \times 10^{-7}$  ( $20^{\circ}C$ , quoted, Montgomery 1993)

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

$< 3.04 \times 10^{-7}$  (calculated-P/C, Howard 1991)

$1.650 \times 10^{-10}$  ( $20^{\circ}C$ , calculated-P/C, Montgomery 1993)

$1.650 \times 10^{-10}$  (calculated-P/C, this work)

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

- 0.85 (shake flask, pH 7, Lichtner 1983)
- 0.52 (selected, Dao et al. 1983; Gerstl & Helling 1987)
- 0.15 (Reinert 1989; quoted, Howard 1991; Montgomery 1993)
- 0.87, -0.84 (pH 7) (Hansch et al. 1995)
- 0.87 (LOGPSTAR or CLOGP data, Sabljic et al. 1995)

Bioconcentration Factor,  $\log BCF$ :

- 0.301 (estimated-S, Lyman et al. 1982; quoted, Howard 1991)
- 0.347 (estimated- $\log K_{ow}$ , Lyman et al. 1982; quoted, Howard 1991)

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

- 2.04 (soil, estimated-molecular topology & QSAR, Sabljic 1984)
- 0.23 (calculated-MCI  $\chi$ , Gerstl & Helling 1987)
- 1.26 (Reinert 1989)
- 2.00 (soil, 20–25°C, selected, Wauchope et al. 1992; Hornsby et al. 1996)
- 1.73–2.31 (quoted, Montgomery 1993)
- 2.00 (estimated-chemical structure, Lohninger 1994)
- 1.25 (soil, calculated-MCI  $\chi$ , Sabljic et al. 1995)

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

Volatilization:

Photolysis:

Oxidation: photooxidation  $t_{1/2} = 3.2\text{--}32$  h in air, based on estimated rate constant for the vapor-phase reaction with hydroxyl radicals in air (Atkinson 1987; quoted, Howard et al. 1991).

Hydrolysis:

Biodegradation: aqueous aerobic  $t_{1/2} = 672\text{--}4032$  h, based on reported half-lives in soil and water (Freed & Haque 1973; Reinert & Rogers 1987; quoted, Howard et al. 1991); aqueous anaerobic  $t_{1/2} = 2688\text{--}16128$  h, based on estimated aqueous aerobic biodegradation half-life (Howard et al. 1991).

Biotransformation:

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

## Half-Lives in the Environment:

Air:  $t_{1/2} = 3.8$  d, based on a theoretical calculation for the vapor-phase reaction with hydroxyl radicals in the atmosphere at 25°C (GEMS 1986; quoted, Howard 1989);

$t_{1/2} = 3.2\text{--}32$  h, based on estimated rate constant for the vapor-phase reaction with hydroxyl radicals in air (Atkinson 1987; quoted, Howard et al. 1991).

Surface water:  $t_{1/2} = 672\text{--}4320$  h, based on estimated aqueous aerobic biodegradation half-life (Howard et al. 1991).

Groundwater:  $t_{1/2} = 1344\text{--}8640$  h, based on estimated aqueous aerobic biodegradation half-life (Howard et al. 1991).<sup>c</sup>

Sediment:

Soil:  $t_{1/2} = 1.4, 1.6, 1.3, 92, 36,$  and  $56$  d with disappearance rates:  $k = 0.495, 0.433, 0.533, 0.0075, 0.0193,$  and  $0.124$  d<sup>-1</sup> at pH 6.0, 7.0, 8.0, 5.3, 6.5, and 7.5 (Hamaker 1972; quoted, Nash 1988);

$t_{1/2} = 1.5$  month at 15°C and  $t_{1/2} = 1.0$  month at 30°C in soils (Freed & Haque 1973);

persistence of one month in soil (Wauchope 1978);

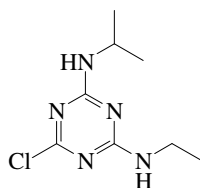
persistence in soil for ca. 2–4 wk (Herbicide Handbook 1989; Tomlin 1994);

$t_{1/2} = 672\text{--}4320$  h, based on estimated aqueous aerobic biodegradation half-life (Howard et al. 1991);

selected field  $t_{1/2} = 14$  d (Wauchope et al. 1992; Hornsby et al. 1996).

Biota:

## 17.1.1.4 Atrazine



Common Name: Atrazine

Synonym: Aatrex, Akikon, Aktikon, Aktinit, Atratol, Atred, Atrex, Candex, Fenamine, Gesaprim, Hungazin, Inakor, Primatol, Primaze, Radazine, Strazine, Triazine A, Vectal, Weedex A, Wonuk, Zeazine

Chemical Name: 2-chloro-4-(ethylamino)-6-(isopropylamino)-1,3,5-triazine; 6-chloro-*N*-ethyl-*N'*-(1-methylethyl)-1,3,5-triazine-diamine

Uses: pre-emergence and post-emergence herbicide to control some annual grasses and broadleaf weeds in corn, fallow land, rangeland, sorghum, noncropland, certain tropical plantations, evergreen nurseries, fruit crops, and lawns.

CAS Registry No: 1912-24-9

Molecular Formula:  $C_8H_{14}ClN_5$

Molecular Weight: 215.684

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

173 (Lide 2003)

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

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

1.187 (Worthing & Hance 1991; Montgomery 1993; Tomlin 1994)

Molar Volume ( $cm^3/mol$ ):

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

Dissociation Constant:

1.68 ( $pK_a$ , Weber 1970; Somasundaram et al. 1991; Bintein & Devillers 1994)

1.70 ( $pK_a$ , Weber et al. 1980; Willis & McDowell 1982; Worthing & Hance 1991; Francioso et al. 1992; Montgomery 1993; Tomlin 1994)

1.60 ( $pK_a$ , Yao & Haag 1991; Haag & Yao 1992)

12.32 ( $pK_b$ , Wauchope et al. 1992; Hornsby et al. 1996)

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

Enthalpy of Fusion,  $\Delta H_{fus}$  ( $kJ/mol$ ):

40.585 (DSC method, Plato 1972)

Entropy of Fusion,  $\Delta S_{fus}$  ( $J/mol\ K$ ):

Fugacity Ratio at  $20^{\circ}C$  (assuming  $\Delta S_{fus} = 56\ J/mol\ K$ ),

F: 0.0353 (mp at  $173^{\circ}C$ )

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

70.0 ( $26^{\circ}C$ , Bailey & White 1965)

50.0 (Günther et al. 1968)

31.1, 34.9, 36.8 ( $26^{\circ}C$ , shake flask-UV at pH 3.0, 7.0. 10.0, Ward & Weber 1968)

98.0 ( $50^{\circ}C$ , Getzen & Ward 1971)

33.0 (shake flask-GC, Hörmann & Eberle 1972)

29.9 (shake flask-UV, Hurle & Freed 1972)

30.0 ( $20^{\circ}C$ , Weber 1972; Worthing & Walker 1987; Worthing & Hance 1991; Burkhard & Guth 1981)

33.0 ( $27^{\circ}C$ , Ashton & Crafts 1973, 1981; Khan 1980; Herbicide Handbook 1989; Pait et al. 1992)

32.0 (Freed 1976; Beste & Humburg 1983; Jury et al. 1983)

31.5 (Spencer 1976)

33.0 (Wauchope 1978; Kenaga 1980; Kenaga & Goring 1980)

35.0 (Weber et al. 1980)

30.0 (shake flask-HPLC, Ellgehausen et al. 1981)

24.0 (Thomas 1982)

70.0 (Windholz 1983)

- 28.0 (20°C, Hartley & Kidd 1987)  
 29.9, 33, 70 (literature data variability, Heller et al. 1989)  
 33.0 (20–25°C, selected, Wauchope et al. 1992; Hornsby et al. 1996)  
 28.0, 33.0 (20°C, 27°C, Montgomery 1993)  
 33.0 (20°C, Tomlin 1994)  
 28.0 (Milne 1995)  
 4012, 4012 (supercooled liquid  $S_L$ : literature derived value LDV, final adjust value FAV, Muir et al. 2004)

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

- $44.0 \times 10^{-5}$ \* (20°C, extrapolated-Antoine eq. from gas saturation-GC measurements, measured range 50–130°C, Friedrich & Stambach 1964)  
 $\log(P/\text{mmHg}) = 13.766 - 5945/(T/K)$ , temp range 50–130°C (gas saturation-GC, data presented in graph and Antoine eq., Friedrich & Stambach 1964)  
 $4.00 \times 10^{-5}$  (20°C, Weber 1972; Worthing 1979; Worthing & Walker 1987, Worthing & Hance 1991; quoted, Khan 1980; Dobbs et al. 1984; Muir 1991)  
 $3.99 \times 10^{-5}$  (20°C, gas saturation, extrapolated from Friedrich & Stambach 1964, Spencer 1976)  
 $4.00 \times 10^{-5}$  (20°C, Hartley & Graham-Bryce 1980; Beste & Humburg 1983)  
 $4.00 \times 10^{-5}$  (20–25°C, Weber et al. 1980)  
 $4.00 \times 10^{-5}$  (20°C, Ashton & Crafts 1981)  
 $1.33 \times 10^{-4}$  (selected, Schnoor & McAvoy 1981)  
 $3.70 \times 10^{-5}$ \* (20°C, extrapolated from gas saturation measurement, Grayson & Fosbracey 1982)  
 $\ln(P/\text{Pa}) = 36.8 - 13778/(T/K)$ , for temp range 51–81.5°C, (Antoine eq., gas saturation, Grayson & Fosbracey 1982)  
 $1.13 \times 10^{-4}$  (Thomas 1982)  
 $4.00 \times 10^{-5}$  (20°C, Hartley & Kidd 1987)  
 $\log(P_s/\text{kPa}) = 12.8909 - 5945/(T/K)$ , temp range 323–403 K, (solid, Antoine eq., Stephenson & Malanowski 1987)  
 $8.70 \times 10^{-5}$  (selected, Nash 1989)  
 $3.99 \times 10^{-5}$ ,  $18.6 \times 10^{-5}$  (20°C, 30°C, Herbicide Handbook 1989)  
 $3.90 \times 10^{-5}$ \* (gas saturation-GC, measured range 40.5–125°C, Rordorf 1989)  
 $\log(P_s/\text{Pa}) = 13.27071 - 6558.5/(T/K)$ ; measured range 40.5–125°C (gas saturation-GC, Rordorf 1989)  
 $\log(P_L/\text{Pa}) = 13.396 - 4803.6/(T/K)$ ; measured range not specified (gas saturation-GC, Rordorf 1989)  
 $4.05 \times 10^{-5}$  (Riederer 1990)  
 $3.85 \times 10^{-5}$  (20–25°C, selected, Wauchope et al. 1992; Hornsby et al. 1996)  
 $4.00 \times 10^{-5}$  (20°C, Montgomery 1993)  
 $2.00 \times 10^{-5}$  (selected, Sieber et al. 1994)  
 $3.90 \times 10^{-5}$  (Tomlin 1994; quoted, Halfon et al. 1996)  
 $6.70 \times 10^{-4}$ \* (40°C, Knudsen effusion method, measured range 40–80°C, Goodman 1997)  
 $\log(P/\text{Pa}) = 16.08 - 6040/(T/K)$ ; temp range 40–80°C, Goodman 1997)  
 0.0096, 0.0096 (supercooled liquid  $P_L$ : literature derived value LDV, final adjust value FAV, Muir et al. 2004)

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

- $6.20 \times 10^{-4}$  (calculated-P/C, Jury et al. 1983, 1984, 1987a; Jury & Ghodrati 1989)  
 $2.90 \times 10^{-4}$  (20°C, calculated-P/C, Suntio et al. 1988)  
 $6.19 \times 10^{-4}$  (calculated-P/C, Taylor & Glotfelty 1988)  
 $5.70 \times 10^{-4}$  (calculated-P/C, Nash 1989)  
 $3.04 \times 10^{-4}$  (Riederer 1990)  
 $2.66 \times 10^{-4}$  (calculated-P/C, Howard 1991)  
 $2.89 \times 10^{-4}$  (20°C, calculated-P/C, Muir 1991)  
 $3.08 \times 10^{-4}$  (20°C, calculated-P/C, Montgomery 1993)  
 $1.00 \times 10^{-3}$  (calculated-P/C, Sieber et al. 1994)  
 $6.20 \times 10^{-4}$  (Gish et al. 1995)  
 $2.88 \times 10^{-4}$  (calculated-P/C, this work)  
 0.518 (final adjust value FAV, Muir et al. 2004)



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

- 2.75 (shake flask-GC, Erkel & Walum 1979)
- 2.63 (HPLC-RT correlation, Veith et al. 1979, 1980; Veith & Kosian 1982)
- 2.35 (Rao & Davidson 1980)
- 2.71 (shake flask-both phases analyzed by GC and UV spec., Brown & Flagg 1981)
- 2.40, 2.21 (HPLC-k' correlation, McDuffie 1981)
- 2.75 (shake flask, Ellgehausen et al. 1981)
- 2.80 (Elgar 1983)
- 2.05 (RP-HPLC-k' correlation, Braumann et al. 1983)
- 2.64 (shake flask-GC, Geyer et al. 1984)
- 2.75 (Hansch & Leo 1985)
- 2.64 (OECD method 1981, Kerler & Schönherr 1988)
- 2.68 (Lopez-Avila et al. 1989)
- 2.61, 2.61 (RP-HPLC-RT correlation, calculated, Finizio et al. 1991)
- 2.34 (Worthing & Hance 1991; Milne 1995)
- 2.10 (shake flask, pH 7, Baker et al. 1992)
- 2.33–2.80 (quoted values, Montgomery 1993)
- 2.75 (recommended, Sangster 1993)
- 2.42 (RP-HPLC-RT correlation, Sicbaldi & Finizio 1993)
- 2.50 (Tomlin 1994)
- 2.27 (shake flask-UV, Liu & Qian 1995)
- 2.61 (selected, Hansch et al. 1995)
- 2.43 (RP-HPLC-RT correlation, Finizio et al. 1997)
- 2.00 (RP-HPLC-RT correlation using short ODP column, Donovan & Pescatore 2002)
- 2.63 ± 0.07, 2.47 ± 0.15, 2.46 ± 0.09 (shake flask, isocratic RP-HPLC-k' correlation, gradient RP-HPLC-k' correlation, Paschke et al. 2004)
- 2.40 (literature derived value LDV, Muir et al. 2004)

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

- 9.08 (final adjust value FAV, Muir et al. 2004)

## Bioconcentration Factor, log BCF:

- 2.00 (vegetation, correlated- $K_{ow}$ , Beynon et al. 1972; quoted, Travis & Arms 1988)
- 1.04 (Metcalf & Sanborn 1975; quoted, Kenaga & Goring 1980; Isensee 1991)
- 1.00 (Isensee 1976)
- 0.50 (whitefish, Burkhard & Guth 1976)
- 0.90 (fathead minnow, Veith et al. 1979)
- 0.30 (catfish, Ellgehausen et al. 1980; quoted, Howard 1991)
- 0.26 (*Daphnia magna*, wet wt. basis, Ellgehausen et al. 1980)
- 0.48 (*Corygonus fera*. at 12°C, Gunkel & Streit 1980)
- 1.93, 0.845 (calculated-S,  $K_{OC}$ , Kenaga 1980)
- < 0.90 (Veith et al. 1980)
- 1.90 (selected, Schnoor & McAvoy 1981)
- 1.93, 1.77 (estimated-S, estimated- $K_{ow}$ , Bysshe 1982)
- 0.90 (fathead minnow, Veith & Kosian 1982)
- 2.00 (mottled sculpin, Lynch et al. 1982)
- 1.60 (activated sludge, Freitag et al. 1984)
- 1.00 (golden ide, Freitag et al. 1985)
- 0.477, 0.954, 0.845, 0.778 (zebrafish: egg, embryo, yolk sac fry, juvenile; Görg & Nagel 1990)
- 0.78 (*Brachydanio rerio*, Görg & Nagel 1990)
- 0.983 (*Hydrilla*, Hinman & Klaine 1992)
- 1.98, 0.748, 0.230 (algae *Scenedesmus acutus*, catfish *Ictalurus melas*, *Daphnia magna*, wet wt basis, Wang et al. 1996)

## Bioaccumulation Factor, log BAF:

- 1.710 (algae, Ellgehausen et al. 1980;)
- 0.329 (catfish, Ellgehausen et al. 1980)
- 0.261 (daphnids, Ellgehausen et al. 1980)
- 1.72, 0.477, 1.60 (algae, fish, sludge, Klein et al. 1984)
- 1.70, < 1.00, 1.60 (algae, fish, sludge, Freitag et al. 1985)

Sorption Partition Coefficient, log  $K_{OC}$  at 25°C or as indicated:

- 2.17 (soil, Hamaker & Thompson 1972)
- 2.09 (average of 4 soils, Rao & Davidson 1979; Davidson et al. 1980)
- 2.81 (calculated, Kenaga & Goring 1980; Kenaga 1980)
- 2.20 (average of soils/sediments, Rao & Davidson 1980)
- 2.21 (average of 56 soils from lit. review, Rao & Davidson 1980)
- 2.33 (a Georgia pond sediment, sorption isotherms by shake flask-GC/ECD, Brown & Flagg 1981)
- 1.59 (a Swiss soil, Burkhard & Guth 1981)
- 3.11, 2.31; 1.94, 2.42 (estimated-S, calculated-S and mp; estimated- $K_{OW}$ , Karickhoff 1981)
- 0.7–1.48 (selected, sediment/water, Schnoor & McAvoy 1981)
- 2.18 (soil, Thomas 1982)
- 2.29–3.18 (Wolf & Jackson 1982)
- 3.23–4.13 (Means & Wijayarathne 1982)
- 2.21 (soil average, Jury et al. 1983)
- 1.63–3.29 (Wauchope & Myers 1985; 1991)
- 2.46 (calculated-MCI  $\chi$ , Gerstl & Helling 1987)
- 2.20 (soil, screening model calculations, Jury et al. 1987a,b; Jury & Ghodrati 1989)
- 1.92 (RP-HPLC- $k'$  correlation, cyanopropyl column, Hodson & Williams 1988)
- 2.21 (estimated as log  $K_{OM}$ , Magee 1991)
- 2.0, 2.18, 2.17–2.81, 2.26 (soil, literature values, Bottoni & Funari 1992)
- 2.27, 2.41, 2.59, 2.16 (soils, no. 1, 2, 3, 4; Francioso et al. 1992)
- 1.81 (soil, HPLC-screening method, mean value from different stationary and mobile phases, Kördel et al. 1993, 1995a,b)
- 2.00 (soil, 20–25°C, selected, Wauchope et al. 1992; quoted, Dowd et al. 1993; Richards & Baker 1993; Wienhold & Gish 1994; Hornsby et al. 1996)
- 1.95–2.71 (quoted values, Montgomery 1993)
- 2.60 (soil with 9.23% organic carbon, Donati et al. 1994)
- 2.04 (agricultural soil, Dousset et al. 1994)
- 2.40 (estimated-chemical structure, Lohninger 1994)
- 2.05 (soil with low organic carbon 0.18%, Roy & Krapac 1994)
- 1.95–2.19 (Tomlin 1994)
- 2.23 (calculated- $K_{OW}$ , Liu & Qian 1995)
- 2.24 (soil, calculated-MCI  $\chi$ , Sabljic et al. 1995)
- 1.81; 2.36 (HPLC-screening method; calculated-PCKOC fragment method, Müller & Kördel 1996)
- 1.00 (sediment/water, Chung et al. 1996)
- 2.64 (Levy wetland soil, sorption equilibrium technique, 24°C, Mersie & Seybold 1996)
- 2.14–2.21; 2.03–2.12 (Teufelsweiher pond sediment: field measurement; exptl laboratory data, Gao et al. 1997)
- 2.19 (sediment from Teufelsweiher pond, batch equilibrium isotherm, Gao et al. 1998)
- 1.93, 1.80–1.85, 1.81 (soil, liquid sewage sludge amended soil, sludge, pH 7.2, batch equilibrium-sorption isotherm, Celis et al. 1998)
- 1.93, 1.83, 1.79 (soil +  $CaCl_2$  at pH 7.2, soil + liquid sewage sludge and dissolved organic matter at pH 7.5, soil + liquid sewage sludge at pH 7.2, batch equilibrium-sorption isotherm, Celis et al. 1998)
- 2.566, 1.72, 1.75, 1.505, 2.40 (first generation Eurosoils ES-1, ES-2, ES-3, ES-4, ES-5, shake flask/batch equilibrium-HPLC/UV, Gawlik et al. 1998, 1999)
- 2.24, 2.45; 2.82., 1.81, 2.81, 1.98, 1.99 (quoted lit., calculated- $K_{OW}$ ; HPLC-screening method with different LC-columns, Szabo et al. 1999)
- 2.154, 1.97, 1.77, 1.61, 2.496 (second generation Eurosoils ES-1, ES-2, ES-3, ES-4, ES-5, shake flask/batch equilibrium-HPLC/UV, Gawlik et al. 1999)

- 1.69 (sandy loam soil, column equilibrium method, 20°C, Xu et al. 1999)
- 2.154, 1.969, 1.769, 1.610, 2.486 (second generation Eurosoils ES-1, ES-2, ES-3, ES-4, ES-5, shake flask/batch equilibrium-HPLC/UV and HPLC-k' correlation, Gawlik et al. 2000)
- 2.24; 2.27, 2.47 (soil, quoted obs.; estimated-class-specific model, estimated-general model using molecular descriptors, Gramatica et al. 2000)
- 2.59, 2.16 (average values for sediments, soils, Delle Site 2001)
- 2.31, 2.17, 2.56 (soils: organic carbon  $OC \geq 0.1\%$ ,  $OC \geq 0.5\%$ ,  $0.1 \leq OC < 0.5\%$ , and pH 3.2–8.2, average, Delle Site 2001)
- 2.34, 2.24, 2.06, 2.59 (soils with organic carbon  $OC \geq 0.5\%$  at: pH 3.2–5.0, pH 5.1–5.9, pH-6.0, pH 4.4–7.7, average, Delle Site 2001)
- 1.77, 2.10 (Kishon river sediments, sorption isotherm, Chefetz et al. 2004)

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

- Volatilization: initial rate constant  $k = 6.4 \times 10^{-4} \text{ h}^{-1}$  and predicted rate constant  $k = 4.2 \times 10^{-4} \text{ h}^{-1}$  from soil with  $t_{1/2} = 1650 \text{ h}$  (Thomas 1982);
- $t_{1/2} = 97 \text{ d}$  (Jury et al. 1983; quoted, Grover 1991);
- rate constants  $k(\text{measured}) = 1100 \text{ d}^{-1}$  and  $k(\text{est.}) = 6000 \text{ d}^{-1}$  (Glottfelty et al. 1989);
- Half-lives from soil surfaces:  $t_{1/2} = 655$  to  $> 1000 \text{ d}$  in peat soil and  $t_{1/2} = 143\text{--}939 \text{ d}$  in sandy soil; half-lives from plant surfaces:  $t_{1/2} = 25.6 \text{ d}$  in bean,  $t_{1/2} = 24.3 \text{ d}$  in turnips and  $t_{1/2} = 14.6 \text{ d}$  in oats at  $20 \pm 1^\circ\text{C}$  (Dörfler et al. 1991)
- Volatilization rate  $k = 1.4 \times 10^{-4} \text{ d}^{-1}$ ,  $2.6 \times 10^{-3} \text{ d}^{-1}$ ,  $4.4 \times 10^{-3} \text{ d}^{-1}$  at 15, 25, 35°C, respectively, for commercial formulation;  $k = 1.2 \times 10^{-5} \text{ d}^{-1}$ ,  $4.8 \times 10^{-4} \text{ d}^{-1}$ ,  $8.1 \times 10^{-4} \text{ d}^{-1}$  at 15, 25, 35°C, respectively, for starch-encapsulated formulation after application (Weinhold et al. 1993)
- Photolysis:  $t_{1/2} = (19 \pm 9) \text{ h}$  under summer sunlight of  $9.1 \text{ h d}^{-1}$  exposure and  $t_{1/2} = 61 \pm 29 \text{ h}$  under spring sunlight of  $3.7 \text{ h d}^{-1}$  exposure in 10 ppm aqueous solutions: (Burkhard et al. 1975);
- $t_{1/2} = 4.9 \text{ h}$  for 10  $\mu\text{g/mL}$  to degrade in 1% acetone solution and  $t_{1/2} = 25 \text{ h}$  for 10  $\mu\text{g/mL}$  to degrade in distilled water both under  $> 290 \text{ nm}$  light (Burkhard & Guth 1976);
- nearsurface direct sunlight photolysis rate constant  $k = 9 \times 10^{-6} \text{ d}^{-1}$  with  $t_{1/2} = 81,000 \text{ d}$  (Schnoor & McAvoy 1981; quoted, Schnoor 1992);
- $t_{1/2} = 2.25 \text{ h}$  for 17–27% of 100  $\mu\text{g/mL}$  to degrade in distilled water under 300 nm light (Tanaka et al. 1981; quoted, Cessna & Muir 1991);
- rate of photolytic degradation was slightly higher in water ( $t_{1/2} = 3\text{--}12 \text{ d}$ ) than in sediments ( $t_{1/2} = 1\text{--}4 \text{ wk}$ ) (Jones et al. 1982; quoted, Montgomery 1993);
- 40 ppb contaminated water in presence of  $\text{TiO}_2$  and  $\text{H}_2\text{O}_2$  degraded to 4 ppb after 15 h by solar irradiation with complete degradation after 75 h (Muszkat et al. 1992)
- $t_{1/2}(\text{aq.}) = 335 \text{ d}$  at pH 7 under natural light;  $t_{1/2} = 17.5 \text{ h}$  at pH 7 using mercury lamp in aqueous solution; soil photolysis  $t_{1/2} = 12 \text{ d}$  under natural light,  $t_{1/2} = 5 \text{ d}$  using mercury lamp and  $t_{1/2} = 45 \text{ d}$  using xenon lamp (Solomon et al. 1996);
- Oxidation: rate constant  $k$ , for gas-phase second order rate constants,  $k_{\text{OH}}$  for reaction with OH radical,  $k_{\text{NO}_3}$  with  $\text{NO}_3$  radical and  $k_{\text{O}_3}$  with  $\text{O}_3$  or as indicated, \*data at other temperatures see reference:
- $k_{\text{OH}} = 147.2 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$  with  $n$  half-life of 2.6 h at 25°C for the vapor-phase reaction with hydroxyl radical in air (Atkinson 1987; quoted, Howard et al. 1991);
- $k(\text{aq.}) = 5.9 \times 10^9 \text{ M}^{-1} \text{ s}^{-1}$  for the reaction (photo-Fenton with reference to acetophenone) with OH radical in aqueous solutions at pH 3.6 and  $24 \pm 1^\circ\text{C}$  (Buxton et al. 1988; quoted, Faust & Hoigné 1990; Haag & Yao 1992)
- $k(\text{aq.}) = (24 \pm 4) \text{ M}^{-1} \text{ s}^{-1}$  for direct reaction with ozone at pH 4 and 26°C;  $k = (13 \pm 1) \text{ M}^{-1} \text{ s}^{-1}$  at pH 4.2 and 21°C and  $k = (24 \pm 4) \text{ M}^{-1} \text{ s}^{-1}$  at pH 4.1 and 19°C in water, with a half-life of 1.5 h at pH 7 (Yao & Haag 1991)
- $k(\text{aq.}) = (2.6 \pm 0.4) \times 10^9 \text{ M}^{-1} \text{ s}^{-1}$  for the reaction (photo-Fenton with reference to acetophenone) with hydroxyl radical in aqueous solutions at pH 3.6 and  $24 \pm 1^\circ\text{C}$  (Haag & Yao 1992)
- $k(\text{aq.}) = 0.82 \times 10^9 \text{ M}^{-1} \text{ s}^{-1}$  for reaction with hydroxyl radical in irradiated field water (Mabury & Crosby 1996)

Hydrolysis:  $t_{1/2} \sim 70$  d at pH 3.1 of citrate buffer;  $t_{1/2} \sim 75$  d at pH 11.1 of carbonate buffer and  $t_{1/2} \sim 2$  d at 3.9 of phosphate buffer + sterile lake sediment in aqueous solutions at 25°C (Armstrong et al. 1967; quoted, Muir 1991)

Over all rate constant  $k = 7.6 \times 10^{-5} \text{ s}^{-1}$  with  $t_{1/2} = 2.5$  h at 25°C and pH 7 (Mabey & Mill 1978)

$t_{1/2} = 3.3, 14, 58, 240, 100, 12.5$ , and  $1.5$  d at pH 1, 2, 3, 4, 11, 12, and 13, respectively, in aqueous buffered solutions in soil at 25°C (Armstrong et al. 1967; quoted, Montgomery 1993);

$t_{1/2} = 244$  d without humic materials,  $t_{1/2} = 1.37$  d with the presence of 2% humic acid at pH 4 and 25°C (Li & Felbeck 1972; quoted, Howard 1991; Montgomery 1993)

$k = 3.9 \times 10^{-5} \text{ M}^{-1} \text{ s}^{-1}$  and  $k = 7.6 \times 10^{-5} \text{ M}^{-1} \text{ s}^{-1}$  with  $t_{1/2} = 66$  and  $81$  d in aqueous solutions of pH 3.1 and 11.1, respectively (Wolfe et al. 1976; quoted, Muir 1991)

$k(\text{aq.}) = 19.9 \text{ d}^{-1}$  at pH 2.9,  $k = 3.99 \text{ d}^{-1}$  at pH 4.5,  $k = 1.74 \text{ d}^{-1}$  at pH 6.0, and  $k = 0.934 \text{ d}^{-1}$  at pH 7.0 with corresponding  $t_{1/2} = 34.8, 174, 398$ , and  $742$  d all at 25°C in  $0.5 \text{ mg mL}^{-1}$  concn. of aqueous fulvic acid (Khan 1978; quoted, Howard 1991; Montgomery 1993)

$k(\text{aq.}) = 28.4 \text{ d}^{-1}$  at pH 2.8,  $k = 12.6 \text{ d}^{-1}$  at pH 4.5,  $k = 3.16 \text{ d}^{-1}$  at pH 6.0, and  $k = 1.23 \text{ d}^{-1}$  at pH 7.0 with corresponding  $t_{1/2} = 24.4, 55.0, 219$ , and  $563$  d all at 25°C in  $1.0 \text{ mg mL}^{-1}$  concn. of aqueous fulvic acid (Khan 1978)

$k(\text{aq.}) = 151 \text{ d}^{-1}$  at pH 2.4,  $k = 43.7 \text{ d}^{-1}$  at pH 4.5,  $k = 13.2 \text{ d}^{-1}$  at pH 6.0, and  $k = 7.93 \text{ d}^{-1}$  at pH 7.0 with corresponding  $t_{1/2} = 4.60, 15.9, 52.5$  and  $87.3$  d all at 25°C in  $5.0 \text{ mg mL}^{-1}$  concn. of aqueous fulvic acid (Khan 1978)

$k(\text{aq.}) = 9.30 \times 10^{-6} \text{ s}^{-1}$  with  $t_{1/2} = 86$  d at 20°C in a buffer at pH 5 (Burkhard & Guth 1981; quoted, Muir 1991)

$t_{1/2} > 3$  months (in sterile buffer solution at pH 7.2) and  $t_{1/2} > 14$  d (in sterile mineral salt solution at pH 7.2) for  $20 \text{ } \mu\text{g mL}^{-1}$  to hydrolyze at 23°C (Geller 1980; quoted, Muir 1991)

$k(\text{alkaline}) = 1 \times 10^{-16} \text{ M}^{-1} \text{ s}^{-1}$  with  $t_{1/2} = 742$  d (Schnoor & McAvoy 1981; quoted, Schnoor 1992)

$t_{1/2} = 1771$  yr at pH 7 and 25°C (Montgomery 1993)

#### Biodegradation:

$t_{1/2} = 64$  d in soil (Armstrong et al. 1967; Dao et al. 1979; quoted, Means et al. 1983)

$t_{1/2} = 3.21$  d in aqueous solution from river die-away tests (Furmidge & Osgerby 1967; quoted, Scow 1982)

$t_{1/2}(\text{aerobic}) > 90$  d for  $10\text{--}20 \text{ } \mu\text{g mL}^{-1}$  to degrade in soil-water suspension (Goswami & Green 1971; quoted, Muir 1991)

$k(\text{aq.}) = 0.019 \text{ d}^{-1}$  by soil incubation die-away studies (Rao & Davidson 1980; quoted, Scow 1982);

$t_{1/2}(\text{aerobic}) > 35$  d for  $0.1\text{--}1.0 \text{ } \mu\text{g mL}^{-1}$  to slowly biodegrade in sediment/water at 25°C (Wolf & Jackson 1982; quoted, Muir 1991)

$t_{1/2} = 36$  and  $110$  d in soil (Jones et al. 1982; quoted, Means et al. 1983)

$t_{1/2} = 71$  d for a 100 d leaching and screening test in 0–10 cm depth of soil (Jury et al. 1983, 1984, 1987a; Jury & Ghodrati 1989; quoted, Grover 1991)

$k = 0.22 \text{ d}^{-1}$  of aerobic degradation rate observed in incubations of river water samples (Lyman et al. 1990; quoted, Hemond & Fechner 1994)

$t_{1/2} = 201$  d with  $12 \text{ mM}$  methanol, for aqueous atrazine using first-order decay rate,  $t_{1/2} = 289$  d with  $6 \text{ mM}$  sodium acetate,  $t_{1/2} = 164$  d with  $6 \text{ mM}$  acetic acid and  $t_{1/2} = 200$  d with  $2 \text{ mM}$  glucose; however  $t_{1/2} = 224$  d in the sample reactors without any organic amendments (Chung et al. 1996)

degradation  $t_{1/2} = 39$  h and  $43$  h by soil micro *Rhodococcus*. sp. NI86/21 with atrazine concn  $4 \text{ } \mu\text{g/mL}$  and  $8 \text{ } \mu\text{g/mL}$  respectively (Van Zwieten & Kennedy 1995)

first order removal of atrazine from sediment organic carbon:  $k = -0.0054 \text{ d}^{-1}$  with  $t_{1/2} = 128$  d in surface sediment 0–6 cm depth,  $k = -0.0016 \text{ d}^{-1}$  with  $t_{1/2} = 433$  d in sub-surface sediment 24–34 cm depth from Blue Heron Pond;  $k = -0.007 \text{ d}^{-1}$  with  $t_{1/2} = 99$  d in surface sediment 0–6 cm depth,  $k = -0.0022 \text{ d}^{-1}$  with  $t_{1/2} = 630$  d in sub-surface sediment 24–34 cm depth from Oyster Rake Pond;  $k = -0.0142 \text{ d}^{-1}$  with  $t_{1/2} = 49$  d in surface sediment 0–6 cm depth,  $k = -0.0009 \text{ d}^{-1}$  with  $t_{1/2} = 770$  d in sub-surface sediment 24–34 cm depth from Trumpet Creeper East Pond, and  $k = -0.0149 \text{ d}^{-1}$  with  $t_{1/2} = 47$  d in surface sediment 0–6 cm depth,  $k = -0.0000 \text{ d}^{-1}$  with  $t_{1/2} = 70$  d in sub-surface sediment 24–34 cm depth from Trumpet Creeper North, Kiawah island (Smalling & Aelion 2004)

50–60% degradation in 35–100 d by anaerobic mixed culture microorganisms with atrazine as sole carbon source (Ghosh & Philip 2004)

#### Biotransformation:

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

$k_2 = 0.0248, 1.26 \text{ h}^{-1}$  (algae, daphnids, Ellgehausen et al. 1980)  
 $k_2 = 27.2 \text{ d}^{-1}$  (catfish, Ellgehausen et al. 1980)  
 $k_1 = 2.4, 30, 19.0 \text{ h}^{-1}$  (zebrafish: egg, yolk sac fry, juvenile; Görges & Nagel 1990)  
 $k_1 = 227.0 \text{ h}^{-1}; k_2 = 2.354 \text{ h}^{-1}$  (algae *Scenedesmus acutus*, Wang et al. 1996)  
 $k_1 = 0.412 \text{ h}^{-1}; k_2 = 0.073 \text{ h}^{-1}$  (catfish *Ictalurus melas*, Wang et al. 1996)  
 $k_1 = 2.027 \text{ h}^{-1}; k_2 = 1.161 \text{ h}^{-1}$  (water flea *Daphnia magna*, Wang et al. 1996)

#### Half-Lives in the Environment:

Air:  $t_{1/2} = 2.6 \text{ h}$ , based on estimated rate constant  $k = 147.2 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$  at  $25^\circ\text{C}$  for the vapor-phase reaction with hydroxyl radical in air (Atkinson 1987; quoted, Howard 1991).

Surface water: estimated  $t_{1/2} \sim 3.21 \text{ d}$  in aqueous solution from river die-away tests (Furmidge & Osgerby 1967; quoted, Scow 1982);

$t_{1/2} = 1\text{--}4 \text{ wk}$  in estuarine systems (Jones et al. 1982; quoted, Meakins et al. 1994);

under laboratory conditions in distilled water and river water was completely degraded after 21.3 and 7.3 h, respectively (Mansour et al. 1989; quoted, Montgomery 1993);

$t_{1/2} = 3.2 \text{ d}$  to 7–8 months in aquatic environments (Eisler 1985; quoted, Day 1991);

measured rate constant  $k = (24 \pm 4) \text{ M}^{-1} \text{ s}^{-1}$  at pH 4.0,  $k = (13 \pm 1) \text{ M}^{-1} \text{ s}^{-1}$  at pH 4.2, for direct reaction with ozone in water at 26 and  $21^\circ\text{C}$ , respectively, with  $t_{1/2} = 1.5 \text{ h}$  at pH 7 (Yao & Haag 1991);

$t_{1/2} = 35.6\text{--}168 \text{ h}$  in surface water system of a small stream in Iowa by water quality analyses (Kolpin & Kalkhoff 1993);

$t_{1/2} = 235 \text{ d}$  at  $6^\circ\text{C}$ ,  $t_{1/2} = 164 \text{ d}$  at  $22^\circ\text{C}$  in darkness,  $t_{1/2} = 59 \text{ d}$  under sunlight conditions for river water at pH 7.3;  $t_{1/2} = 130 \text{ d}$  at  $22^\circ\text{C}$  in darkness for filtered river water at pH 7.3 and  $t_{1/2} = 200 \text{ d}$  at  $22^\circ\text{C}$  in darkness,  $t_{1/2} = 169 \text{ d}$  under sunlight conditions for seawater, pH 8.1 (Lartiges & Garrigues 1995)

Groundwater:  $t_{1/2} = 6\text{--}15 \text{ months}$  for  $0.72\text{--}10 \mu\text{g mL}^{-1}$  to biodegrade slowly at  $25^\circ\text{C}$  (Weidener 1974; quoted, Muir 1991)

reported half-lives or persistence,  $t_{1/2} = 60\text{--}150, 71, 74$ , and  $130 \text{ d}$  (Bottoni & Funari 1992)

Sediment:  $t_{1/2} = 145 \text{ d}$  in a Wisconsin Lake sediment (Armstrong et al. 1967; quoted, Jones et al. 1982; Means et al. 1983) and  $t_{1/2} \sim 30 \text{ d}$  for Chesapeake Bay sediment (Ballantine et al. 1978; quoted, Jones et al. 1982);

$t_{1/2} = 7\text{--}28 \text{ d}$  for  $0.1 \mu\text{g mL}^{-1}$  to rapid degrade in both aerobic and low oxygen systems in estuarine sediment/water at  $12\text{--}35^\circ\text{C}$  (Jones et al. 1982, quoted, Muir 1991);

$t_{1/2}(\text{aerobic}) > 35 \text{ d}$  for  $0.1\text{--}1.0 \mu\text{g mL}^{-1}$  to slowly biodegrade in sediment/water at  $25^\circ\text{C}$  (Wolf & Jackson 1982; quoted, Muir 1991)

$t_{1/2} = 60\text{--}120 \text{ d}$  in surface sediment,  $t_{1/2} = 60\text{--}223 \text{ d}$  in subsurface sediment

biodegradation  $t_{1/2} = 47\text{--}128 \text{ d}$  in the surface and  $t_{1/2} = 70\text{--}770$  in subsurface sediment (Smalling & Aelion 2004)

Soil: half-lives in aqueous buffered solutions in soil at  $25^\circ\text{C}$  and pH 1, 2, 3, 4, 11, 12, and 13 were reported to be 3.3, 14, 58, 240, 100, 12.5, and 1.5 d, respectively (Armstrong et al. 1967; quoted, Montgomery 1993);

$t_{1/2} = 3\text{--}5 \text{ yr}$  in agricultural soils (Armstrong et al. 1967; quoted, Jones et al. 1982);

estimated persistence of 10 months in soil (Kearney et al. 1969; quoted, Jury et al. 1987a);

$t_{1/2} = 1.73$ , and  $244 \text{ d}$  at  $25^\circ\text{C}$  and pH 4 with and without fulvic acid (2%) (Li & Felbeck 1972; quoted, Montgomery 1993);

persistence of 10 months in soil (Edwards 1973; quoted, Morrill et al. 1982);

$t_{1/2} = 6.0 \text{ months}$  at  $15^\circ\text{C}$  and  $t_{1/2} = 2.0 \text{ months}$  at  $30^\circ\text{C}$  in soils (Freed & Haque 1973);

persistence of 12 months (Wauchope 1978);

correlated  $t_{1/2} = 37 \text{ d}$  at pH 5.1–7.0, and  $t_{1/2} = 28 \text{ d}$  at pH 7.7–8.2 (Boddington Barn soil, Hance 1979),

$t_{1/2} \sim 30 \text{ d}$  at pH 4.6–5.3 and  $t_{1/2} = 40 \text{ d}$  at pH 6.3–8.0 (Triangle soil, Hance 1979);

$t_{1/2} = 37 \text{ d}$  in agricultural soils (Dao et al. 1979; quoted, Jones et al. 1982);

estimated first-order  $t_{1/2} = 36.5 \text{ d}$  from biodegradation rate constant  $k = 0.019 \text{ d}^{-1}$  by soil incubation die-away studies (Rao & Davidson 1980; quoted, Scow 1982);

$t_{1/2} = 53$  and  $113 \text{ d}$  at pH 6.5 at  $22^\circ\text{C}$  in a Hatzenbühl soil at pH 4.8 and Neuhofen soil, respectively (Burkhard & Guth 1981; quoted, Montgomery 1993);

$t_{1/2} = 1\text{--}6 \text{ months}$  (Jones et al. 1982; quoted, Meakins et al. 1994);

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

biodegradation  $t_{1/2} = 71 \text{ d}$  from screening model calculations (Jury et al. 1984; 1987a,b; Jury & Ghodrati 1989);

$t_{1/2} \sim 6\text{--}10$  wk (Hartley & Kidd 1987; quoted, Montgomery 1993);

field  $t_{1/2} = 4$  wk by using lysimeters (Bowman 1990);

half-lives from soil surfaces:  $t_{1/2} = 655$  to  $> 1000$  d in peat soil and  $t_{1/2} = 143\text{--}939$  d in sandy soil at  $20 \pm 1^\circ\text{C}$  (Dörfler et al. 1991);

degradation rate constant  $k = (1.20 \pm 0.097) \times 10^{-2} \text{ d}^{-1}$  with  $t_{1/2} = 57.8$  d in control soil and  $k = (1.01 \pm 0.034) \times 10^{-2} \text{ d}^{-1}$  with  $t_{1/2} = 68.6$  d in pretreated soil once only in the laboratory (Walker & Welch 1991);

$t_{1/2} \sim 21$  d based on extractable residues in microcosm studies, compared to  $t_{1/2} = 14$  d in surface field soil (Winkelmann & Klaine 1991);

selected field  $t_{1/2} = 60$  d (Wauchope et al. 1992; quoted, Dowd et al. 1993; Richards & Baker 1993; Hornsby et al. 1996);

soil  $t_{1/2} = 130$  d (quoted, Pait et al. 1992);

field  $t_{1/2} = 35\text{--}50$  d in soil and water but may be longer under cold or dry conditions;  $t_{1/2} = 105$  to  $> 200$  d under groundwater conditions, depending on test system (Wood et al. 1991; quoted, Tomlin 1994);

reported  $t_{1/2} = 60\text{--}150$  d, 71 d, 74 d and 130 d (Bottoni & Funari 1992);

first-order  $k = -0.017$  to  $-0.003 \text{ d}^{-1}$  with corresponding  $t_{1/2} = 41$  d in the 0- to 30-cm soil to  $t_{1/2} = 231$  d in the 90 to 120-cm soil in Ames, Iowa (Kruger et al. 1993);

dissipation  $t_{1/2} = 71$  d from soil surface (Gish et al. 1995);

$t_{1/2} = 60$  d (selected, Halfon et al. 1996).

$t_{1/2} = 60$  d (Gao et al. 1997)

Biota:  $t_{1/2} = 0.03$  h in algae,  $t_{1/2} = 1.52$  d in catfish and  $t_{1/2} = 9.5$  h in daphnids (Ellgehausen et al. 1980);

biochemical  $t_{1/2} = 64$  d from screening model calculations (Jury et al. 1987b);

$t_{1/2} = 25.6$  d in bean,  $t_{1/2} = 24.3$  d in turnips and  $t_{1/2} = 14.6$  d in oats at  $20 \pm 1^\circ\text{C}$  from plant surfaces (Dörfler et al. 1991).

**TABLE 17.1.1.4.1**

**Reported vapor pressures of atrazine at various temperatures and the coefficients for the vapor pressure equations**

log P = A – B/(T/K)		(1)	ln P = A – B/(T/K)		(1a)		
log P = A – B/(C + t/°C)		(2)	ln P = A – B/(C + t/°C)		(2a)		
log P = A – B/(C + T/K)		(3)					
log P = A – B/(T/K) – C·log (T/K)		(4)					
Friedrich & Stambach 1964		Grayson & Fosbracey 1982		Rordorf 1989		Goodman 1997	
gas saturation-GC		gas saturation-GC		gas saturation-GC		Knudsen effusion method	
t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa
20	4.0 × 10 <sup>-5</sup>	51.0	0.0040	25	3.9 × 10 <sup>-5</sup>	40	6.7 × 10 <sup>-4</sup>
	extrapolated	55.5	0.0048	50	1.9 × 10 <sup>-3</sup>	50	2.2 × 10 <sup>-3</sup>
measured range 50–130°C		63.0	0.0095	75	0.056	60	9.5 × 10 <sup>-3</sup>
Antoine eq.		66.0	0.0337	100	1.0	70	0.030
eq. 1	P/mmHg	66.7	0.023	125	13.0	80	0.098
A	13.766	76.5	0.0713				
B	5945	81.5	0.117	eq. 1	P <sub>g</sub> /Pa	eq. 1	P/Pa
		20	3.7 × 10 <sup>-5</sup>	A	17.583	A	16.08
				B	6558.5	B	6040
		eq. 1a	P/Pa	for temp range 40–125°C			
		A	36.80				
		B	13.778				
					liquid		
				eq. 1	P <sub>L</sub> /Pa		
				A	13.2701		
				B	4626.79		

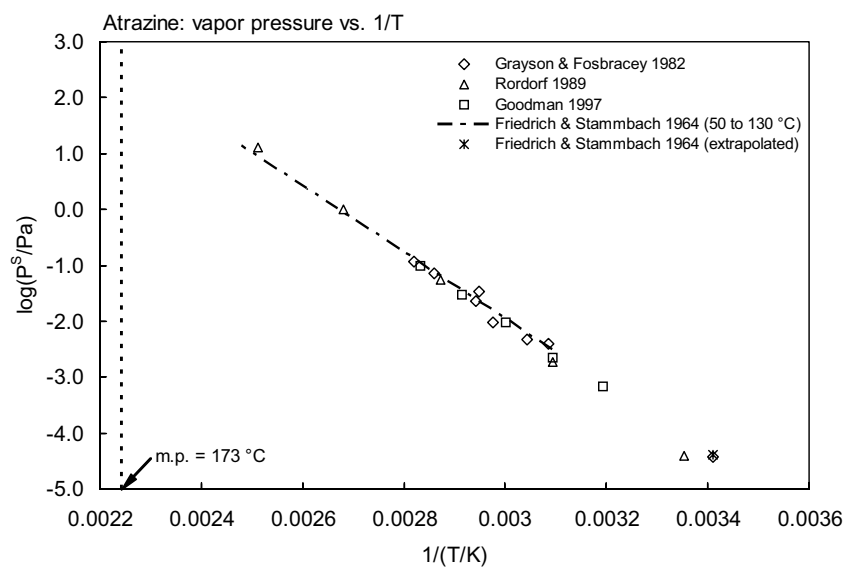
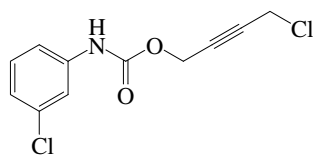


FIGURE 17.1.1.4.1 Logarithm of vapor pressure versus reciprocal temperature for atrazine.

## 17.1.1.5 Barban



Common Name: Barban

Synonym: Barbamate, Barbane, Carbine, Carbyne, CBN, Chlorinat

Chemical Name: carbamic acid, (3-chlorophenyl)-, 4-chloro-2-butynyl ester; 4-chlorobut-2-ynyl 3-chloro-carbanilate; 4-chloro-2-butynyl 3-chlorophenylcarbamate

Uses: herbicide for post-emergence control of wild oats in wheat, barley, broad beans, field beans, soybeans, peas, sugar beet, flax, lucerne, lentils, mustard, oilseed rape, sunflowers, etc.

CAS Registry No: 101-27-9

Molecular Formula:  $C_{11}H_9Cl_2NO_2$

Molecular Weight: 258.101

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

75 (Khan 1980; Herbicide Handbook 1989; Lide 2003)

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

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

1.403 ( $25^{\circ}C$ , Hartley & Kidd 1987)

Molar Volume ( $cm^3/mol$ ):

262.8 (calculated-Le Bas method at normal boiling point, this work)

Dissociation Constant  $pK_a$ :

Enthalpy of Vaporization,  $\Delta H_v$  ( $kJ/mol$ ):

109.1 (Rordorf 1989)

Enthalpy of Fusion,  $\Delta H_{fus}$  ( $kJ/mol$ ):

26.8 (Rordorf 1989)

Entropy of Fusion,  $\Delta S_{fus}$  ( $J/mol K$ ):

Fugacity Ratio at  $25^{\circ}C$  (assuming  $\Delta S_{fus} = 56 J/mol K$ ), F: 0.323 (mp at  $75^{\circ}C$ )

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

15.0 (Swezey & Nex 1961)

11.0 ( $20^{\circ}C$ , Weber 1972; Worthing & Walker 1987)

11.0 (Martin & Worthing 1977; Ashton & Crafts 1981; Hartley & Kidd 1987; Worthing & Walker 1987; Herbicide Handbook 1989, Budavari 1989; Milne 1995)

11.0 ( $20$ – $25^{\circ}C$ , selected, Augustijn-Beckers et al. 1994; Hornsby et al. 1996)

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

$1.33 \times 10^{-3}$  ( $20^{\circ}C$ , Weber 1972; Worthing & Walker 1987)

$5.00 \times 10^{-5}$  (Hartley & Kidd 1987)

$1.60 \times 10^{-4}$  (Worthing & Walker 1987)

$5.05 \times 10^{-5}$  (Herbicide Handbook 1989)

$3.50 \times 10^{-5}$ ,  $1.0 \times 10^{-3}$ , 0.019, 0.240, 2.20 ( $25$ ,  $50$ ,  $70$ ,  $100$ ,  $125^{\circ}C$ , gas saturation-GC, Rordorf 1989)

$\log(P_L/Pa) = 14.669 - 5703.8/(T/K)$ ; measured range  $72$ – $150^{\circ}C$  (gas saturation-GC, Rordorf 1989)

$5.07 \times 10^{-5}$  ( $20$ – $25^{\circ}C$ , selected, Augustijn-Beckers et al. 1994; Hornsby et al. 1996)

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

0.00117 ( $20^{\circ}C$ , calculated-P/C, Muir 1991)

1.17 (calculated-P/C as per Worthing & Walker 1987, Majewski & Capel 1995)

0.00117 (calculated-P/C, this work)



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

2.68 (selected, Gerstl & Helling 1987)

Bioconcentration Factor,  $\log BCF$ :

2.20 (calculated-S, Kenaga 1980)

Sorption Partition Coefficient,  $\log K_{oc}$  at 25°C or as indicated:

3.06 (soil, calculated-S, Kenaga 1980)

2.66 (calculated-MCI  $\chi$ , Gerstl & Helling 1987)

3.00 (20–25°C, estimated, Augustijn-Beckers et al. 1994; Hornsby et al. 1996)

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

Volatilization: estimated  $t_{1/2} = 6690$  d from 1 m depth of water at 20°C (Muir 1991).

Photolysis:  $t_{1/2} = 2.25$  h for 22–99% of 10  $\mu\text{g/ml}$  to degrade in distilled water under 300 nm light (Tanaka et al. 1981; quoted, Cessna & Muir 1991).

Oxidation:

Hydrolysis:

Biodegradation:

Biotransformation:

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

Half-Lives in the Environment:

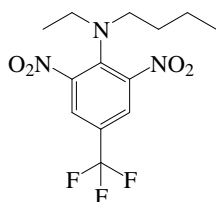
Soil: estimated persistence of 2 months (Kearney et al. 1969; quoted, Jury et al. 1987);

persistence of 2 weeks in soil (Edwards 1973; quoted, Morrill et al. 1982);

persistence of about 3 weeks in soil (Herbicide Handbook 1989);

selected field  $t_{1/2} = 5$  d (Augustijn-Beckers et al. 1994; Hornsby et al. 1996).

## 17.1.1.6 Benefin



Common Name: Benefin

Synonym: Balan, Bonalan, benfluralin

Chemical Name: *N*-butyl-*N*-ethyl- $\alpha,\alpha,\alpha$ -trifluoro-2,6-dinitro-*p*-toluidine

Uses: as pre-emergence herbicide for the control of annual grasses and broadleaf weeds in chicory, cucumbers, endive, groundnuts, lettuce, lucerne, and other foliage crops.

CAS Registry No: 1861-40-1

Molecular Formula:  $C_{13}H_{16}F_3N_3O_4$

Molecular Weight: 335.279

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

66 (Lide 2003)

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

121–122 (0.5 mmHg), 148–149 at 7 mmHg (Tomlin 1994)

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

1.28 (tech., Tomlin 1994)

Molar Volume ( $cm^3/mol$ ):

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

Dissociation Constant  $pK_a$ :

Enthalpy of Fusion,  $\Delta H_{fus}$  (kJ/mol):

38.70 (DSC method, Plato & Glasgow 1969)

Entropy of Fusion,  $\Delta S_{fus}$  (J/mol K):

Fugacity Ratio at  $25^{\circ}C$  (assuming  $\Delta S_{fus} = 56$  J/mol K), F: 0.396 (mp at  $66^{\circ}C$ )

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

< 1.0 (Ashton & Crafts 1973)

0.50 (Weber et al. 1980)

1.0 ( $20^{\circ}C$ , selected, Suntio et al. 1988)

0.10 (Herbicide Handbook 1983; Tomlin 1994)

0.10 ( $20$ – $25^{\circ}C$ , selected, Hornsby et al. 1996)

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

0.00519 ( $30^{\circ}C$ , Ashton & Crafts 1973)

0.0104 (Herbicide Handbook 1983)

0.0040 ( $20^{\circ}C$ , estimated, Suntio et al. 1988)

0.0087 (Tomlin 1994)

0.0088 ( $20$ – $25^{\circ}C$ , selected, Hornsby et al. 1996)

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

1.34 ( $20^{\circ}C$ , calculated-P/C, Suntio et al. 1988)

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

5.34 (selected, Magee 1991)

5.29 ( $20^{\circ}C$ , pH 7, Tomlin 1994)

5.29 (pH 7, selected, Hansch et al. 1995)

Bioconcentration Factor, log BCF:

3.36 (calculated-S per Kenaga 1980, this work)

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

- 4.03 (quoted exptl., Sabljic 1987)
- 4.03, 3.75 (quoted, estimated; Magee 1991)
- 3.95 (soil, Hornsby et al. 1996)
- 2.96 (2.59–3.33) (soil: organic carbon OC  $\geq 0.5\%$ , average, Delle Site 2001)

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

## Volatilization:

Photolysis: atmospheric and aqueous photolysis half-lives were estimated to be 288–864 h (Howard et al. 1991).

Oxidation: photooxidation  $t_{1/2} \sim 0.782$ –7.82 h based on reaction with OH radicals in air (Howard et al. 1991).

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

Biodegradation: aerobic  $t_{1/2} \sim 504$ –2880 h in soil, and anaerobic soil  $t_{1/2} = 144$ –480 h (Howard et al. 1991).

## Biotransformation:

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

## Half-Lives in the Environment:

Air:  $t_{1/2} = 0.782$ –7.82 h based on estimated reaction with OH radicals in the gas-phase (Howard et al. 1991).

Surface water:  $t_{1/2} = 288$ –864 h based on observed photolysis by sunlight (Howard et al. 1991).

Groundwater:  $t_{1/2} = 144$ –5760 h based on unacclimated aqueous aerobic and anaerobic biodegradation half-lives (Howard et al. 1991).

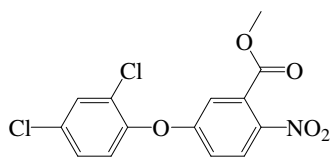
## Sediment:

Soil:  $t_{1/2} = 504$ –2880 h based on aerobic solid die-away test data (Howard et al. 1991);

field  $t_{1/2} = 40$  d (Hornsby et al. 1996).

## Biota:

## 17.1.1.7 Bifenox



Common Name: Bifenox

Synonym: MC-4379, Modown

Chemical Name: benzoic acid, 5-(2,4-dichlorophenoxy)-2-nitro-, methyl ester; methyl-5-(2,4-dichlorophenoxy)-2-nitrobenzoate

Uses: selective pre-emergence and post-emergence herbicide to effectively control a wide variety of broadleaf weeds in corn, grain, sorghum, maize, rice, and soybeans.

CAS Registry No: 42576-02-3

Molecular Formula:  $C_{14}H_9Cl_2NO_5$

Molecular Weight: 342.131

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

85 (Lide 2003)

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

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

1.155 (Ashton & Crafts 1981; Herbicide Handbook 1989; Montgomery 1993)

Molar Volume ( $cm^3/mol$ ):

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

Dissociation Constant  $pK_a$ :

Enthalpy of Vaporization,  $\Delta H_v$  (kJ/mol):

90.5 (Rordorf 1989)

Enthalpy of Fusion,  $\Delta H_{fus}$  (kJ/mol):

26.4 (Rordorf 1989)

Entropy of Fusion,  $\Delta S_{fus}$  (J/mol K):

74.0 (Rordorf 1989)

Fugacity Ratio at  $25^{\circ}C$  (assuming  $\Delta S_{fus} = 56$  J/mol K), F: 0.258 (mp at  $85^{\circ}C$ )

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

0.35 ( $20^{\circ}C$ , Weber 1972; Worthing & Walker 1987)

0.35 (Martin & Worthing 1977; Herbicide Handbook 1978)

0.35 (Ashton & Crafts 1981; Herbicide Handbook 1989; Budavari 1989)

0.35 ( $30^{\circ}C$ , Worthing & Walker 1987)

0.35 (Hartley & Kidd 1987; Worthing & Hance 1991; Montgomery 1993; Tomlin 1994; Milne 1995)

0.398 ( $20$ – $25^{\circ}C$ , selected, Wauchope et al. 1992; Lohninger 1994; Hornsby et al. 1996)

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

0.00032 ( $20^{\circ}C$ , Weber 1972; Worthing & Walker 1987)

0.00032 ( $30^{\circ}C$ , Ashton & Crafts 1981; Worthing & Hance 1991; Tomlin 1994)

0.00032 ( $30^{\circ}C$ , Hartley & Kidd 1987; Budavari 1989; Montgomery 1993)

$5.40 \times 10^{-6}$ ,  $2.0 \times 10^{-4}$ ,  $4.40 \times 10^{-3}$ , 0.064, 0.67 ( $25$ ,  $50$ ,  $70$ ,  $100$ ,  $125^{\circ}C$ , gas saturation-GC, Rordorf 1989)

$\log (P_s/Pa) = 14.996 - 6040.4/(T/K)$ ; measured range  $36.9$ – $85.5^{\circ}C$  (solid, gas saturation-GC, Rordorf 1989)

$\log (P_L/Pa) = 13.815 - 5582.5/(T/K)$ ; measured range  $90.5$ – $175^{\circ}C$  (liquid, gas saturation-GC, Rordorf 1989)

0.00032 ( $20$ – $25^{\circ}C$ , selected, Wauchope et al. 1992; Hornsby et al. 1996)

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

0.321 ( $20^{\circ}C$ , calculated-P/C, Muir 1991)

0.011 (calculated-P/C, Montgomery 1993)

0.313 (calculated-P/C, this work)

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

- 5.63 (selected, Dao et al. 1983)
- 4.50 (Worthing & Hance 1991)
- 4.48 (Montgomery 1993; Tomlin 1994)
- 4.48 (selected, Hansch et al. 1995)
- 5.24 (RP-HPLC-RT correlation using short ODP column, Donovan & Pescatore 2002)

Bioconcentration Factor,  $\log BCF$ :

- 2.30 (static water, Metcalf & Sanborn 1975; quoted, Kenaga & Goring 1980; Isensee 1991)
- 3.05 (calculated-S, Kenaga 1980; quoted, Isensee 1991)

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

- 3.89 (soil, calculated per Kenaga & Goring, Kenaga 1980)
- 4.0 (soil, 20–25°C, estimated, Wauchope et al. 1992; Hornsby et al. 1996)
- 2.24–4.39 (Montgomery 1993)
- 4.0 (estimated-chemical structure, Lohninger 1994)
- 2.70–4.36 (Tomlin 1994)

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

Volatilization: estimated  $t_{1/2} = 29.8$  d from 1 m depth of water at 30°C (Muir 1991).

Photolysis: with < 5% degradation by UV light of 290–400 nm in 48 h (Worthing & Hance 1991).

Oxidation:

Hydrolysis: stable in aqueous solution at pH 5.0–7.3 but rapidly hydrolyzed at pH 9.0 both at 22°C (Worthing & Hance 1991).

Biodegradation:  $t_{1/2} = 2$ –5 d for 10 µg/mL to biodegrade in flooded soil at 30°C (Ohyama & Kuwatsuka 1978; quoted, Muir 1991).

Biotransformation:

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

## Half-Lives in the Environment:

Soil:  $t_{1/2} = 2$ –5 d for 10 µg/mL to biodegrade in flooded soil at 30°C (Ohyama & Kuwatsuka 1978; quoted, Muir 1991);

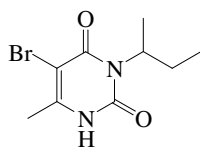
average  $t_{1/2} = 7$ –14 d in soils (Hartley & Kidd 1987; Herbicide Handbook 1989; quoted, Montgomery 1993);

selected field  $t_{1/2} = 7.0$  d (Wauchope et al. 1992; Hornsby et al. 1996);

average  $t_{1/2} = 7$ –14 d (Herbicide Handbook 1989);

$t_{1/2} \sim 5$ –7 d in soil (Tomlin 1994).

## 17.1.1.8 Bromacil



Common Name: Bromacil

Synonym: Borea, Bromax, Bromazil, Cynogan, Hyvar, Hyvarex, Krovar I or II, Nalkil, Uragan, Urox B, Uron HX, Weed Blast

Chemical Name: 5-bromo-3-*sec*-butyl-6-methyluracil; 5-bromo-6-methyl-3-(1-methylpropyl)-2,4-(1*H*,3*H*)pyrimidinedione

Uses: Herbicide applied to soil to control annual and perennial grasses, broadleaf weeds, and general vegetation on uncropped land; also used for selective weed control in apple, asparagus, cane fruit, hops, and citrus crops.

CAS Registry No: 314-40-9

Molecular Formula: C<sub>9</sub>H<sub>13</sub>BrN<sub>2</sub>O<sub>2</sub>

Molecular Weight: 261.115

Melting Point (°C):

158 (Lide 2003)

Boiling Point (°C):

Density (g/cm<sup>3</sup> at 20°C):

1.55 (25°C, Hartley & Kidd 1987; Herbicide Handbook 1989; Worthing & Hance 1991; Montgomery 1993)

1.59 (23°C, Tomlin 1994)

1.55 (Milne 1995)

Molar Volume (cm<sup>3</sup>/mol):

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

Dissociation Constant pK<sub>a</sub>:

9.10 (Wauchope et al. 1992; Hornsby et al. 1996)

< 7.0 (Montgomery 1993)

9.27 (Tomlin 1994)

Enthalpy of Fusion, ΔH<sub>fus</sub> (kJ/mol):

Entropy of Fusion, ΔS<sub>fus</sub> (J/mol K):

Fugacity Ratio at 25°C (assuming ΔS<sub>fus</sub> = 56 J/mol K), F: 0.0496 (mp at 158°C)

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

815 (Bailey & White 1965; Khan 1980; Hartley & Kidd 1987; Montgomery 1993; Milne 1995)

815 (Melnikov 1971; Spencer 1973; Herbicide Handbook 1978; Herbicide Handbook 1989)

815 (20°C, Weber 1972; Worthing & Walker 1987, Worthing & Hance 1991)

820 (Beste & Humburg 1983; Jury et al. 1983)

1064 (shake flask-GC or LSC, Gerstl & Mingelgrin 1984; Gerstl & Helling 1987)

626, 775, 1043 (4, 25, 40°C, shake flask-LSS, Madhun et al. 1986)

700 (20–25°C, selected, Wauchope et al. 1992; Lohninger 1994; Hornsby et al. 1996)

700, 807, 1287 (at pH 7, 5, 9, Tomlin 1994)

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

5 × 10<sup>-5</sup> (20°C, Weber 1972; Worthing & Walker 1987)

3 × 10<sup>-5</sup> (estimated, USEPA 1975)

0.107 (100°C, Khan 1980)

2.9 × 10<sup>-5</sup> (Jury et al. 1983)

0.00033 (Hartley & Kidd 1987; Worthing & Hance 1991)

4 × 10<sup>-5</sup> (20–25°C, selected, Wauchope et al. 1992)

3.3 × 10<sup>-5</sup> (Montgomery 1993)

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

- $9.17 \times 10^{-6}$  (Beste & Humburg 1983; Jury et al. 1983)
- $9.17 \times 10^{-5}$  (calculated-P/C, Jury et al. 1984, 1987a; Jury & Ghodrati 1989)
- 0.0019 ( $20^\circ\text{C}$ , selected, Suntio et al. 1988)
- $1.06 \times 10^{-5}$  ( $20^\circ\text{C}$ , calculated-P/C, Muir 1991)
- $1.06 \times 10^{-5}$  (calculated-P/C, Montgomery 1993)

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

- 2.02 (Rao & Davidson 1980)
- 1.33 (selected, Dao et al. 1983)
- 1.84 (shake flask-GC or LSC, Gerstl & Mingelgrin 1984)
- 1.84, 1.87, 1.90 (4, 25,  $40^\circ\text{C}$ , shake flask-LSS, Madhun et al. 1986)
- 1.85 (selected, Gerstl & Helling 1987)
- 2.11 selected, Magee 1991; Devillers et al. 1996)
- 1.84–2.04 (Montgomery 1993)
- 2.11 (selected, Sangster 1993)
- 1.87, 1.88, 1.63 (at pH 7, 5, 9, Tomlin 1994)
- 2.11 (recommended, Hansch et al. 1995)

Bioconcentration Factor,  $\log \text{BCF}$ :

- 0.505 (measured, Kenaga 1980)
- 2.27 (calculated-S, Kenaga 1980)
- 0.477 (calculated- $K_{\text{OC}}$ , Kenaga 1980)
- 0.51 (*Pimephales promelas*, Call et al. 1987)

Sorption Partition Coefficient,  $\log K_{\text{OC}}$  at  $25^\circ\text{C}$  or as indicated:

- 1.86 (soil, Hamaker & Thompson 1972)
- 3.13 (soil, calculated as per Kenaga & Goring 1980, Kenaga 1980)
- 1.86 (Rao & Davidson 1980)
- 2.33, 1.34, 1.63 (estimated-S, calculated-S and mp, calculated- $K_{\text{OW}}$ , Karickhoff 1981)
- 1.61 (sediments average-Freundlich adsorption, Corwin & Farmer 1984)
- 1.41–2.46 (California lake sediments, Corwin & Farmer 1984)
- 1.98, 1.88 (4,  $25^\circ\text{C}$ , Semiahmoo soil, in  $\mu\text{mol}/\text{kg}$  OC, batch equilibrium method-LSS, Madhun et al. 1986)
- 2.11, 1.88 (4,  $25^\circ\text{C}$ , Adkins soil, in  $\mu\text{mol}/\text{kg}$  OC, Madhun et al. 1986)
- 1.90, 1.66, 1.75; 1.86, 1.89, 1.34 (estimated- $K_{\text{OW}}$ ; S, Madhun et al. 1986)
- 1.53, 2.73 (quoted, calculated-MCI  $\chi$ , Gerstl & Helling 1987)
- 1.86 (soil, screening model calculations, Jury et al. 1987a,b; Jury & Ghodrati 1989; Carsel 1989)
- 2.56 (calculated-MCI  $\chi$ , Bahnick & Doucette 1988)
- 1.86, 1.80 (reported, estimated as  $\log K_{\text{OM}}$ , Magee 1991)
- 1.53, 1.86, 3.13 (soil, quoted values, Bottoni & Funari 1992)
- 1.51 (soil,  $20$ – $25^\circ\text{C}$ , selected, Wauchope et al. 1992; Hornsby et al. 1996)
- 1.51 (Montgomery 1993)
- 2.09 (estimated-chemical structure, Lohninger 1994)
- 1.60 (quoted or calculated-QSAR MCI  $\chi$ , Sabljic et al. 1995)
- 1.43, 1.72 (average values for sediments, soils, Delle Site 2001)
- 1.48, 1.46, 1.53 (soils: organic carbon  $\text{OC} \geq 0.1\%$ ,  $\text{OC} \geq 0.5\%$ ,  $0.1 \leq \text{OC} < 0.5\%$ , and pH 6.3–7.9, average, Delle Site 2001)
- 1.80, 1.72 (soils: organic carbon  $\text{OC} \geq 0.1\%$ ,  $\text{OC} \geq 0.5\%$ , and pH  $\leq 7.3$  undissociated, average, Delle Site 2001)

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

- Volatilization: estimated  $t_{1/2} \sim 10,000$  d from 1 m depth of water at  $20^\circ\text{C}$  (Muir 1991).
- Photolysis: 115 ppb contaminated water in the presence of  $\text{TiO}_2$  and  $\text{H}_2\text{O}_2$  photodegraded to 6 ppb by 15 h solar irradiation with complete degradation after 75 h (Muszkat et al. 1992).
- Oxidation:
- Hydrolysis:

Biodegradation:  $t_{1/2} = 350$  d for 100 d leaching and screening test in 0–10 cm depth of soil (Rao & Davidson 1980; quoted, Jury et al. 1983, 1984, 1987a).

Biotransformation:

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

#### Half-Lives in the Environment:

Air:

Surface water:

Ground water: reported  $t_{1/2} = 150$ –158 and 350 d (Bottoni & Funari 1992)

Sediment:

Soil:  $t_{1/2} = 7.0$  months at 15°C and  $t_{1/2} = 4.5$  months at 30°C in soils (Freed & Haque 1973);

rate constant  $k = 0.0038 \text{ d}^{-1}$  with biodegradation  $t_{1/2} = 350$  d under field conditions (Rao & Davidson 1980; quoted, Jury et al. 1984);

$t_{1/2} = 350$  d from screening model calculations (Jury et al. 1987a,b; Jury & Ghodrati 1989);

$t_{1/2} > 100$  d (Willis & McDowell 1982)

$t_{1/2} \sim 5429$ –46200 d in loamy sand and peat at 25–35°C as follows (Madhum & Freed 1987):

$t_{1/2} = 46200$ , 12391, and 5856 d at 25, 30, and 35°C, respectively, at herbicide concn at 5 µg/kg, while  $t_{1/2} = 18851$ , 9925, and 7588 d at 25, 30, and 35°C, respectively, at herbicide concn at 100 µg/kg in an Adkins loamy sand; however, the half-lives in peat.  $t_{1/2} = 5429$ , 6789, and 8044 d at 25, 30, and 35°C, respectively, at herbicide concn at 5 µg/kg while  $t_{1/2} = 6293$ , 5986, and 6784 d at 25, 30, and 35°C, respectively, at herbicide concn at 100 µg/kg in a Semiahoo mucky peat (Madhun & Freed 1987)

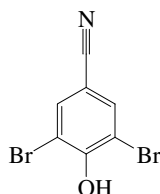
selected field  $t_{1/2} = 60$  d (Wauchope et al. 1992; Hornsby et al. 1996);

$t_{1/2} = 150$ –180d and 350 d (Bottoni & Funari 1992).

Biota: biochemical  $t_{1/2} = 350$  d from screening model calculations (Jury et al. 1987a,b; Jury & Ghodrati 1989).



## 17.1.1.9 Bromoxynil



Common Name: Bromoxynil

Synonym: Brittox, Brominal, Brominex, Brominil, Broxynil, Bucril, Chipco crab-kleen, ENT 20852, Nu-lawn weeder, Oxytril M, Partner

Chemical Name: 3,5-dibromo-4-hydroxybenzonitrile; 4-cyano-2,6-dibromophenol

Uses: herbicide for post-emergence control of annual broadleaf weeds and it is often used in combination with other herbicides to extend the spectrum of control.

CAS Registry No: 1689-84-5

Molecular Formula:  $C_7H_3Br_2NO$

Molecular Weight: 276.913

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

190 (Khan 1980; Herbicide Handbook 1989; Montgomery 1993; Lide 2003)

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

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

Molar Volume ( $cm^3/mol$ ):

176.7 (calculated-Le Bas method at normal boiling point, this work)

Dissociation Constant  $pK_a$ :

4.20 (radiometer/pH meter, Cessna & Grover 1978)

4.06 (Herbicide Handbook 1989; Montgomery 1993)

4.06 (Budavari 1989; Worthing & Hance 1991)

3.86 (Tomlin 1994)

Enthalpy of Fusion,  $\Delta H_{fus}$  ( $kJ/mol$ ):

31.80 (DSC method, Plato 1972)

Entropy of Fusion,  $\Delta S_{fus}$  ( $J/mol K$ ):

Fugacity Ratio at  $25^{\circ}C$  (assuming  $\Delta S_{fus} = 56 J/mol K$ ), F: 0.0241 (mp at  $190^{\circ}C$ )

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

130 ( $20-25^{\circ}C$ , Spencer 1973)

131 (Kenaga 1980)

< 200 (Khan 1980)

130 ( $20-25^{\circ}C$ , Ashton & Crafts 1981)

130 (Hartley & Kidd 1987; Montgomery 1993; Tomlin 1994; Milne 1995)

130 (Worthing & Walker 1987, Worthing & Hance 1991)

130 ( $20-25^{\circ}C$ , Herbicide Handbook 1989)

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

< 0.0010 ( $20^{\circ}C$ , Hartley & Kidd 1987; Tomlin 1994)

0.00064 (Herbicide Handbook 1989)

0.00064 (Montgomery 1993)

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

0.14180 ( $20-25^{\circ}C$ , calculated-P/C, Montgomery 1993)

$1.36 \times 10^{-3}$  (calculated-P/C, this work)

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

2.60 (selected, Dao et al. 1983)

< 2.00 (Herbicide Handbook 1989)

< 2.00 (Montgomery 1993)

Bioconcentration Factor, log BCF:

1.60 (calculated, Kenaga 1980)

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

2.48 (soil, quoted from Kenaga 1980, Bottoni & Funari 1992)

2.48 (calculated, Montgomery 1993)

2.86, 3.06 (soil, quoted exptl.; estimated-general model using molecular descriptors, Gramatica et al. 2000)

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

Volatilization:

Photolysis: rate constant of degradation in water,  $k = 1.04 \times 10^{-3} \text{ s}^{-1}$  at pH 8.3 and  $k = 1.08 \times 10^{-3} \text{ s}^{-1}$  at pH 11.6 (Kochany 1992).

Oxidation:

Hydrolysis:

Biodegradation:  $t_{1/2} \sim 24 \text{ h}$  for  $0.03 \text{ }\mu\text{g/mL}$  to biodegrade in runoff water at  $20\text{--}25^\circ\text{C}$  (Brown et al. 1984; quoted, Muir 1991).

Biotransformation:

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

Half-Lives in the Environment:

Air:

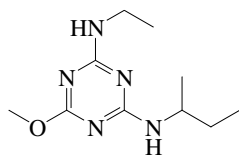
Surface water:  $t_{1/2} \sim 24 \text{ h}$  for  $0.03 \text{ }\mu\text{g mL}^{-1}$  to biodegrade in runoff water at  $20\text{--}25^\circ\text{C}$  (Brown et al. 1984; quoted, Muir 1991).

Ground water: reported  $t_{1/2} = 10 \text{ d}$  (Bottoni & Funari 1992)

Sediment:

Soil:  $t_{1/2} \sim 10 \text{ d}$  in soil (Hartley & Kidd 1987; Worthing & Hance 1991; quoted, Bottoni & Funari 1992; Montgomery 1993; Tomlin 1994);.

Biota:

17.1.1.10 *sec*-Bumeton

Common Name: *sec*-Bumeton

Synonym: etazine, GS14254, secbumeton

Chemical Name: *N*-ethyl-6-methoxy-*N'*-(1-methylpropyl)-1,3,5-triazine-2,4-diamine

CAS Registry No: 26259-45-0

Uses: herbicide

Molecular Formula: C<sub>10</sub>H<sub>19</sub>N<sub>3</sub>O

Molecular Weight: 225.291

Melting Point (°C):

87 (Lide 2003)

Boiling Point (°C):

Density (g/cm<sup>3</sup> at 20°C):

1.105 (Hartley & Kidd 1987; Worthing & Walker 1987)

Molar Volume (cm<sup>3</sup>/mol):

Dissociation Constant pK<sub>a</sub>:

4.4 (Worthing 1987)

4.4, 4.36 (Augustijn-Beckers et al. 1994; Hornsby et al. 1996)

Enthalpy of Fusion, ΔH<sub>fus</sub> (kJ/mol):

Entropy of Fusion, ΔS<sub>fus</sub> (J/mol K):

Fugacity Ratio at 25°C (assuming ΔS<sub>fus</sub> = 56 J/mol K), F: 0.246 (mp at 87°C)

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

620 (quoted, Kenaga & Goring 1980)

620 (Ashton & Crafts 1981)

600 (20°C, Hartley & Kidd 1987; Worthing & Walker 1987)

600 (20–25°C, selected, Augustijn-Beckers et al. 1994; Hornsby et al. 1996)

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

9.7 × 10<sup>-4</sup> (20°C, Ashton & Crafts 1981; Worthing & Walker 1987)

9.71 × 10<sup>-4</sup> (20°C, Hartley & Kidd 1987)

9.7 × 10<sup>-4</sup> (20–25°C, selected, Augustijn-Beckers et al. 1994; Hornsby et al. 1996)

Henry's Law Constant (Pa·m<sup>3</sup>/mol):

Octanol/Water Partition Coefficient, log K<sub>ow</sub>:

3.20 (LOGPSTAR or CLOGP data, Sabljic et al. 1995)

Octanol/Air Partition Coefficient, log K<sub>OA</sub>:

Bioconcentration Factor, log BCF or log K<sub>B</sub>:

1.20 (fish, Kenaga 1980b)

Sorption Partition Coefficient, log K<sub>OC</sub>:

2.54 (soil, calculated, Kenaga & Goring 1980)

2.11 (soil, calculated, Kenaga 1980b)

2.18 (soil, pH 7, Augustijn-Beckers et al. 1994; Hornsby et al. 1996)

2.78; 2.29 (soil: quoted, calculated-MCI χ, Meylan et al. 1992)

2.78 (soil, calculated-MCI χ, Sabljic et al. 1995)

2.78; 2.78, 2.55 (soil, estimated-class-specific model, estimated-general model using molecular descriptors, Gramatica et al. 2000)

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

Hydrolysis: on hydrolysis at 20°C,  $t_{1/2} \sim 30$  d at pH 1,  $t_{1/2} = 75$  d at pH 13 (Worthing & Walker 1987).

Half-Lives in the Environment:

Air:

Surface water: on hydrolysis at 20°C,  $t_{1/2} \sim 30$  d at pH 1,  $t_{1/2} = 75$  d at pH 13 (Worthing & Walker 1987).

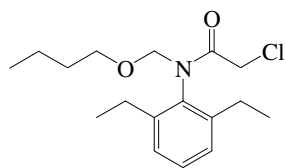
Ground water:

Sediment:

Soil: field  $t_{1/2} \sim 60$  d (estimated, Augustijn-Beckers et al. 1994; Hornsby et al. 1996).

Biota:

## 17.1.1.11 Butachlor



Common Name: Butachlor

Synonym: Butanex, Butanox, CP 53619, Lambast, Machete, Pillarsete

Chemical Name: N-butoxymethyl-2-chloro-2'-diethylacetanilide; N-(butoxymethyl)-2-chloro-N-(2,6-diethylphenyl)-acetamide

Uses: herbicide for pre-emergence control of most annual grasses, some broadleaf weeds, and many aquatic weeds in both seeded and transplanted rice.

CAS Registry No: 23184-66-9

Molecular Formula:  $C_{17}H_{26}ClNO_2$

Molecular Weight: 311.847

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

$< -5.0$  (Hartley & Kidd 1987; Worthing & Hance 1991; Tomlin 1994; Milne 1995; Lide 2003)

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

156 (at 0.5 mmHg, Ashton & Crafts 1981; Herbicide Handbook 1989; Tomlin 1994; Milne 1995)

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

1.07 ( $25^{\circ}C$ , Ashton & Crafts 1981; Hartley & Kidd 1987; Herbicide Handbook 1989; Tomlin 1994; Milne 1995)

Molar Volume ( $cm^3/mol$ ):

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

Dissociation Constant  $pK_a$ :

Enthalpy of Fusion,  $\Delta H_{fus}$  ( $kJ/mol$ ):

Entropy of Fusion,  $\Delta S_{fus}$  ( $J/mol K$ ):

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

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

23 ( $20^{\circ}C$ , Weber 1972; Worthing 1987)  
 20 (Martin & Worthing 1977)  
 23 ( $24^{\circ}C$ , Ashton & Crafts 1981; Herbicide Handbook 1989)  
 20 ( $20^{\circ}C$ , Hartley & Kidd 1987; Tomlin 1994; Milne 1995)  
 23 ( $24^{\circ}C$ , Worthing & Walker 1987, Worthing & Hance 1991)  
 23 ( $20-25^{\circ}C$ , selected, Augustijn-Beckers et al. 1994; Hornsby et al. 1996)

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

0.0007 ( $20^{\circ}C$ , Weber 1972; Worthing & Walker 1987)  
 0.0006 (Ashton & Crafts 1981; Herbicide Handbook 1989)  
 0.0006 (Hartley & Kidd 1987; Worthing & Hance 1991; Tomlin 1994)  
 0.0006 ( $20-25^{\circ}C$ , selected, Augustijn-Beckers et al. 1994; Hornsby et al. 1996)

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

0.00817 ( $20^{\circ}C$ , calculated-P/C, Muir 1991)  
 0.00814 (calculated-P/C, this work)

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

4.50 (quoted and recommended, Hansch et al. 1995; quoted, Sabljic et al. 1995)

Bioconcentration Factor,  $\log BCF$ :

2.06 (calculated-S, Kenaga 1980)  
 1.03, 0.756 (18, 9  $\mu g/L$  concn in water; carp, 3-5 d exposure, Wang et al. 1992)

0.38, 0.845 (10, 1 µg/L concn in water; tilapia, 3–5 d exposure, Wang et al. 1992)  
0.447, 0.845 (10, 1 µg/L concn in water; loach, 3–5 d exposure, Wang et al. 1992)  
1.76, 2.02 (2.5, 1.25 µg/L concn in water; grass carp, 3–5 d exposure, Wang et al. 1992)  
1.71, 1.90 (5, 2.5 µg/L concn in water; eel, 3–5 d exposure, Wang et al. 1992)  
1.99, 2.34 (2.4, 0.4 µg/L concn in water; black silver carp, 3–5 d exposure, Wang et al. 1992)  
0.041, 0.778 (100, 10 µg/L concn in water; freshwater clam, 3–5 d exposure, Wang et al. 1992)

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

2.92 (calculated-solubility, Kenaga 1980)  
2.85 (20–25°C, selected, Augustijn-Beckers et al. 1994; Hornsby et al. 1996)  
2.86 (soil, calculated-MCI  $\chi$ , Sabljic et al. 1995)

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

Volatilization: estimated  $t_{1/2} \sim 1049$  d from 1 m depth of water at 20°C (Muir 1991).

Photolysis:  $t_{1/2} = 0.8$ –5.4 h in distilled water (Chen et al. 1982; quoted, Cessna & Muir 1991).

Oxidation:

Hydrolysis:  $t_{1/2} > 2.5$  months for 2 µg/mL to hydrolyze in phosphate buffer at pH 6 and borate buffer at pH 9 both at 25°C (Chen & Chen 1979; quoted, Muir 1991).

Biodegradation:

Biotransformation:

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

Half-Lives in the Environment:

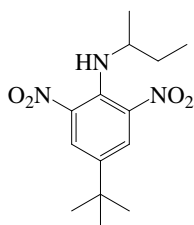
Soil: persists for 6–10 wk in soil (Hartley & Kidd 1987; Tomlin 1994);

$t_{1/2} = 4$  to 8 d depending upon soil type (Herbicide Handbook 1989);

persists in soil 42–70 d (Worthing & Hance 1991);

selected field  $t_{1/2} = 12$  d (Augustijn-Beckers et al. 1994; Hornsby et al. 1996).

## 17.1.1.12 Butralin



Common Name: Butralin

Synonym: Amex, Butalin, Rutralin, Sector, Tamex

Chemical Name: N-*sec*-butyl-4-*tert*-butyl-2,6-dinitroaniline; 4-(1,1-dimethylethyl)-N-(1-methylpropyl)-2,6-dinitrobenzenamine

Uses: herbicide for pre-emergence control of annual broadleaf weeds and grasses in cotton, beans, barley, rice, soybeans, alliums, vines, ornamentals and orchards of fruit and nut trees; also to control suckers on tobacco.

CAS Registry No: 33629-47-9e

Molecular Formula:  $C_{14}H_{21}N_3O_4$

Molecular Weight: 295.335

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

60 (Lide 2003)

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

134–136 (at 0.5 mmHg, Hartley & Kidd 1987; Worthing & Hance 1991; Tomlin 1994; Milne 1995)

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

Molar Volume ( $cm^3/mol$ ):

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

Dissociation Constant  $pK_a$ :

Enthalpy of Fusion,  $\Delta H_{fus}$  (kJ/mol):

Entropy of Fusion,  $\Delta S_{fus}$  (J/mol K):

Fugacity Ratio at  $25^{\circ}C$  (assuming  $\Delta S_{fus} = 56$  J/mol K), F: 0.454 (mp at  $60^{\circ}C$ )

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

1.0 (Herbicide Handbook 1978)  
 1.0 (Khan 1980)  
 10 ( $24^{\circ}C$ , Ashton & Crafts 1981)  
 1.0 ( $24^{\circ}C$ , Hartley & Kidd 1987; Tomlin 1994; Milne 1995)  
 1.0 ( $24$ – $26^{\circ}C$ , Worthing & Walker 1987, Worthing & Hance 1991)  
 1.0 (Budavari 1989)

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

0.002 (Ashton & Crafts 1981)  
 0.0017 (Hartley & Kidd 1987; Worthing & Hance 1991; Tomlin 1994)  
 0.0017 (Budavari 1989)

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

0.502 (calculated-P/C, this work)

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

4.54 (selected, Dao et al. 1983)  
 5.16 (quoted LOGPSTAR or CLOGP data, Sabljic et al. 1995)

Bioconcentration Factor, log BCF:

2.79 (calculated-S, Kenaga 1980; quoted, Isensee 1991)  
 2.80 (calculated- $K_{oc}$ , Kenaga 1980)

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

- 3.64 (calculated, Kenaga & Goring 1980; quoted, Kenaga 1980)
- 3.91 (soil, Kenaga & Goring 1980; quoted, Sabljic 1987; Bahnick & Doucette 1988)
- 3.75 (calculated-MCI  $\chi$ , Bahnick & Doucette 1988)
- 3.98 (soil, calculated-MCI  $^1\chi$ , Sabljic et al. 1995)
- 3.98; 3.38 (soil, quoted exptl.; estimated-general model using molecular descriptors, Gramatica et al. 2000)

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

Volatilization:

Photolysis:  $t_{1/2} = 8$  h for 25% of 2000  $\mu\text{g/mL}$  to degrade in methanol under sunlight (Plimmer & Klingebiel 1974; quoted, Cessna & Muir 1991).

Oxidation:

Hydrolysis:

Biodegradation:  $t_{1/2} = 24$  d for 0.5  $\mu\text{g/mL}$  to biodegrade in soil at 20–42°C (Savage 1978; quoted, Muir 1991).

Biotransformation:

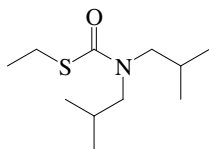
Bioconcentration, Uptake ( $k_1$ ) and Elimination ( $k_2$ ) Rate Constants:

## Half-Lives in the Environment:

Soil:  $t_{1/2} = 24$  d for 0.5  $\mu\text{g/mL}$  to biodegrade in soil at 20–42°C (Savage 1978; quoted, Muir 1991).



## 17.1.1.13 Butylate



Common Name: Butylate

Synonym: Butilate, diisocarb, Genate, R 1910, Sutan

Chemical Name: *S*-ethyl-diisobutylthiocarbamate; *S*-ethyl-bis(2-methylpropylcarbamothioate

Uses: herbicide to control annual grass weeds in maize, by pre-plant soil incorporation; also to control some broadleaf weeds.

CAS Registry No: 2008-41-5

Molecular Formula:  $C_{11}H_{23}NO_S$

Molecular Weight: 217.372

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

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

137.5–138 (at 21 mmHg, Hartley & Kidd 1987; Worthing & Hance 1991; Tomlin 1994; Milne 1995)

71.0 (at 10 mmHg, Herbicide Handbook 1989)

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

0.9402 ( $25^{\circ}C$ , Hartley & Kidd 1987; Herbicide Handbook 1989; Worthing & Hance 1991; Tomlin 1994)

0.9417 (Milne 1995)

Molar Volume ( $cm^3/mol$ ):

280.9 (calculated-Le Bas method at normal boiling point, Suntio et al. 1988)

Dissociation Constant  $pK_a$ :

Enthalpy of Fusion,  $\Delta H_{fus}$  ( $kJ/mol$ ):

Entropy of Fusion,  $\Delta S_{fus}$  ( $J/mol K$ ):

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

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

45.0 (Kenaga 1980; Weber et al. 1980)

45.0 ( $22^{\circ}C$ , Ashton & Crafts 1981; Hartley & Kidd 1987; Herbicide Handbook 1989)

46.0 ( $20^{\circ}C$ , Worthing & Walker 1987, Worthing & Hance 1991)

44.0 ( $20$ – $25^{\circ}C$ , selected, Wauchope et al. 1992; Hornsby et al. 1996)

36.0 ( $20^{\circ}C$ , Tomlin 1994)

45.0 ( $22^{\circ}C$ , Milne 1995)

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

1.73 (Ashton & Crafts 1973)

0.096 ( $20^{\circ}C$ , Hartley & Graham-Bryce 1980)

1.733 (Herbicide Handbook 1983, 1989)

0.287 ( $20^{\circ}C$ , GC-RT correlation, Kim 1985)

0.10 ( $20^{\circ}C$ , selected, Suntio et al. 1988)

0.17 (Worthing & Hance 1991)

1.733 ( $20$ – $25^{\circ}C$ , selected, Wauchope et al. 1992; Hornsby et al. 1996)

1.73 (Tomlin 1994)

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

0.560 ( $20^{\circ}C$ , calculated-P/C, Suntio et al. 1988)

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

4.15 (Worthing & Hance 1991; Tomlin 1994; Milne 1995)

4.15 (recommended, Hansch et al. 1995)

4.17, 4.01, 3.45 (RP-HPLC-RT correlation, CLOGP, calculated-S, Finizio et al. 1997)

## Bioconcentration Factor, log BCF:

- 1.86 (calculated-S, Kenaga 1980)
- 3.06 (calculated- $K_{OW}$  as per Kenaga 1980, this work)

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

- 2.73 (soil, Kenaga 1980)
- 2.73, 4.09 (quoted values, Bottoni & Funari 1992)
- 2.60 (soil, 20–25°C, selected, Wauchope et al. 1992)
- 2.60 (estimated-chemical structure, Lohninger 1994)
- 2.11 (soil, calculated-MCI  $^1\chi$ , Sabljic et al. 1995)
- 2.39, 2.13 (soil, estimated-class specific model, estimated-general model using molecular descriptors, Gramatica et al. 2000)

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

## Half-Lives in the Environment:

Air:

Surface water:

Ground water: reported half-lives or persistence,  $t_{1/2}$  = 11–21 d (Bottoni & Funari 1992)

Sediment:

Soil: measured dissipation rate  $k$  = 3.6 d<sup>-1</sup> (Nash 1983; quoted, Nash 1988);

estimated dissipation rate  $k$  = 23 and 0.61 d<sup>-1</sup> (Nash 1988);

$t_{1/2}$  = 1.5–3.0 wk in several soils under crop growing conditions (Herbicide Handbook 1989);

selected field  $t_{1/2}$  = 13 d (Wauchope et al. 1992; quoted, Richards & Baker 1993; Hornsby et al. 1996)

reported  $t_{1/2}$  = 11–21 d (Bottoni & Funari 1992);

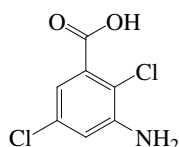
soil  $t_{1/2}$  = 12 d (quoted, Pait et al. 1992);

$t_{1/2}$  = 1.5–10 wk in soil and water (Tomlin 1994);

soil  $t_{1/2}$  = 13 d (selected, Halfon et al. 1996).

Biota: disappear from the stems and leaves of corn plants 7 to 14 d after application (Herbicide Handbook 1989).

## 17.1.1.14 Chloramben



Common Name: Chloramben

Synonym: ACP-M-728, Amiben, Amoben, Chlorambed, Chlorambene, M-728, NCI-C00055, Ornamental weeder, Vegaben, Vegiben

Chemical Name: 3-amino-2,5-dichlorobenzoic acid

Uses: pre-emergence or pre-plant herbicide used in many vegetable and field crops to control annual broadleaf weeds and grasses.

CAS Registry No: 133-90-4

Molecular Formula:  $C_7H_5Cl_2NO_2$

Molecular Weight: 206.027

Melting Point (°C):

200 (Lide 2003)

Boiling Point (°C):

Density ( $g/cm^3$  at 20°C):

Molar Volume ( $cm^3/mol$ ):

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

Dissociation Constant  $pK_a$ :

3.40 (Hornsby et al. 1996)

Enthalpy of Fusion,  $\Delta H_{fus}$  (kJ/mol):

38.91 (DSC method, Plato 1972)

Entropy of Fusion,  $\Delta S_{fus}$  (J/mol K):

Fugacity Ratio at 25°C (assuming  $\Delta S_{fus} = 56$  J/mol K), F: 0.0192 (mp at 200°C)

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

700 (Spencer 1973; Ashton & Crafts 1981)

700 (Martin & Worthing 1977; Herbicide Handbook 1978; 1989)

700 (Hartley & Kidd 1987; Budavari 1989; Montgomery 1993; Milne 1995)

700 (Worthing & Walker 1987, Worthing & Hance 1991; Tomlin 1994; Majewski & Capel 1995)

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

0.933 (100°C, Segal & Sutherland 1967; Spencer 1976)

0.93 (100°C, Hartley & Kidd 1987; Worthing & Hance 1991; Tomlin 1994)

52.7 (Worthing & Walker 1987)

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

0.274 (calculated-P/C as per Worthing 1987)

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

1.11 (quoted, Rao & Davidson 1980)

1.46 (selected, Dao et al. 1983)

-2.64 (selected, Gerstl & Helling 1987)

1.11 (Magee 1991)

1.11 (Montgomery 1993)

1.11 (Log P database of Hansch & Leo 1987, Sangster 1993)

1.90 (CLOGPSTAR or CLOGP data, Sabljic et al. 1995)

Bioconcentration Factor,  $\log BCF$ :

1.18 (calculated-S, Kenaga 1980)

-0.097 (calculated- $K_{OC}$ , Kenaga 1980)

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

- 1.32 (soil, Harris & Warren 1964; Farmer 1976)
- 2.08 (soil, calculated as per Kenaga & Goring 1980, Kenaga 1980)
- 1.78 (calculated-MCI  $\chi$ , Gerstl & Helling 1987)
- 1.32 (reported as  $\log K_{OM}$ , Magee 1991)
- 2.28 (Montgomery 1993)
- 1.56 (selected, Lohninger 1994)
- 1.48 (soil, calculated-MCI  $^1\chi$ , Sabljic et al. 1995)

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

Volatilization:

Photolysis:  $t_{1/2} = 6$  h for 206  $\mu\text{g/mL}$  to degrade in distilled water under sunlight (Sheets 1963; quoted, Cessna & Muir 1991);

$t_{1/2} < 2$  d for 16  $\mu\text{g/mL}$  to degrade in distilled water under sunlight (Hahn et al. 1969; quoted, Cessna & Muir 1991).

Oxidation:

Hydrolysis:

Biodegradation:  $t_{1/2} > 70$  d for 50  $\mu\text{g/mL}$  to degrade in incubated soil with nutrient medium of 3 g/L (Schliebe et al. 1965; quoted, Muir 1991).

Biotransformation:

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

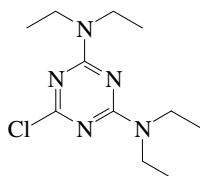
Half-Lives in the Environment:

Soil: estimated persistence of 3 months (Kearney et al. 1969; quoted, Jury et al. 1987);

$t_{1/2} = 36, 38, 41$ , and 20 d with disappearance rates:  $k = 0.0193, 0.0182, 0.0169$  and  $0.0347 \text{ d}^{-1}$  at pH 4.3, 5.3, 6.5 and 7.5 (Hamaker 1972; quoted, Nash 1988);

persistence in soil is of 6–8 wk (Hartley & Kidd 1987; Herbicide Handbook 1989; quoted, Montgomery 1993).

## 17.1.1.15 Chlorazine



Common Name: Chlorazine

Synonym:

Chemical Name: 6-chloro-*N,N,N',N'*-tetraethyl-1,3,5-triazine-2,4-diamine

Uses: herbicide

CAS Registry No: 580-48-3

Molecular Formula:  $C_{11}H_{20}ClN_5$

Molecular Weight: 257.764

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

27 (Howard 1991; Lide 2003)

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

154–156/4.0 mmHg (Howard 1991)

Density ( $g/cm^3$ ):

Acid Dissociation Constants,  $pK_a$ :

1.74 ( $pK_a$  of conjugate acid, Howard 1991)

Molar Volume ( $cm^3/mol$ ):

Enthalpy of Fusion,  $\Delta H_{fus}$  (kJ/mol):

Entropy of Fusion,  $\Delta S_{fus}$  (J/mol K):

Fugacity Ratio at  $25^{\circ}C$ , (assuming  $\Delta S_{fus} = 56$  J/mol K), F: 0.956 (mp at  $27^{\circ}C$ )

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

23.7, 22.2, 21.4 ( $26^{\circ}C$ , shake flask-UV at pH 3.0, 7.0, 10.0, Ward & Weber 1968)

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

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

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

3.236 (estimated, Howard 1991)

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

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

2.033 (estimated-S, Howard 1991)

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

2.90 (calculated-S, Howard 1991)

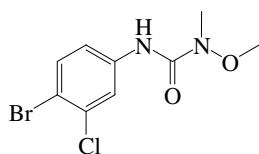
Environmental Fate Rate Constants,  $k$ , and Half-Lives,  $t_{1/2}$ :

Hydrolysis: may be more important at low pH (Howard 1991).

Half-Lives in the Environment:

Air:  $t_{1/2} = 2.5$  h for the vapor phase reaction with OH radicals (estimated, Howard 1991).

## 17.1.1.16 Chlorbromuron



Common Name: Chlorbromuron

Synonym: Maloran

Chemical Name: 3-(4-bromo-3-chlorophenyl)-1-methoxy-1-methylurea

Uses: herbicide

CAS Registry No: 13360-45-7

Molecular Formula:  $C_9H_{10}BrClN_2O_2$

Molecular Weight: 293.544

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

96 (Lide 2003)

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

Density ( $g/cm^3$ ): 1.69 (Tomlin 1994)

Acid Dissociation Constants,  $pK_a$ :

Molar Volume ( $cm^3/mol$ ):

Enthalpy of Fusion,  $\Delta H_{fus}$  ( $kJ/mol$ ):

Entropy of Fusion,  $\Delta S_{fus}$  ( $J/mol\ K$ ):

Fugacity Ratio at  $25^{\circ}C$ , (assuming  $\Delta S_{fus} = 56\ J/mol\ K$ ) F: 0.201 (mp at  $96^{\circ}C$ )

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

50 (Kenaga & Goring 1980, Kenaga 1980a; Ashton & Crafts 1981)

35 ( $20^{\circ}C$ , Spencer 1982; Worthing 1983; Hartley & Kidd 1987; Tomlin 1994)

35; 27.4 (quoted; calculated-MCI  $\chi$ , Patil 1994)

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

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

$5.33 \times 10^{-5}$  ( $20^{\circ}C$ , Ashton & Crafts 1981)

$5.3 \times 10^{-5}$  (Spencer 1982; Worthing 1983; Hartley & Kidd 1987; Tomlin 1994)

$5.33 \times 10^{-5}$  (selected,  $20$ – $25^{\circ}C$ , Augustijn-Beckers et al. 1994; Hornsby et al. 1996)

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

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

3.06 (quoted, Rao & Davidson 1980)

3.09 (shake flask, Brigg 1981)

3.09; 3.26 (quoted lit.; calculated-MCI  $\chi$ , Patil 1994)

3.09 (recommended, Hansch et al. 1995)

2.86, 2.99, 3.45 (RP-HPLC-RT correlation, CLOGP, HPLC- $k'$  correlation, Finizio et al. 1997)

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

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

1.83, 1.40 (quoted, calculated, Kenaga 1980b)

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

2.66 (soil, Kenaga & Goring 1980)

2.66, 2.71 (quoted, calculated- $K_{ow}$ , Kenaga 1980b)

3.00 (mean value of 5 soils, Rao & Davidson 1980)

2.34, 2.94 (quoted, calculated-MCI  $\chi$ , Gerstl & Helling 1987)

2.19–3.61 (range of reported data, Augustijn-Beckers et al. 1994)

- 2.70 (estimated and recommended, soil, Augustjin-Beckers et al. 1994; Hornsby et al. 1996)  
2.70 (soil, calculated-MCI  $^1\chi$ , Sabljic et al. 1995)  
2.70, 2.97 (soil, estimated-class-specific model, estimated-general model using molecular descriptors, Gramatica et al. 2000)  
2.54, 2.55 (soils: organic carbon OC  $\geq 0.1\%$ , OC  $\geq 0.5\%$ , average, Delle Site 2001)

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

Hydrolysis: slowly hydrolyzed in neutral, slightly acidic, and slightly alkaline media (Hartley & Kidd 1987; Tomlin 1994).

Half-Lives in the Environment:

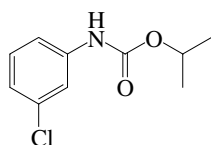
Soil: persists in soil > 56 d (Worthing 1983);

$t_{1/2} = 45$  d (Hartley & Kidd 1987);

$t_{1/2} = 45\text{--}120$  d (Tomlin 1994);

$t_{1/2} = 21\text{--}45$  d and 40 d (range of reported values and recommended field half-life, Augustjin-Beckers et al. 1994; Hornsby et al. 1996)

## 17.1.1.17 Chlorpropham



Common Name: Chlorpropham

Synonym: Beet-Kleen, Bud-nip, Chlor-IFC, Chloro-IPC, CIPC, Ebanil, ENT 18060, Fasco Wy-hoe, Furloe, Nexoval, Prevenol, Preweed, Sprout-nip, Taterpex

Chemical Name: isopropyl N-(3-chlorophenyl) carbamate; isopropyl 3-chlorocarbamate

Uses: pre-emergent and post-emergent herbicide used to regulate plant growth and control weeds in carrot, onion, garlic, and other crops.

CAS Registry No: 101-21-3

Molecular Formula:  $C_{10}H_{12}ClNO_2$

Molecular Weight: 213.661

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

41 (Lide 2003)

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

149 (at 2 mmHg, Budavari 1989)

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

1.180 ( $30^{\circ}C$ , Hartley & Kidd 1987; Herbicide Handbook 1989; Worthing & Hance 1991; Montgomery 1993; Tomlin 1994)

1.5388 (Budavari 1989)

Molar Volume ( $cm^3/mol$ ):

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

Enthalpy of Vaporization,  $\Delta H_v$  (kJ/mol):

88.67 (Rordorf 1989)

Enthalpy of Fusion,  $\Delta H_{fus}$  (kJ/mol):

20.50 (DSC method, Plato & Glasgow 1969)

16 (Rordorf 1989)

Entropy of Fusion,  $\Delta S_{fus}$  (J/mol K):

Fugacity Ratio at  $25^{\circ}C$  (assuming  $\Delta S_{fus} = 56$  J/mol K), F: 0.697 (mp at  $41^{\circ}C$ )

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

0.470 (Brust 1966)

102.3 (shake flask-GC, Freed et al. 1967)

108 ( $20^{\circ}C$ , Günther et al. 1968)

89 ( $20^{\circ}C$ , Weber 1972; Martin & Worthing 1977; Worthing & Walker 1987)

2.0 (Spencer 1973; quoted, Shiu et al. 1990)

88 (Martin & Worthing 1977; Herbicide Handbook 1978, 1989)

0.70 ( $19^{\circ}C$ , shake flask-GC, Bowman & Sans 1979)

0.73 ( $20^{\circ}C$ , shake flask-GC, Bowman & Sans 1983a,b)

88 (Khan 1980; Ashton & Crafts 1981)

80–102 (Weber et al. 1980)

89 (Hartley & Kidd 1987; Worthing & Hance 1991; Tomlin 1994)

89 (selected, Gerstl & Helling 1987; Montgomery 1993; Lohninger 1994)

2.0 ( $20^{\circ}C$ , Worthing & Walker 1987)

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

0.00050 ( $20^{\circ}C$ , Weber 1972; Worthing & Walker 1987)

0.00133 (extrapolated, Spencer 1976)

0.00133 (Khan 1980)

0.00133 (Ashton & Crafts 1981; Herbicide Handbook 1989)

0.00100 ( $20^{\circ}C$ , selected, Suntio et al. 1988)



0.012, 0.30, 5.0, 56, 470 (25, 50, 70, 100, 125°C, gas saturation-GC, Rordorf 1989)

$\log (P_s/Pa) = 16.402 - 5467.7/(T/K)$ ; measured range 44.9–140°C (solid, gas saturation-GC, Rordorf 1989)

$\log (P_L/Pa) = 13.753 - 4631.9/(T/K)$ ; measured range 44.9–140°C (liquid, gas saturation-GC, Rordorf 1989)

0.00130 (selected, Taylor & Spencer 1990)

0.00107 (20–25°C, selected, Wauchope et al. 1992; Hornsby et al. 1996)

0.00133 (estimated, Montgomery 1993)

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

0.0021 (20°C, calculated-P/C, Suntio et al. 1988)

0.0032 (20°C, calculated-P/C, Muir 1991)

0.0021 (20–25°C, calculated-P/C, Montgomery 1993)

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

3.06 (Rao & Davidson 1980; Karickhoff 1981)

3.42 (selected, Dao et al. 1983; Gerstl & Helling 1987)

3.51 (shake flask, Mitsutake et al. 1986)

3.10 (selected, Suntio et al. 1988)

3.51 (recommended, Sangster 1993)

3.09 (calculated, Patil 1994)

3.51 (recommended, Hansch et al. 1995)

Bioconcentration Factor,  $\log BCF$ :

1.70 (calculated-S, Kenaga 1980)

1.52 (calculated- $K_{oc}$ , Kenaga 1980)

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

2.77 (soil, Hamaker & Thompson 1972)

2.57 (soil, calculated-S as per Kenaga & Goring 1980, Kenaga 1980)

2.85, 2.80 (estimated-S, Karickhoff 1981)

3.17, 3.08 (estimated-S and mp, Karickhoff 1981)

2.67 (estimated- $K_{ow}$ , Karickhoff 1981)

2.31 (calculated-MCI  $\chi$ , Gerstl & Helling 1987)

2.32 (calculated-MCI  $\chi$  and fragment contribution method, Meylan et al. 1992)

2.60 (soil, 20–25°C, estimated, Wauchope et al. 1992; Hornsby et al. 1996)

2.77, 2.91 (Montgomery 1993)

2.60 (estimated-chemical structure, Lohninger 1994)

2.53 (soil, calculated-MCI  $\chi$ , Sabljic et al. 1995)

2.40, 2.05 (soil, estimated-class-specific model, estimated-general model using molecular descriptors, Gramatica et al. 2000)

2.62 (2.37–2.87) (soil: organic carbon OC  $\geq$  0.5%, average, Delle Site 2001)

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

Volatilization:  $t_{1/2} = 2220$  d from 1-m depth of water at 20°C (estimated, Muir 1991).

Photolysis:  $t_{1/2} = 130$  h for 4  $\mu\text{g/mL}$  to degrade in distilled water under  $> 280$  nm light (Guzik 1978; quoted, Cessna & Muir 1991)

direct photolysis  $t_{1/2} = 121$  d in distilled water pH 5–7 for a mid-summer day at latitude of 40° (Wolfe et al. 1978)

$t_{1/2} = 2.25$  h for 21–76% of 80  $\mu\text{g/mL}$  to degrade in distilled water under 300 nm light (Tanaka et al. 1981; quoted, Cessna & Muir 1991).

Oxidation:

Hydrolysis:  $t_{1/2} > 4$  months for 4274  $\mu\text{g/mL}$  to hydrolyze in phosphate buffer at pH 5–9 and 20°C (El-Dib & Aly 1976; quoted, Muir 1991)

$k(\text{alkaline}) = 2.0 \times 10^{-5} \text{ M}^{-1} \text{ s}^{-1}$  at 27°C,  $1.9 \times 10^{-4} \text{ M}^{-1} \text{ s}^{-1}$  at 50°C,  $6.4 \times 10^{-4} \text{ M}^{-1} \text{ s}^{-1}$  at 70°C; with  $t_{1/2} > 1 \times 10^4$  d at pH 5, 7 and 9 (Wolfe et al. 1978)

$t_{1/2} > 1$  wk for 2.10  $\mu\text{g/mL}$  to hydrolyze in natural waters at 67°C (Schnoor et al. 1982; quoted, Muir 1991).

#### Biodegradation:

$t_{1/2}(\text{aerobic}) = 10\text{--}75$  d for 0.1–5.4  $\mu\text{g/mL}$  to biodegrade in activated sludge (Schwartz 1967; quoted, Muir 1991)

$k = (3.6\text{--}6.7) \times 10^{-10}$  mL cell<sup>-1</sup> d<sup>-1</sup> of different river water samples (Paris et al. 1978; quoted, Scow 1982)

$t_{1/2} = 120$  d by fungi *Aspergillus fumigatus* and  $t_{1/2} = 2.9$  d by bacteria at 28°C (Wolfe et al. 1978)

$k = 2.5 \times 10^{-4}$  L (mg M)<sup>-1</sup> h<sup>-1</sup> with  $t_{1/2} = 120$  d for 2–25  $\mu\text{g/mL}$  fungus *Aspergillus fumigatus*;  $k = 0.1$  L (mg M)<sup>-1</sup> h<sup>-1</sup> with  $t_{1/2} = 2.9$  d for bacteria *Pseudomonas striata* to biodegrade in stream water at pH 7 and 28°C (Wolfe et al. 1978; quoted, Muir 1991)

$k = (1.6\text{--}1.8) \times 10^{-8}$  mL cell<sup>-1</sup> d<sup>-1</sup> of different river water samples (Steen et al. 1979; quoted, Scow 1982)

$k = (2.6 \pm 0.72) \times 10^{-14}$  L cell<sup>-1</sup> h<sup>-1</sup> in North American waters (Paris et al. 1981; quoted, Battersby 1990)

$k = (1.3\text{--}4.9) \times 10^{-4}$  L org<sup>-1</sup> h<sup>-1</sup> with  $t_{1/2}(\text{aerobic}) = 190$  h for 0.1–1.0  $\mu\text{g/mL}$  to biodegrade in lake water at 22°C (Schnoor et al. 1982; quoted, Muir 1991)

$k = (1.4\text{--}4.2) \times 10^{-13}$  L org<sup>-1</sup> h<sup>-1</sup> for 75  $\mu\text{g/mL}$  to biodegrade at 28°C in natural and sediment waters (Steen et al. 1982; quoted, Muir 1991);

$t_{1/2}(\text{aerobic}) > 4$  months for 6–7  $\mu\text{g/mL}$  to biodegrade in river water at 25°C (Stepp et al. 1985; quoted, Muir 1991).

#### Biotransformation:

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

#### Half-Lives in the Environment:

##### Air:

Surface water: rate constant  $k = 3.6\text{--}6.7 \times 10^{-10}$  mL cell<sup>-1</sup> d<sup>-1</sup> from measurements of different river water samples (Paris et al. 1978; quoted, Scow 1982);

hydrolysis  $t_{1/2} > 1 \times 10^4$  d based on neutral and alkaline hydrolysis assuming pseudo-first order kinetics; direct photolysis  $t_{1/2} = 121$  d assuming a quantum efficiency of 1 and for a mid-summer day at altitude 40°, and biolysis  $t_{1/2} = 120$  d for 1mg/L of fungus and  $t_{1/2} = 2.9$  d for bacteria at 28°C (Wolfe et al. 1978);

$k = (1.6\text{--}1.8) \times 10^{-8}$  mL cell<sup>-1</sup> d<sup>-1</sup> from measurements of different river water samples (Steen et al. 1979; quoted, Scow 1982);

aerobic  $t_{1/2} = 190$  h for 0.1–1.0  $\mu\text{g/mL}$  to biodegrade in lake water with biodegradation rate of  $(1.3\text{--}4.9) \times 10^{-4}$  L org<sup>-1</sup> h<sup>-1</sup> at 22°C (Schnoor et al. 1982; quoted, Muir 1991);

aerobic  $t_{1/2} > 4$  months for 6–7  $\mu\text{g mL}^{-1}$  to biodegrade in river water at 25°C (Stepp et al. 1985; quoted, Muir 1991).

##### Ground water:

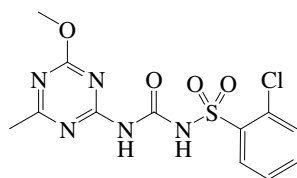
Sediment: aerobic half-life of 10–75 d for 0.1–5.4  $\mu\text{g/mL}$  to biodegrade in activated sludge (Schwartz 1967; quoted, Muir 1991).

Soil:  $t_{1/2} = 65$  and 30 d soil at 15 and 29°C, respectively (Hartley & Kidd 1987; Herbicide Handbook 1989; quoted, Montgomery 1993; Tomlin 1994);

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

##### Biota:

## 17.1.1.18 Chlorsulfuron



Common Name: Chlorsulfuron

Synonym: DPX 4189, Finesse, Glean, Telar

Chemical Name: 2-chloro-*N*-(((4-methoxy-6-methyl-1,3,5-triazin-2-yl)amino)-carbonyl)-benzenesulfonamide;  
1-(*o*-chlorophenyl)-3-(4-methoxy-6-methyl-*s*-triazin-2-yl)urea

Uses: herbicide to control broadleaf weeds and some grass weeds.

CAS Registry No: 64902-72-3

Molecular Formula: C<sub>12</sub>H<sub>12</sub>ClN<sub>5</sub>O<sub>4</sub>S

Molecular Weight: 357.773

Melting Point (°C):

176 (Lide 2003)

Boiling Point (°C):

192 (dec., Herbicide Handbook 1989; Montgomery 1993)

Density (g/cm<sup>3</sup> at 20°C):

Molar Volume (cm<sup>3</sup>/mol):

Dissociation Constant pK<sub>a</sub>:

3.6 (Herbicide Handbook 1989; Worthing & Hance 1991; Montgomery 1993; Tomlin 1994)

Enthalpy of Fusion, ΔH<sub>fus</sub> (kJ/mol):

Entropy of Fusion, ΔS<sub>fus</sub> (J/mol K):

Fugacity Ratio at 25°C (assuming ΔS<sub>fus</sub> = 56 J/mol K), F: 0.0330 (mp at 176°C)

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

300 (at pH 5, Hartley & Kidd 1987; Worthing & Hance 1991; Tomlin 1994; Milne 1995)  
27900 (at pH 7, Hartley & Kidd 1987; Worthing & Hance 1991; Tomlin 1994; Milne 1995)  
28000 (at pH 7 with ionic strength 0.05, Herbicide Handbook 1989)  
7000 (20–25°C, at pH 7, selected, Wauchope et al. 1992; quoted, Majewski & Capel 1995)  
7000 (20–25°C, at pH 7, selected, Hornsby et al. 1996)  
60, 7000 (at pH 5, pH 7, Montgomery 1993)  
32000 (selected, Armbrust 2000)

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

6.10 × 10<sup>-4</sup> (Hartley & Kidd 1987)  
6.13 × 10<sup>-4</sup> (Herbicide Handbook 1989)  
3.00 × 10<sup>-9</sup> (Worthing & Hance 1991; Tomlin 1994)  
1.98 × 10<sup>-2</sup> (20–25°C, Wauchope et al. 1992)  
3.11 × 10<sup>-9</sup> (Montgomery 1993)  
6.13 × 10<sup>-4</sup> (20–25°C, selected, Hornsby et al. 1996)

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

3.60 × 10<sup>-11</sup> (calculated-P/C, Montgomery 1993)  
1.98 × 10<sup>-5</sup> (20–25°C, calculated-P/C as per Wauchope et al. 1992, Majewski & Capel 1995)  
6.79 × 10<sup>-6</sup> (selected, Armbrust 2000)

Octanol/Water Partition Coefficient, log K<sub>ow</sub>:

-0.84, 0.17, 1.09 (pH 8.4, pH 7.1, pH 4.5, UV, Ribo 1988)  
-0.88, 1.05 (pH 8.4, pH 4.5, HPLC, Ribo 1988)  
-1.34, 0.74 (pH 7, pH 4.5, Hay 1990)

2.20 (Grayson & Kleier 1990)  
 -1.0 (Montgomery 1993)  
 -0.88, 1.05, -1.34, 0.74, 2.20 (reported values, Sangster 1993)  
 -1.00 (at pH 7, Tomlin 1994)  
 0.74, -1.34 (lit. values, Hansch et al. 1995)  
 2.14 (LOGPSTAR or CLOGP data, Sabljic et al. 1995)

Bioconcentration Factor, log BCF:

0.622 (calculated-S as per Kenaga 1980, this work)

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

1.02 (Flanagan silt loam, Montgomery 1993)  
 1.60 (Tomlin 1994)  
 2.19 (calculated-MCI  $^1\chi$ , Sabljic et al. 1995)  
 1.60 (at pH 7, selected, Hornsby et al. 1996)  
 1.56 (selected, Armbrust 2000)

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

Volatilization:

Photolysis: assuming first-order kinetics, calculated  $t_{1/2} \sim 186$  h for 33  $\mu\text{g/mL}$  to degrade in distilled water,  $t_{1/2} = 31$  h for creek water,  $t_{1/2} = 136$  h for silica gel and  $t_{1/2} = 115$  h for montmorillonit under sunlight (Herrmann et al. 1985; quoted, Cessna & Muir 1991);  
 under indoor conditions  $t_{1/2} = 92$  h in methanol,  $t_{1/2} = 78$  h in distilled water but  $t_{1/2} = 18$  h in natural creek water (Herrmann et al. 1985);  
 reported  $t_{1/2} = 18$  h in distilled water at  $> 290$  nm (Montgomery 1993)  
 aqueous photolysis rate constant,  $k = 5.0 \times 10^{-4} \text{ h}^{-1}$  (Armbrust 2000).

Oxidation:

Hydrolysis:  $t_{1/2} = 4\text{--}8$  wk at  $20^\circ\text{C}$  and pH 5.7–7.0 (Hartley & Kidd 1987; Worthing & Hance 1991; Montgomery 1993; Tomlin 1994);

stable aqueous hydrolysis rates at pH 7, 9; measured hydroxy radical rate constant for chlorsulfuron  $6.9 \times 10^{12} \text{ M}^{-1}/\text{h}$  (Armbrust 2000).

Biodegradation: aerobic rate constant,  $k = 1.44 \times 10^{-3} \text{ h}^{-1}$  (Armbrust 2000).

Biotransformation:

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

Half-Lives in the Environment:

Soil: hydrolysis rates will be increased by warm soil temperatures at low pH and in the presence of moisture with an average  $t_{1/2} = 4\text{--}6$  wk under growing conditions (Hartley & Kidd 1987; Herbicide Handbook 1989)  
 $t_{1/2} = 4\text{--}6$  wk for degradation in soil via hydrolysis followed by microbial degradation (Hartley & Kidd 1987; quoted, Montgomery 1993; Tomlin 1994);

degradation rate constants:  $k = 0.033 \text{ d}^{-1}$  at depth 0–20 cm with  $t_{1/2} = 21$  d,  $k = 0.0315 \text{ d}^{-1}$  at depth 20–40 cm with  $t_{1/2} = 22$  d and for depth 40–60 cm with  $t_{1/2} > 150$  d (Soakwaters soil, Walker et al. 1989);

degradation  $k = 0.0116 \text{ d}^{-1}$  at depth 0–20 cm with  $t_{1/2} = 60$  d,  $k = 0.0120 \text{ d}^{-1}$  at depth 20–40 cm with  $t_{1/2} = 58$  d, and  $k = 0.0076 \text{ d}^{-1}$  at depth 40–60 cm with  $t_{1/2} = 91$  d (Wharf ground soil, Walker et al. 1989);

degradation  $k = 0.0126 \text{ d}^{-1}$  at depth 0–20 cm with  $t_{1/2} = 55$  d,  $k = 0.0073 \text{ d}^{-1}$  at depth 20–40 cm with  $t_{1/2} = 95$  d, and  $k = 0.0056 \text{ d}^{-1}$  at depth 40–60 cm with  $t_{1/2} = 124$  d (Cottage Field soil, Walker et al. 1989);

degradation  $k = 0.0147 \text{ d}^{-1}$  at depth 0–20 cm with  $t_{1/2} = 47$  d,  $0.0116 \text{ d}^{-1}$  at depth 20–40 cm with  $t_{1/2} = 60$  d, and  $k = 0.0047 \text{ d}^{-1}$  at depth 40–60 cm with  $t_{1/2} = 147$  d (Hunts Mill soil, Walker et al. 1989);

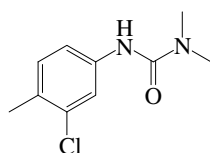
degradation  $0.0094 \text{ d}^{-1}$  (depth 0–20 cm with  $t_{1/2} = 74$  d),  $0.0096 \text{ d}^{-1}$  (depth 20–40 cm with  $t_{1/2} = 72$  d) and  $0.0082 \text{ d}^{-1}$  (depth 40–60 cm with  $t_{1/2} = 85$  d) (Bottom Barn soil, Walker et al. 1989);

degradation  $k = 0.0141 \text{ d}^{-1}$  at depth 0–20 cm with  $t_{1/2} = 49$  d,  $k = 0.0126 \text{ d}^{-1}$  at depth 20–40 cm with  $t_{1/2} = 55$  d, and  $k = 0.0089 \text{ d}^{-1}$  at depth 40–60 cm with  $t_{1/2} = 78$  d (Long Ashton soil, Walker et al. 1989);

degradation  $k = 0.0144 \text{ d}^{-1}$  at depth 0–20 cm with  $t_{1/2} = 48$  d,  $k = 0.0126 \text{ d}^{-1}$  at depth 20–40 cm with  $t_{1/2} = 55$  d, and  $k = 0.0124 \text{ d}^{-1}$  at depth 40–60 cm with  $t_{1/2} = 56$  d (Norfolk Agricultural Station soil, Walker et al. 1989)

degradation  $k = 0.0248 \text{ d}^{-1}$  at depth 0–20 cm with  $t_{1/2} = 28 \text{ d}$ ,  $k = 0.0289 \text{ d}^{-1}$  at depth 20–40 cm with  $t_{1/2} = 24 \text{ d}$ , and  $k = 0.0347 \text{ d}^{-1}$  at depth 40–60 cm with  $t_{1/2} = 20 \text{ d}$  (Norfolk Agricultural Station soil, Walker et al. 1989); selected field  $t_{1/2} = 40 \text{ d}$  (Hornsby et al. 1996).

## 17.1.1.19 Chlorotoluron



Common Name: Chlorotoluron

Synonym: C 2242, Clortokem, Deltarol, Dicuran, Highuron, Higaluron, Tolurex

Chemical Name: 3-(3-chloro-*p*-tolyl)-1,1-dimethylurea; *N'*-(3-chloro-4-methylphenyl)-*N,N*-dimethylurea

Uses: herbicide to control pre- and post-emergent annual grasses and broadleaf weeds in winter cereals, particularly wheat and barley.

CAS Registry No: 15545-48-9

Molecular Formula: C<sub>10</sub>H<sub>13</sub>ClN<sub>2</sub>O

Molecular Weight: 212.675

Melting Point (°C):

147 (Lide 2003)

Boiling Point (°C):

Density (g/cm<sup>3</sup> at 20°C):

1.40 (Tomlin 1994)

Molar Volume (cm<sup>3</sup>/mol):

192 (modified Le Bas method at normal boiling point, Spurlock & Biggar 1994)

Dissociation Constant pK<sub>a</sub>:

Enthalpy of Fusion, ΔH<sub>fus</sub> (kJ/mol):

Entropy of Fusion, ΔS<sub>fus</sub> (J/mol K):

Fugacity Ratio at 25°C (assuming ΔS<sub>fus</sub> = 56 J/mol K), F: 0.0635 (mp at 147°C)

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

10.0 (20°C, Spencer 1973)

70.0 (Martin & Worthing 1977)

10.0 (20°C, Khan 1980)

70.0 (20°C, Ashton & Crafts 1981)

56.4, 80.6, 99.1 (4, 25, 40°C, shake flask-liquid scintillation spectrometer LSS, Madhun et al. 1986)

70.0 (20°C, Hartley & Kidd 1987; Worthing & Walker 1991)

90.0 (Spurlock 1992; Spurlock & Biggar 1994)

10660 (calculated, Patil 1994)

74.0 (Tomlin 1994)

49.3 (predicted-AQUAFAC, Lee et al. 1996)

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

4.8 × 10<sup>-6</sup> (20°C, Khan 1980)

1.7 × 10<sup>-5</sup> (20°C, Ashton & Crafts 1981)

1.7 × 10<sup>-5</sup> (20°C, Hartley & Kidd 1987)

1.7 × 10<sup>-5</sup> (Tomlin 1994; selected, Halfon et al. 1996)

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

5.17 × 10<sup>-5</sup> (20°C, calculated-P/C, this work)

Octanol/Water Partition Coefficient, log K<sub>ow</sub>:

2.41 (shake flask-UV, Briggs 1981)

2.54 (Dao et al. 1983; Spurlock 1992; Spurlock & Biggar 1994)

2.33, 2.34, 2.32 (4, 25, 40°C, shake flask-liquid scintillation spectrometer LSS, Madhun et al. 1986)

2.41 (shake flask, Mitsutake et al. 1986)

2.0 (shake flask, pH 7, Baker et al. 1992)

- 2.241 (calculated, Evelyne et al. 1992)
- 2.41 (recommended, Sangster 1993)
- 2.25 (RP-HPLC-RT correlation, Sicbaldi & Finizio 1993)
- 0.26 (calculated, Patil 1994)
- 2.50 (Tomlin 1994)
- 2.41 (recommended, Hansch et al. 1995)
- 2.38, 2.44 (shake flask-UV, calculated-RP-HPLC-k' correlation, Liu & Qian 1995)
- 2.25, 2.49, 2.42 (RP-HPLC-RT correlation, CIOGP, calculated-S, Finizio et al. 1997)
- 2.0 (RP-HPLC-RT correlation using short ODP column, Donovan & Pescatore 2002)

#### Bioconcentration Factor, log BCF:

- 1.75 (calculated-S, Kenaga 1980)
- 2.09, 2.16 (cuticle/water 24 h: tomato, pepper, Chaumat et al. 1991)
- 2.01, 2.15 (cuticle/water 24 h: box tree, pear, Chaumat et al. 1991)
- 1.30 (cuticle/water 24 h: vanilla, Chaumat et al. 1991)
- 2.09, 2.16 (cuticle/water: tomato, pepper, Evelyne et al. 1992)

#### Sorption Partition Coefficient, log K<sub>OC</sub>:

- 2.62 (soil, calculated-S, Kenaga 1980)
- 1.78 (reported as log K<sub>OM</sub>, Briggs 1981)
- 2.75, 2.62 (4°C, 25°C, Semiahmoo soil, in µmol/kg OC, batch equilibrium-sorption isotherm-liquid scintillation spectrometer LSS, Madhun et al. 1986)
- 2.57, 2.43 (4°C, 25°C, Adkins soil, in µmol/kg OC, batch equilibrium method-LSS, Madhun et al. 1986)
- 2.48, 2.18; 2.54, 2.50 (estimated-K<sub>OW</sub>; solubility, Madhun et al. 1986)
- 2.81, 2.58 (exptl., calculated-K<sub>OW</sub>, Liu & Qian 1995)
- 2.02 (soil, calculated-MCI <sup>1</sup>χ, Sabljic et al. 1995)
- 2.02; 2.05, 2.15 (soil, quoted obs.; estimated-class-specific model, estimated-general model using molecular descriptors, Gramatica et al. 2000)
- 2.00, 2.00 (soils: organic carbon OC ≥ 0.1%, OC ≥ 0.5%, average, Delle Site 2001)
- 2.14, 2.36 (Kishon river sediments, sorption isotherm, Chefetz et al. 2004)

#### Environmental Fate Rate Constants, k, or Half-Lives, t<sub>1/2</sub>:

Volatilization:

Photolysis:

Oxidation:

Hydrolysis: calculated t<sub>1/2</sub> > 200 d at pH 5, 7, 9 and 30°C (Tomlin 1994).

Biodegradation: Biological degradation rate followed a first order kinetics with t<sub>1/2</sub> = 21.6 d by raw water microflora from River Nile, t<sub>1/2</sub> = 13.8 d by raw water microflora + sewage (El-Dib & Abou-Waly 1998)

Biotransformation: 4% of the selected 90 strains of micromycetes mostly isolated from soil-soil fungi, depleted 50% of chlorotoluron (100 mg/L) in 5-d experiment. (Vroumsia et al. 1996)

Bioconcentration, Uptake (k<sub>1</sub>) and Elimination (k<sub>2</sub>) Rate Constants:

#### Half-Lives in the Environment:

Air:

Surface water: Biological degradation t<sub>1/2</sub> = 21.6 d by raw water microflora from River Nile, t<sub>1/2</sub> = 13.8 d by raw water microflora + sewage (El-Dib & Abou-Waly 1998)

Ground water:

Sediment:

Soil: t<sub>1/2</sub> = 4 wk in the moist silty loam at (25 ± 1)°C (Smith & Briggs 1978);

t<sub>1/2</sub> ~ 200–4000 d in loamy sand and peat for 25–35°C as follows (Madhum & Freed 1987):

t<sub>1/2</sub> = 4340, 904, and 381 d at 25, 30, and 35°C, respectively, at herbicide concn at 5 µg/kg, while t<sub>1/2</sub> = 1335, 524, and 266 d at 25, 30, and 35°C, respectively, at herbicide concn at 100 µg/kg in an Adkins loamy sand; however, the half-lives in peat. t<sub>1/2</sub> = 2306, 1245, and 618 d at 25, 30, and 35°C, respectively, at herbicide concn at 5 µg/kg while t<sub>1/2</sub> = 1949, 1024, and 582 d at 25, 30, and 35°C, respectively, at herbicide concn at 100 µg/kg in a Semiahmoo mucky peat (Madhum & Freed 1987)

degradation by microorganism in biometer systems,  $t_{1/2} = 93$  d in silty sand standard metabolism experiments,  $t_{1/2} = 140$  d corrected standard conditions,  $t_{1/2} = 110$  d in simulated outdoor conditions;  $t_{1/2} = 40$  d in silty loam standard conditions,  $t_{1/2} = 60$  d corrected standard conditions,  $t_{1/2} = 31$  d in simulated outdoor conditions; at constant soil moisture and 20°C. Degradation by microorganism in small lysimeter systems:  $t_{1/2} = 52$  d outdoor fallow,  $t_{1/2} = 14$  d outdoor barley in silty sand, and  $t_{1/2} = 49$  d outdoor fallow,  $t_{1/2} = 38$  d outdoor barley in silty loam (Rüdel et al. 1993)

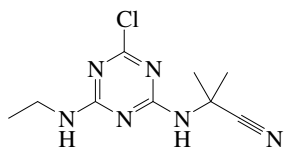
$t_{1/2} = 30\text{--}40$  d in soil (Tomlin 1994);

$t_{1/2} = 135$  d (selected, Halfon et al. 1996).

Biota:



## 17.1.1.20 Cyanazine



Common Name: Cyanazine

Synonym: Bladex, 90DF, DW 3418, Fortrok, Fortrol, Payze, SD 15418, WL 19805

Chemical Name: 2-(4-chloro-6-ethylamino-1,3,5-triazin-2-ylamino)-2-methyl-propionitrile

Uses: herbicide to control annual grasses and broadleaf weeds in cereals, cotton, maize, onions, peanuts, peas, potatoes, soybeans, sugar cane, and wheat fallow.

CAS Registry No: 21725-46-2

Molecular Formula:  $C_9H_{13}ClN_6$

Molecular Weight: 240.692

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

168 (Lide 2003)

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

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

Molar Volume ( $cm^3/mol$ ):

Dissociation Constant:

1.00 ( $pK_a$ , Weber et al. 1980; Willis & McDowell 1982)

12.9 ( $pK_b$ , Wauchope et al. 1992; Hornsby et al. 1996)

0.63, 1.1 ( $pK_a$ , Montgomery 1993)

Enthalpy of Fusion,  $\Delta H_{fus}$  (kJ/mol):

Entropy of Fusion,  $\Delta S_{fus}$  (J/mol K):

Fugacity Ratio at  $25^{\circ}C$  (assuming  $\Delta S_{fus} = 56$  J/mol K), F: 0.0395 (mp at  $168^{\circ}C$ )

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

171 (Melnikov 1971; Wauchope 1978; Weber et al. 1980; Ashton & Crafts 1981)

171 (Martin & Worthing 1977; Herbicide Handbook 1978; Worthing & Walker 1987, Worthing & Hance 1991; Majewski & Capel 1995)

150 (selected, Schnoor & McAvoy 1981; Schnoor 1992)

171 (Hartley & Kidd 1987; Montgomery 1993; Tomlin 1994)

160 ( $23^{\circ}C$ , Herbicide Handbook 1989)

171 (Budavari 1989; Milne 1995)

170 ( $20$ – $25^{\circ}C$ , selected, Wauchope et al. 1992; Hornsby et al. 1996)

6046 (calculated, Patil 1994)

45 (calculated-group contribution fragmentation method, Kühne et al. 1995)

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

$2.13 \times 10^{-7}$  ( $20^{\circ}C$ , Ashton & Crafts 1973; 1981; Spencer 1982; Herbicide Handbook 1989)

$2.67 \times 10^{-7}$  ( $20$ – $25^{\circ}C$ , Weber et al. 1980)

$5.33 \times 10^{-7}$  (selected, Schnoor & McAvoy 1981; Schnoor 1992)

$1.00 \times 10^{-5}$  ( $20^{\circ}C$ , extrapolated from gas saturation measurement, Grayson & Fosbracey 1982)

$\ln(P/Pa) = 25.7 - 10913/(T/K)$ , temp range  $65.7$ – $92^{\circ}C$ , (Antoine eq., gas saturation, Grayson & Fosbracey 1982)

$2.00 \times 10^{-7}$  ( $20^{\circ}C$ , Hartley & Kidd 1987; Worthing & Hance 1991; Tomlin 1994; Majewski & Capel 1995)

$5.21 \times 10^{-6}$  (Worthing & Walker 1987)

$1.33 \times 10^{-6}$  ( $30^{\circ}C$ , Herbicide Handbook 1989)

$2.13 \times 10^{-7}$  ( $20^{\circ}C$ , Budavari 1989)

$2.13 \times 10^{-7}$  ( $20$ – $25^{\circ}C$ , selected, Wauchope et al. 1992; Hornsby et al. 1996)

$2.13 \times 10^{-7}$  ( $20^{\circ}C$ , Montgomery 1993)

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

- 2816 (20– $25^\circ\text{C}$ , calculated-P/C, Montgomery 1993)
- $2.87 \times 10^{-7}$  (calculated-P/C as per Worthing & Walker 1987, Majewski & Capel 1995)
- $3.00 \times 10^{-7}$  (calculated-P/C, this work)

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

- 2.18 (Kenaga & Goring 1980)
- 2.24 (shake flask-GC, Brown & Flagg 1981)
- 1.80, 1.66 (RP-HPLC-RT correlation, calculated, Finizio et al. 1991)
- 2.22 (selected, Magee 1991)
- 1.80, 2.24 (Montgomery 1993)
- 2.22 (recommended, Sangster 1993)
- 0.79 (calculated, Patil 1994)
- 2.10 (Tomlin 1994)
- 2.22 (recommended, Hansch et al. 1995)
- 2.04 (shake flask-UV, Liu & Qian 1995)
- 1.64, 1.29, 3.02 (RP-HPLC-RT correlation, CLOGP, calculated-S, Finizio et al. 1997)
- 1.70 (RP-HPLC-RT correlation using short ODP column, Donovan & Pescatore 2002)

Bioconcentration Factor,  $\log \text{BCF}$ :

- 1.53 (calculated-S, Kenaga 1980)
- 1.00 (calculated- $K_{\text{OC}}$ , Kenaga 1980)
- 1.48 (selected, Schnoor & McAvoy 1981; Schnoor 1992)

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

- 2.30 (Kenaga 1980; Kenaga & Goring 1980; Karickhoff 1981; Sabljic 1987; Bahnick & Doucette 1988)
- 2.41 (soil, calculated-S as per Kenaga & Goring 1980, Kenaga 1980)
- 2.26 (Georgia's Hickory Hill pond sediment, Brown & Flagg 1981)
- 2.71, 1.75, 1.85 (estimated-S, calculated-S and mp, calculated- $K_{\text{OW}}$ , Karickhoff 1981)
- 0.48–1.48 (selected, sediment/water, Schnoor & McAvoy 1981; Schnoor 1992)
- 2.57, 2.26 (soil, quoted, Madhun et al. 1986)
- 2.36, 2.09; 2.33, 1.75 (estimated-reported  $K_{\text{OW}}$ s; estimated-reported solubilities, Madhun et al. 1986)
- 2.23 (soil, screening model calculations, Jury et al. 1987b)
- 2.35 (calculated-MCI  $\chi$ , Bahnick & Doucette 1988)
- 2.30, 2.16 (reported, estimated as  $\log K_{\text{OM}}$ , Magee 1991)
- 2.23, 2.26, 2.30 (soil, quoted values, Bottoni & Funari 1992)
- 2.28 (soil, 20– $25^\circ\text{C}$ , selected, Wauchope et al. 1992; quoted, Richards & Baker 1993; Hornsby et al. 1996)
- 1.58–2.63 (Montgomery 1993)
- 2.54 (selected, Lohninger 1994)
- 2.05, 2.11 (exptl., calculated- $K_{\text{OW}}$ , Liu & Qian 1995)
- 2.28 (soil, calculated-MCI  $^1\chi$ , Sabljic et al. 1995)
- 2.28; 2.33, 2.25 (soil, quoted obs.; estimated-class-specific model, estimated-general model using molecular descriptors, Gramatica et al. 2000)
- 2.14, 2.19 (soils: organic carbon  $\text{OC} \geq 0.1\%$ ,  $\text{OC} \geq 0.5\%$ , pH 5.6–8.0, average, Delle Site 2001)

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

Volatilization:

Photolysis:

Oxidation:

Hydrolysis: alkaline chemical hydrolysis  $t_{1/2} > 365$  d (Schnoor & McAvoy 1981; quoted, Schnoor 1992).

Biodegradation: aerobic  $t_{1/2} = 14$  d for  $0.06 \mu\text{g/mL}$  to degrade in pond water and  $t_{1/2} > 28$  d in pond sediment both at 10– $20^\circ\text{C}$  (Roberts 1974; quoted, Muir 1991).

Biotransformation:

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

## Half-Lives in the Environment:

## Air:

Surface water: aerobic  $t_{1/2} = 14$  d for 0.06  $\mu\text{g/mL}$  to degrade in pond water at 10–20°C (Roberts 1974; quoted, Muir 1991).

Ground water: reported half-lives or persistence,  $t_{1/2} = 10$ –29, 14 and 108 d (Bottoni & Funari 1992)

Sediment: aerobic  $t_{1/2} > 28$  d for 0.06  $\mu\text{g/mL}$  to slowly degrade in pond sediment at 10–20°C (Roberts 1974; quoted, Muir 1991).

Soil:  $t_{1/2} \sim 2$  wk in soil (Beynon et al. 1972; quoted, Tomlin 1994);

persistence of 12 months in soil (Wauchope 1978);

$t_{1/2} = 13.5$  d from screening model calculations (Jury et al. 1987b);

$t_{1/2} = 12$ –15 d in sandy loam soils and  $t_{1/2} = 20$ –25 d in silt and clay loam soils (Herbicide Handbook 1989; quoted, Montgomery 1993);

disappearance  $t_{1/2} = 181$  d from the upper 15 cm on a clay loam Ontario soil in 1987 and  $t_{1/2} = 90$  d in 1988 with  $t_{1/2}(\text{calc}) = 27$  and 12 d, respectively (Frank et al. 1991);

reported  $t_{1/2} = 10$ –29 d, 13 d and 108 d (Bottoni & Funari 1992);

selected field  $t_{1/2} = 14$  d (Wauchope et al. 1992; quoted, Richards & Baker 1993; Hornsby et al. 1996)

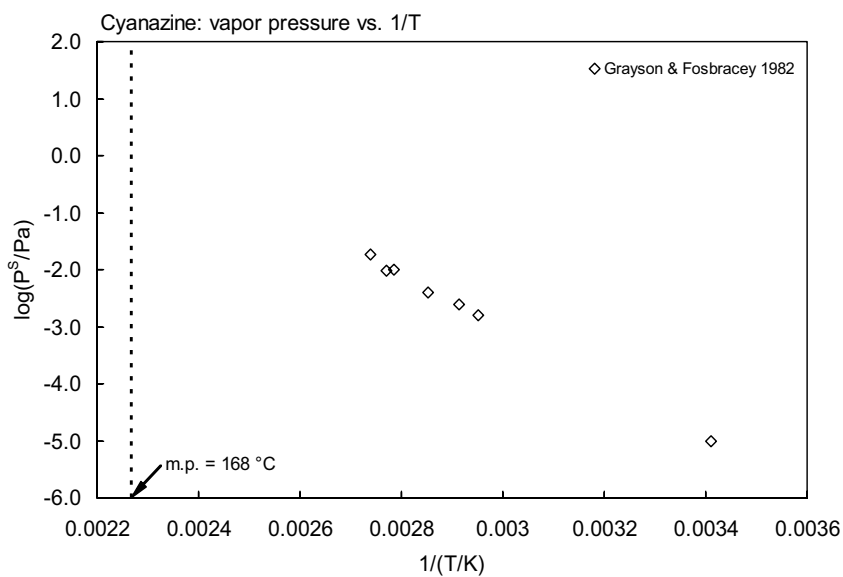
soil  $t_{1/2} = 19$  d (Pait et al. 1992).

Biota: biochemical  $t_{1/2} = 13.5$  d from screening model calculations (Jury et al. 1987b).

**TABLE 17.1.1.20.1**  
**Reported vapor pressures of cyanazine at various temperatures**

Grayson & Fosbracey 1982

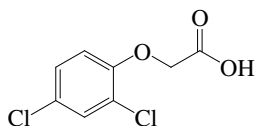
gas saturation-GC	
$t/^{\circ}\text{C}$	P/Pa
65.7	0.0016
70.0	0.0025
77.5	0.0040
85.8	0.0101
87.8	0.0096
92.0	0.0181
20	$1. \times 10^{-5}$
$\ln P = A - B/(T/K)$	
	P/Pa
A	25.7
B	10913



**FIGURE 17.1.1.20.1** Logarithm of vapor pressure versus reciprocal temperature for cyanazine.

## 17.1.1.21 2,4-D

(See also [Chapter 13](#), Carboxylic Acids)



Common Name: 2,4-D

Synonym: 2,4-Dichlorophenoxyacetic acid

Chemical Name: 2,4-dichlorophenoxyacetic acid

Uses: post-emergence control of annual and perennial broadleaf weeds in cereals, maize, sorghum, grassland, established turf, grass seed crops, orchards, cranberries, asparagus, sugar cane, rice, forestry, and on noncropland, etc.

CAS Registry No: 94-75-7

Molecular Formula:  $C_8H_6Cl_2O_3$ ,  $Cl_2C_6H_3OCH_2COOH$

Molecular Weight: 221.038

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

140.5 (Hartley & Kidd 1987; Howard 1991; Tomlin 1994; Lide 2003)

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

160 (at 0.4 mmHg, Dean 1985)

215 (Neely & Blau 1985)

Density ( $g/cm^3$  at  $25^{\circ}C$ ):

1.565 ( $30^{\circ}C$ , Neely & Blau 1985; Tomlin 1994)

1.416 (Montgomery 1993)

Molar Volume ( $cm^3/mol$ ):

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

Dissociation Constant,  $pK_a$ :

2.73 (potentiometric method, Nelson & Faust 1969)

2.87 (spectrophotometric method, Cessna & Grover 1978)

2.80 (Reinert & Rogers 1984; selected, Wauchope et al. 1992)

2.64 (Dean 1985; Haag & Yao 1992; Lee et al. 1993)

2.61–3.31 (Howard 1991)

2.97 (Sangster 1993)

3.10 (Kollig 1993)

2.64–3.31 (Montgomery 1993)

Enthalpy of Vaporization,  $\Delta H_v$  (kJ/mol):

93.89 (Rordorf 1989)

Enthalpy of Fusion  $\Delta H_{fus}$  (kJ/mol):

38.074 (DSC method, Plato & Glasgow 1969)

39.6 (Rordorf 1989)

Entropy of Fusion,  $\Delta S_{fus}$  (J/mol K):

Fugacity Ratio at  $25^{\circ}C$  (assuming  $\Delta S_{fus} = 56$  J/mol K), F: 0.0736 (mp at  $140.5^{\circ}C$ )

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

890 (Hodgman 1952; Hamaker 1975; Verschueren 1983; Montgomery 1993)

522 (shake flask-UV, Leopold et al. 1960)

725 (Bailey & White et al. 1965)

725, 400, 900, 550 (Gunther et al. 1968)

900 (Herbicide Handbook 1974; Wauchope 1978; Kenaga 1980a,b; Kenaga & Goring 1980)

600 ( $20^{\circ}C$ , Khan 1980)

620–900 (Weber et al. 1980)

470 ( $20$ – $25^{\circ}C$ , pH 5.6, Geyer et al. 1981)

633, 812 (15,  $25^{\circ}C$ , shake flask method, average values of 5 laboratories, OECD 1981)

620 ( $20^{\circ}C$ , Hartley & Kidd 1983, 1987)

620	(Worthing & Walker 1983)
609	(Gerstl & Helling 1987)
400	(20°C, selected, Suntio et al. 1988)
703	(Gustafson 1989)
682	(Yalkowsky et al. 1987)
540–890	(Nyholm et al. 1992)
900, 600, 890, 703, 1072	(Wauchope et al. 1992)
890	(20–25°C, selected, Wauchope et al. 1992)
311	(pH 1, Tomlin 1994)

Vapor Pressure (Pa at 25°C or as indicated and reported temperature dependence equations):

$8.0 \times 10^{-5}$	(Hamaker 1975)
0.180–1.69	(transpiration method, Spencer 1976)
53.0	(160°C, Hartley & Kidd 1983, 1987)
$8.0 \times 10^{-5}$	(recommended, Neely & Blau 1985; Lyman 1985)
1.0	(20°C, selected, Suntio et al. 1988)
$6.0 \times 10^{-6}$	(selected, Nash 1989)
$4.10 \times 10^{-5}$ , $2.0 \times 10^{-3}$ , 0.058, 1.10, 13.0	(25, 50, 70, 100, 125°C, gas saturation-GC, Rordorf 1989)
$\log (P_s/\text{Pa}) = 17.56 - 6544.1/(T/K)$	; measured range 70.2–135°C (solid, gas saturation-GC, Rordorf 1989)
$\log (P_L/\text{Pa}) = 13.558 - 4904.6/(T/K)$	; measured range 140–196°C (liquid, gas saturation-GC, Rordorf 1989)
0.20, 0.0032	(quoted, estimated from Henry's law constant, Howard 1991)
$5.6 \times 10^{-5}$	(selected, Mackay & Stiver 1991)
1.40, $3.2 \times 10^{-3}$	(quoted, estimated from HLC, Howard 1991)
$1.33 \times 10^{-5}$ , $8.0 \times 10^{-5}$ , $1.07 \times 10^{-3}$ ; $1.07 \times 10^{-3}$	(20–25°C, quoted lit; selected, Wauchope et al. 1992)
0.627	(Montgomery 1993)
0.011	(Tomlin 1994)

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

$1.36 \times 10^{-5}$	(calculated-P/C, Jury et al. 1983)
$1.39 \times 10^{-5}$	(calculated-P/C, Jury et al. 1987a, Jury & Ghodrati 1989)
0.55	(20°C, calculated-P/C, Suntio et al. 1988)
0.0015	(calculated, Nash 1989)
$1.03 \times 10^{-3}$	(calculated-bond contribution, Howard 1991)
6.80, 0.853	(pH 1, pH 7 at 20°C, wetted wall column-GC, Rice et al. 1997b)
$1.82 \times 10^{-7}$	(quoted lit., Armbrust 2000)

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

2.81	(shake flask-UV, Fujita et al. 1964)
2.59	(electrometric titration, Freese et al. 1979)
1.57	(Kenaga & Goring 1980; Kenaga 1980b)
2.74	(selected, Dao et al. 1983)
2.81	(20°C, Verschueren 1983)
1.57, 4.88	(shake flask-OECD 1981 Guidelines, Geyer et al. 1984)
2.65	(shake flask, log P Database, Hansch & Leo 1987)
2.50	(OECD 1981 method, Kerler & Schönherr 1988)
2.649	(liquid/liquid-countercurrent-chromatography, Ilchmann et al. 1993)
2.81	(recommended, Sangster 1993)
1.44–4.18	(quoted lit. range, Montgomery 1993)
2.58–2.83	(pH 1, Tomlin 1994)
2.81	(selected, Hansch et al. 1995)
0.59	(RP-HPLC-RT correlation, CLOGP, Calculated-S, Finizio et al. 1997)

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

Bioconcentration Factor,  $\log BCF$ :

- 1.11, -0.097 (calculated-S,  $K_{OW}$ , Kenaga 1980a)
- 2.46, 1.30 (beef fat, fish, Kenaga 1980b)
- 0.778, 1.94 (alga *Chlorella*: exptl. 24 h exposure, calculated-S, Geyer et al. 1981)
- 0.778 (algae, Freitag et al. 1982)
- < 1.00 (golden orfe, Freitag et al. 1982)
- 1.23 (activated sludge, Freitag et al. 1982)
- 0.0 (fish, microcosm conditions, Garten & Trabalka 1983;)
- 0.778, 1.23 (algae, calculated- $K_{OW}$ , Geyer et al. 1984)
- 1.23 (algae, Geyer et al. 1984)
- 1.11 (calculated, Isensee 1991)
- 5.00 (bluegill sunfish and channel catfish, Howard 1991)
- 2.70 (frog tadpoles, Howard 1991)
- 3.0, -2.52 (pH 7.8, seaweeds, Howard 1991)
- 0.778, 0.85 (quoted: alga, fish, Howard 1991)
- 0.0, 0.505 (catfish *Ictalurus melas*, water flea *Daphnia magna*, wet wt basis, Wang et al. 1996)

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

- 1.51 (Hamaker 1975)
- 1.30, 2.0 (quoted, calculated, Kenaga 1980a)
- 1.30, 2.11 (quoted, Kenaga & Goring 1980)
- 1.30 (quoted, Kenaga 1980b)
- 1.76 (quoted, average value of 3 soils, McCall et al. 1980)
- 2.25, 2.04, 2.35 (soil I-very strongly acid sandy soil pH 4.5–5.5, soil II-moderately or slightly acid loamy soil pH 5.6–6.5, soil III-slightly alkaline loamy soil pH 7.1–8.0, OECD 1981)
- 1.29 (soil, Neely & Blau 1985)
- 1.30 (soil, screening model calculations, Jury et al. 1987a,b; Jury & Ghodrati 1989)
- 1.61 (soil, quoted, Sabljic 1987)
- 1.75, 2.00 (quoted, calculated-MCI  $\chi$ , Gerstl & Helling 1987)
- 2.59 (HPLC- $k'$  correlation, cyanopropyl column, mobile phase buffered to pH 3, Hodson & Williams 1988)
- 1.00, 1.23, 2.29 (sediment, Alfisol soil, Podzol soil, von Oepen et al. 1991)
- 1.30–1.78, 1.30–2.0, 1.72 (soil, quoted lit. values, Bottoni & Funari 1992)
- 1.30, 1.78, 1.51, 1.26, 1.72, 1.75, 1.76 (soil, quoted values, Wauchope et al. 1992)
- 1.30 (soil, selected, Wauchope et al. 1992)
- 0.68 (calculated- $K_{OW}$ , Kollig 1993)
- 1.68–2.73 (Montgomery 1993)
- 1.66 (calculated-QSAR MCI  $\chi$ , Sabljic et al. 1995)
- 2.09, 1.04, 1.40, 0.778 (first generation Eurosoils ES-1, ES-2, ES-3, ES-4, shake flask/batch equilibrium-HPLC/UV, Gawlik et al. 1998, 1999)
- 1.65, 1.36, 1.37, 0.899 (second generation Eurosoils ES-1, ES-2, ES-3, ES-4, shake flask/batch equilibrium-HPLC/UV, Gawlik et al. 1999)
- 1.652 (second generation Eurosoil ES-1, HPLC- $k'$  correlation, Gawlik et al. 2000)
- 1.68 (soil, quoted, Armbrust 2000)
- 1.79, 1.77 (soils: organic carbon OC  $\geq$  0.1%, OC  $\geq$  0.5%, pH 2.8–8.0, average, Delle Site 2001)
- 2.16, 2.13 (soils: organic carbon OC  $\geq$  0.1%, OC  $\geq$  0.5%, pH 2.8–5.0, average, Delle Site 2001)
- 1.68, 1.68 (soils: organic carbon OC  $\geq$  0.1%, OC  $\geq$  0.5%, pH > 5.0, average, Delle Site 2001)

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

- Volatilization: volatilization from water is negligible, calculated volatilization  $t_{1/2} = 660$  d (from 1 cm) and  $t_{1/2} = 7.1$  yr (from 10 cm) from soil (Howard 1991).

Photolysis: aqueous photolysis  $t_{1/2} = 2\text{--}4$  d when irradiated at 356 nm,  $t_{1/2} = 50$  min in water when irradiated at 254 nm and  $t_{1/2} = 29\text{--}43$  d when exposed to September sunlight (Howard 1991); aqueous photolysis rate constant,  $k = 2.2 \times 10^{-3} \text{ h}^{-1}$  (Armbrust 2000).

**Oxidation:**

photooxidation  $t_{1/2} = 1.8\text{--}18$  h, based on estimated rate constant for the vapor-phase reaction with hydroxyl radical in air (Howard et al. 1991)

$k(\text{aq.}) = (1.0\text{--}2.3) \text{ M}^{-1} \text{ s}^{-1}$  for direct reaction with ozone in water at pH 1.5–2.9 and  $21 \pm 1^\circ\text{C}$ , with  $t_{1/2} = 3.9$  h at pH 7 (Yao & Haag 1991).

$k(\text{calc}) = 5.0 \times 10^9 \text{ M}^{-1} \text{ s}^{-1}$  (Haag & Yao 1992)

$k_{\text{OH}}(\text{aq.}) = 1.6 \times 10^9 \text{ M}^{-1} \text{ s}^{-1}$  for reaction with hydroxyl radical in irradiated field water both in the laboratory and sunlit rice paddies (Mabury & Crosby 1996; quoted, Armbrust 2000);

$k_{\text{OH}}(\text{aq.}) = 8.4 \times 10^{12} \text{ M}^{-1} \text{ h}^{-1}$  at pH 5, 7, 9; measured hydroxyl radical rate constant for 2,4-D, (Armbrust 2000)

Hydrolysis: no hydrolyzable groups and rate constant at neutral pH is zero (Kollig et al. 1987; selected, Howard et al. 1991); generally resistant to hydrolysis, may become important at pH > 8 (Howard 1991).

**Biodegradation:**

$k = 0.7\text{--}14.0 \text{ d}^{-1}$  and  $t_{1/2} = 10$  to > 50 d in clear to murky river water with lag time ranges from 6–12 d (Nesbitt & Watson 1980a);

$t_{1/2} = 4$  d in river with nutrient and suspended sediments and  $t_{1/2} = 10$  d with a lag time of 5 d for filtered river water (Nesbitt & Watson 1980b);

degradation kinetics not first-order, time for 50% decomposition in six soils: Commerce 5 d, Catlin 1.5 d, Keith 3.9 d, Cecil 3.0 d, Walla-Walla 2.5 d and Fargo 8.5 d, with an average time of 4 d (McCall et al. 1981)

aerobic degradation  $k = 0.3 \times 10^{-3} \text{ h}^{-1}$  with  $t_{1/2} = 97.0$  d for control system,  $k = 9.5 \times 10^{-3} \text{ h}^{-1}$  with  $t_{1/2} = 3.1$  d for metabolism,  $k = 16.2 \times 10^{-3} \text{ h}^{-1}$  with  $t_{1/2} = 1.8$  d for co-metabolism; anaerobic degradation  $k = 0.24 \times 10^{-3} \text{ h}^{-1}$  with  $t_{1/2} = 120$  d for control system,  $k = 0.21 \times 10^{-3} \text{ h}^{-1}$  with  $t_{1/2} = 135$  d for metabolism,  $k = 0.42 \times 10^{-3} \text{ h}^{-1}$  with  $t_{1/2} = 69$  d for co-metabolism, by a mixture of microorganisms from activated sludge, soil and sediment in cyclone fermentors (Liu et al. 1981)

$k = (3.6\text{--}28.8) \times 10^{-6} \text{ mL cell}^{-1} \text{ d}^{-1}$  in natural water (Paris et al. 1981; quoted, Klečka 1985)

$k < 0.14\text{--}0.07 \text{ d}^{-1}$  in river water at  $25^\circ\text{C}$  (Nesbitt & Watson 1980; quoted, Klečka 1985)

$k = (0.058 \pm 0.006) \text{ d}^{-1}$  in lake water at  $29^\circ\text{C}$  (Subba-Rao et al. 1982; quoted, Klečka 1985)

$k = 0.08\text{--}0.46 \text{ d}^{-1}$  in soil at  $25^\circ\text{C}$  (McCall et al. 1981; quoted, Klečka 1985);

$t_{1/2}(\text{aq. aerobic}) = 240\text{--}1200$  h, based on unacclimated aerobic river die-away test data (Nesbitt & Watson 1980; selected, Howard et al. 1991);

$t_{1/2}(\text{anaerobic}) = 672\text{--}4320$  h, based on unacclimated aqueous screening test data (Liu et al. 1981; selected, Howard et al. 1991);

$k = 0.035 \text{ d}^{-1}$  in die-away test,  $k = 0.029 \text{ d}^{-1}$  in  $\text{CO}_2$  evolution test, in soil and  $k = 6.9 \times 10^{-1} \text{ mL (g bacteria)}^{-1} \text{ d}^{-1}$  by activated sludge cultures (Scow 1982);

$t_{1/2} = 18$  to over 50 d in clear river water, and  $t_{1/2} = 10$  to 25 d in muddy river water with lag times of 6 to 12 d; degradation with a mixture of microorganisms from activated sludge, soil, and sediments lead to half-lives of 1.8–3.1 d under aerobic conditions and 69–135 d under anaerobic conditions (Howard 1991)

$k(\text{aerobic}) = 5.25 \times 10^{-3} \text{ h}^{-1}$  (Armbrust 2000).

**Biotransformation:**

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

$k_1 = 0.0092 \text{ h}^{-1}$ ;  $k_2 = 0.0092 \text{ h}^{-1}$  (catfish *Ictalurus melas*, Wang et al. 1996)

$k_1 = 0.8560 \text{ h}^{-1}$ ;  $k_2 = 0.2690 \text{ h}^{-1}$  (Water flea *Daphnia magna*, Wang et al. 1996)

**Half-Lives in the Environment:**

Air:  $t_{1/2} = 1.8\text{--}18$  h, based on estimated rate constant for the reaction with OH radical (Howard et al. 1991); photooxidation  $t_{1/2} = 23.9$  h for reactions with OH radical in air (Howard 1991).

Surface water:  $t_{1/2} = 48\text{--}96$  h, based on reported photolysis half-lives for aqueous solution irradiated at UV wavelength of 356 nm (Baur & Bovey 1974; selected, Howard et al. 1991);

degradation  $t_{1/2} = 14$  d in sensitized, filtered and sterilized river water, based on sunlight photolysis test of  $1 \mu\text{g mL}^{-1}$  in distilled water (Zepp et al. 1975; quoted, Cessna & Muir 1991);

$t_{1/2} = 1.8$  and  $3.1$  d for cometabolism and metabolism, respectively, easily degraded under aerobic conditions;  $t_{1/2} = 69$  and  $135$  d under anaerobic conditions (Liu et al. 1981);



typical biodegradation  $t_{1/2} = 10$  to  $< 50$  d with longer expected in oligotrophic waters, photolysis  $t_{1/2} = 29$ –43 d for water solutions irradiated at sunlight (Howard 1991);

degraded relatively slowly when incubated in natural waters or in soil/sediment suspensions, with  $t_{1/2} \sim 6$  to 170 d (Muir 1991);

rate constant  $k(\text{exptl}) = (1.0$ – $2.3) \text{ M}^{-1} \text{ s}^{-1}$  for direct reaction with ozone in water at pH 1.5–2.9 and 21°C, with  $t_{1/2} = 3.9$  h at pH 7 (Yao & Haag 1991);

rate constant  $k(\text{calc}) = 5 \times 10^9 \text{ M}^{-1} \text{ s}^{-1}$  for the reaction with hydroxyl radical in aqueous solution (Haag & Yao 1992);

$t_{1/2} = 2$ –4 d when irradiated at  $\lambda = 356$  nm in aqueous solution (Montgomery 1993).

Ground water:  $t_{1/2} = 480$ –4320 h, based on estimated unacclimated aqueous aerobic and anaerobic biodegradation half-lives (Howard et al. 1991)

reported  $t_{1/2} = 4, 15, 1$ –35, 7–21 d (Bottoni & Funari 1992)

Sediment:  $t_{1/2} < 1$  d for degradation in sediments and lake muds (Howard 1991);

degraded relatively slowly when incubated in natural waters or in soil/sediment suspensions, with  $t_{1/2} = 6$  to 170 d (Muir 1991).

Soil: degradation  $t_{1/2} = 5.0$  and 4.0 d in Quachita Highlands' forest and grassland soil respectively,  $t_{1/2} = 4$  d in Gross Timbers Forest soil, average  $t_{1/2} = 4$  d in 3 soils (shake flask, Altom & Stritzke 1973);

field  $t_{1/2} = 5.2$  d in Arid range (Lane et al. 1977; quoted, Nash 1983);

field  $t_{1/2} = 19$  d in Dykland soil (Stewart & Gaul 1977; quoted, Nash 1983);

lab.  $t_{1/2} = 5.5$  d in Naff soil (Wilson & Cheng 1978; quoted, Nash 1983);

microagroecosystem  $t_{1/2} = 11$  d for granular application to bluegrass turf (Nash & Beall 1980)

non-persistent in soil with  $t_{1/2} < 20$  d (Willis & McDowell 1982);

microagroecosystem  $t_{1/2} = 3$  d in moist fallow soil (Nash 1983);

$t_{1/2} = 15$  d in soil (Jury et al. 1983, 1987a,b; Jury & Ghodrati 1989);

persistence of one month in soil (Jury et al. 1987);

$t_{1/2} = 240$ –1200 h, based on estimated unacclimated aqueous aerobic biodegradation half-life (Howard et al. 1991);

biodegradation  $t_{1/2} < 1$  d to several weeks,  $t_{1/2} = 3.9$  and 11.5 d in 2 moist soils and  $t_{1/2} = 9.4$  to 254 d in the same soils under dry conditions (Howard 1991);

degraded relatively slowly when incubated in natural waters or in soil/sediment suspensions, with  $t_{1/2} = 6$  to 170 d (Muir 1991);

reported  $t_{1/2} = 4, 15, 1$ –35 and 7–21 d (Bottoni & Funari 1992);

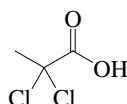
field  $t_{1/2} = 2$ –16 d, with a selected value of 10 d (Wauchope et al. 1992);

soil  $t_{1/2} = 18$  d (Pait et al. 1992);

rate constants for Amsterdam silt loam at soil depth 0–30 cm:  $k = 0.0053 \text{ d}^{-1}$  at 10°C,  $k = 0.0046 \text{ d}^{-1}$  at 17°C and  $k = 0.0127 \text{ d}^{-1}$  at 24°C with corresponding first-order  $t_{1/2} = 7, 7,$  and 2 d; at soil depth 30–60 cm:  $k = 0.00012 \text{ d}^{-1}$  at 10°C,  $k = 0.0044 \text{ d}^{-1}$  at 17°C and  $k = 0.0077 \text{ d}^{-1}$  at 24°C with corresponding first-order  $t_{1/2} = 273, 8,$  and 4 d; and at soil depth 60–120 cm:  $k = 0.00005 \text{ d}^{-1}$  at 10°C,  $k = 0.0013 \text{ d}^{-1}$  at 17°C and  $k = 0.0022 \text{ d}^{-1}$  at 24°C with corresponding first-order  $t_{1/2} = 593, 25,$  and 12 d (Veeh et al. 1996).

Biota: depuration  $t_{1/2} = 13.8$  h in daphnids,  $t_{1/2} = 1.32$  d in catfish (Ellgehausen et al. 1980).

## 17.1.1.22 Dalapon



Common Name: Dalapon

Synonym: Alatex, Basinex P, Crisapon, D-Granulat, Dawpon-Rae, Ded-Weed, Dowpon, DPA, Gramevin, Kenapon, Liropon, Proprop, Radapon

Chemical Name: 2,2-dichloropropanoic acid; 2,2-dichloropropionic acid;  $\alpha$ -dichloropropanoic acid;  $\alpha,\alpha$ -dichloropropionic acid

Uses: selective systemic herbicide to control perennial and annual grasses on noncropland, fruits, vegetables, and some aquatic weeds.

CAS Registry No: 75-99-0

Molecular Formula:  $C_3H_4Cl_2O_2$

Molecular Weight: 1432.969

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

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

185–190 (Herbicide Handbook 1989; Worthing & Hance 1991; Tomlin 1994)

98–99 (sodium salt at 20 mmHg, Budavari 1989)

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

1.389 (Nelson & Faust 1969; quoted, Kenaga 1974; Montgomery 1993)

1.389 ( $22.8^{\circ}C$ , Herbicide Handbook 1989)

1.4014 (Budavari 1989; Milne 1995)

Molar Volume ( $cm^3/mol$ ):

Dissociation Constant  $pK_a$ :

1.84 (potentiometric titration, Nelson & Faust 1969; Freed 1976; Hornsby et al. 1996)

1.74 (Kenaga 1974; quoted, Howard 1991)

1.74–1.84 (Worthing & Hance 1991; Tomlin 1994)

2.06 (Yao & Haag 1991; Haag & Yao 1992)

1.84 (free acid, Montgomery 1993)

Enthalpy of Fusion,  $\Delta H_{fus}$  ( $kJ/mol$ ):

Entropy of Fusion,  $\Delta S_{fus}$  ( $J/mol K$ ):

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

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

900000 (Woodford & Evans 1963; Bailey & White 1965)

> 800000 (Kenaga 1974)

502000 (Martin & Worthing 1977)

450000 (Weber et al. 1980; Budavari 1989)

501200 (Garten & Trabalka 1983)

431850 (selected, Gerstl & Helling 1987)

900000 (sodium salt, Worthing & Walker 1987, Worthing & Hance 1991)

500000 (Reinert 1989)

450000–900000 (Montgomery 1993)

900000 ( $20$ – $25^{\circ}C$ , selected, Hornsby et al. 1996)

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

16.0 (calculated from high temp., Foy 1976)

$1.0 \times 10^{-5}$  (Worthing & Hance 1991; Tomlin 1994)

0.0 ( $20$ – $25^{\circ}C$ , selected, Hornsby et al. 1996)

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

$6.50 \times 10^{-3}$  (Hine & Mookerjee 1975)

0.608 (calculated, Montgomery 1993)

$4.56 \times 10^{-3}$  (calculated-P/C as per Howard 1991, Majewski & Capel 1995)

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

0.76 (Kenaga 1974)  
 0.78 (Kenaga 1980)  
 1.34 (selected, Dao et al. 1983)  
 -2.76 (selected, Gerstl & Helling 1987)  
 1.48 (Reinert 1989)  
 0.78 (selected, Hansch et al. 1995)  
 1.47 (LOGSTAR or CLOGP data, Sabljic et al. 1995)

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

Bioconcentration Factor,  $\log BCF$ :

0.477 (dalapon sodium salt in fish, Kenaga 1974)  
 -0.444 (calculated-S, Kenaga 1980; quoted, Isensee 1991)  
 0.301 (estimated- $K_{OW}$ , Lyman et al. 1982; quoted, Howard 1991)

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

0.477 (soil, calculated-S as per Kenaga & Goring 1980, Kenaga 1980)  
 0.97 (calculated-MCI  $\chi$ , Gerstl & Helling 1987)  
 2.13 (Reinert 1989)  
 0.48, 2.13 (soil, quoted values, Bottoni & Funari 1992)  
 0.27–2.18 (calculated, Montgomery 1993)  
 0.40 (soil, calculated-MCI  $1\chi$ , Sabljic et al. 1995)  
 0.0 (soil, 20–25°C, selected, Hornsby et al. 1996)

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

Volatilization:

Photolysis:

Oxidation:

photooxidation  $t_{1/2} = 289\text{--}2893$  h in air, based on an estimated rate constant for the vapor-phase reaction with hydroxyl radical in air (Atkinson 1987; quoted, Howard et al. 1991);

$k(aq.) = 4.6 \times 10^8 \text{ M}^{-1} \text{ s}^{-1}$  for the reaction (photo-Fenton with reference to acetophenone) with hydroxyl radical in aqueous solutions at pH 3.4 and at  $24 \pm 1^\circ\text{C}$  (Buxton et al. 1988; quoted, Faust & Hoigné 1990; Haag & Yao 1992)

$k(aq.) \leq 0.005 \text{ M}^{-1} \text{ s}^{-1}$  for direct reaction with ozone in water at pH 6.4 and  $22^\circ\text{C}$ , with a half-life of  $> 2$  yr at pH 7 (Yao & Haag 1991).

$k(aq.) = (7.3 \pm 0.3) \times 10^7 \text{ M}^{-1} \text{ s}^{-1}$  for the reaction (photo-Fenton with reference to acetophenone) with hydroxyl radical in aqueous solutions at pH 3.4 and at  $24 \pm 1^\circ\text{C}$  (Haag & Yao 1992).

Hydrolysis:

Biodegradation: aqueous aerobic  $t_{1/2} = 336\text{--}1440$  h, based on unacclimated aerobic soil grab sample data (Corbin & Upchurch 1967; Kaufman & Doyle 1977; quoted, Howard et al. 1991);

rate constant  $k = 0.047 \text{ d}^{-1}$  by soil incubation die-away studies (Rao & Davidson 1980; quoted, Scow 1982);

aqueous anaerobic  $t_{1/2} = 1344\text{--}5760$  h, based on estimated aqueous aerobic biodegradation half-life (Howard et al. 1991).

Biotransformation:

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

Half-Lives in the Environment:

Air:  $t_{1/2} = 289\text{--}2893$  h, based on an estimated rate constant for the vapor-phase reaction with hydroxyl radical in air (Atkinson 1987; quoted, Howard et al. 1991).

Surface water:  $t_{1/2} = 336\text{--}1440$  h, based on estimated aqueous aerobic biodegradation half-life (Howard et al. 1991);

measured rate constant  $k \leq 0.0005 \text{ M}^{-1} \text{ s}^{-1}$  for direct reaction with ozone in water at pH 6.4 and 22°C, with a  $t_{1/2} \geq 2 \text{ yr}$  at pH 7 (Yao & Haag 1991).

Groundwater:  $t_{1/2} = 672\text{--}2880 \text{ h}$ , based on estimated aqueous aerobic biodegradation half-life (Howard et al. 1991).

reported  $t_{1/2} = 30 \text{ d}$  (Bottoni & Funari 1992)

Sediment:

Soil:  $t_{1/2} = 7\text{--}8 \text{ d}$  in soil (Kaufman 1966; quoted, Kaufman 1976);

persistence across 43 soils from  $< 2 \text{ wk}$  to  $> 8 \text{ wk}$  (Day et al. 1963; quoted, Kaufman 1976);

$t_{1/2} = 336\text{--}1440 \text{ h}$ , based on unacclimated aerobic soil grab sample data (Corbin & Upchurch 1967; Kaufman & Doyle 1977; quoted, Howard et al. 1991);

estimated persistence of 8 months (Kearney et al. 1969; quoted, Jury et al. 1987);

persistence of 8 wk in soil (Edwards 1973; quoted, Morrill et al. 1982);

persistence of about 2 wk in growing season in most agricultural soils (Herbicide Handbook 1974; quoted, Kaufman 1976);

estimated first-order  $t_{1/2} = 15 \text{ d}$  from biodegradation rate constant  $k = 0.047 \text{ d}^{-1}$  by soil incubation die-away studies (Rao & Davidson 1980; quoted, Scow 1982);

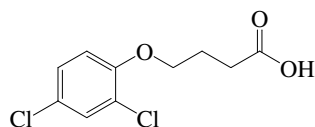
non-persistent in soil with  $t_{1/2} < 20 \text{ d}$  (Willis & McDowell 1982);

reported half-life or persistence, 30 d (Verschuren 1983; Bottoni & Funari 1992);

field  $t_{1/2} = 30 \text{ d}$  at 20–25°C (selected, Hornsby et al. 1996).

Biota:

## 17.1.1.23 2,4-DB



Common Name: 2,4-DB

Synonym: Butoxon, Butyrac, Butyrac 118, Embutox, Legumex D

Chemical Name: 4-(2,4-dichlorophenoxy)butanoic acid; 4-(2,4-dichlorophenoxy)butyric acid

Uses: herbicide for post-emergence control of many annual and perennial broadleaf weeds in lucerne, clovers, undersown cereals, grassland, forage legumes, soybeans, and groundnuts.

CAS Registry No: 94-82-6

Molecular Formula:  $C_{10}H_{10}Cl_2O_3$

Molecular Weight: 249.090

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

118 (Lide 2003)

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

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

Molar Volume ( $cm^3/mol$ ):

254.2 (calculate-Le Bas method at normal boiling point)

Dissociation Constant  $pK_a$ :

5.95 (Bailey & White 1965; Que Hee et al. 1981)

4.80 (Worthing & Walker 1987; Hornsby et al. 1996)

Enthalpy of Vaporization,  $\Delta H_v$  ( $kJ/mol$ ):

91.29 (Rordorf 1989)

Enthalpy of Fusion,  $\Delta H_{fus}$  ( $kJ/mol$ ):

33.6 (Rordorf 1989)

Entropy of Fusion,  $\Delta S_{fus}$  ( $J/mol K$ ):

Fugacity Ratio at  $25^{\circ}C$  (assuming  $\Delta S_{fus} = 56 J/mol K$ ), F: 0.122 (mp at  $118^{\circ}C$ )

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

82.3 (Bailey & White 1965)

53 (rm. temp., Melnikov 1971)

46 (Martin & Worthing 1977; Worthing & Walker 1987, Worthing & Hance 1991)

46 (Weber et al. 1980)

46 (Hartley & Kidd 1987; Budavari 1989; Milne 1995)

46 ( $20-25^{\circ}C$ , selected, Hornsby et al. 1996)

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

negligible (Hartley & Kidd 1987)

$1.0 \times 10^{-5}$ ,  $5.90 \times 10^{-4}$ , 0.019, 0.38, 5.20 ( $25, 50, 70, 100, 125^{\circ}C$ , gas saturation-GC, Rordorf 1989)

$\log (P_g/Pa) = 17.692 - 6760.5/(T/K)$ ; measured range  $80-120^{\circ}C$  (solid, gas saturation-GC, Rordorf 1989)

$\log (P_L/Pa) = 12.682 - 4768.7/(T/K)$ ; measured range  $125-196^{\circ}C$  (liquid, gas saturation-GC, Rordorf 1989)

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

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

3.53 (shake flask-HPLC/UV, Jafvert et al. 1990)

3.53 (selected, Hansch et al. 1995)

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

Bioconcentration Factor,  $\log BCF$ :

1.85 (calculated-S, Kenaga 1980)

2.21 (calculated- $\log K_{ow}$  as per Mackay 1982, this work)

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

- 2.72 (soil, calculated-S, Kenaga 1980)
- 1.3 (organic carbon, Wauchope et al. 1991)
- 2.64 (20–25°C, estimated, Hornsby et al. 1996)

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

Volatilization:

Photolysis:

Oxidation: photooxidation  $t_{1/2} = 6\text{--}60$  h in air, based on an estimated rate constant for the vapor-phase reaction with hydroxyl radicals in air (Atkinson 1987; quoted, Howard et al. 1991).

Hydrolysis: stable in distilled water for 40 d (Chau & Thomson 1978; quoted, Howard et al. 1991).

Biodegradation: aqueous aerobic  $t_{1/2} = 24\text{--}168$  h, based on unacclimated soil grab sample data (Smith 1978; quoted, Howard et al. 1991); aqueous anaerobic  $t_{1/2} = 96\text{--}672$  h, based on estimated unacclimated aqueous aerobic biodegradation half-life (Howard et al. 1991).

Biotransformation:

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

Half-Lives in the Environment:

Air:  $t_{1/2} = 6\text{--}60$  h, based on an estimated rate constant for the vapor-phase reaction with hydroxyl radicals in air (Atkinson 1987; Howard et al. 1991).

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

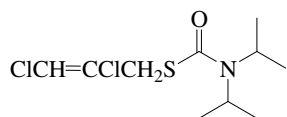
Groundwater:  $t_{1/2} = 48\text{--}336$  h, based on estimated unacclimated aqueous aerobic biodegradation half-life (Howard et al. 1991)  
reported  $t_{1/2} < 7$  d (Bottoni & Funari 1992)

Sediment:

Soil:  $t_{1/2} = 24\text{--}168$  h, based on unacclimated soil grab sample data (Smith 1978; quoted, Howard et al. 1991)  
selected  $t_{1/2} = 10$  d (Wauchope et al. 1991; quoted, Dowd et al. 1993);  
 $t_{1/2} < 7$  d (Worthing & Hance 1991; Bottoni & Funari 1992);  
field  $t_{1/2} = 5$  d (20–25°C, selected, Hornsby et al. 1996).

Biota:

## 17.1.1.24 Diallate



Common Name: Diallate

Synonym: Avadex, CP 15336, DATC, Pyradex

Chemical Name: *S*-(2,3-dichloroallyl)diisopropyl(thiocarbamate); *S*-(2,3-dichloro-2-propenyl)bis(1-methylethyl)-carbamothioate

Uses: pre-emergent and selective herbicide to control wild oats and blackgrass in barley, corn, flax, lentils, peas, potatoes, soybeans, and sugar beets.

CAS Registry No: 2303-16-4

Molecular Formula:  $C_{10}H_{17}Cl_2NOS$

Molecular Weight: 270.219

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

25–30 (Herbicide Handbook 1989; Montgomery 1993)

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

97 (at 0.15 mmHg, Herbicide Handbook 1989)

108 (at 0.25 mmHg, Herbicide Handbook 1989; Montgomery 1993)

150 (at 9 mmHg, Howard 1991; Milne 1995; Montgomery 1993)

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

1.188 ( $25^{\circ}C$ , Hartley & Kidd 1987; Montgomery 1993)

Molar Volume ( $cm^3/mol$ ):

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

Dissociation Constant  $pK_a$ :

Enthalpy of Fusion,  $\Delta H_{fus}$  (kJ/mol):

Entropy of Fusion,  $\Delta S_{fus}$  (J/mol K):

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

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

40.0 (Günther et al. 1968)

14.0 (Ashton & Crafts 1973, 1981)

40.0 (rm. temp., Spencer 1973; Khan 1980)

40.0 (Martin & Worthing 1977; Hartley & Kidd 1987; Montgomery 1993; Milne 1995)

14.0 (Herbicide Handbook 1978; Herbicide Handbook 1989; Montgomery 1993)

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

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

52.5 (Garten & Trabalka 1983)

14.0 ( $20$ – $25^{\circ}C$ , selected, Augustijn-Beckers et al. 1994; Hornsby et al. 1996)

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

0.020 (Ashton & Crafts 1973; Herbicide Handbook 1989)

0.0117 ( $20^{\circ}C$ , Hartley & Graham-Bryce 1980)

0.0337 ( $20^{\circ}C$ , GC-RT correlation, Kim 1985)

0.020 (Hartley & Kidd 1987)

0.013 ( $20^{\circ}C$ , selected, Suntio et al. 1988)

0.020 ( $20^{\circ}C$ , Montgomery 1993)

0.020 ( $20$ – $25^{\circ}C$ , selected, Augustijn-Beckers et al. 1994; Hornsby et al. 1996)

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

0.250 ( $20^{\circ}C$ , calculated-P/C, Suntio et al. 1988)

0.385 (calculated-P/C, Howard 1991)

0.253 ( $20$ – $25^{\circ}C$ , calculated-P/C, Montgomery 1993)

0.108 (calculated-P/C, this work)

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

5.23 (estimated, USEPA 1988; quoted, Howard 1991)  
 3.29 (calculated, Montgomery 1993)  
 3.67 (LOGPSTAR or CLOGP data, Sabljic et al. 1995)

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

Bioconcentration Factor, log BCF:

2.15 (calculated-S, Kenaga 1980; quoted, Howard 1991; Isensee 1991)  
 2.08 (calculated- $K_{OC}$ , Kenaga 1980)

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

3.28 (soil, Grover 1974)  
 2.96, 2.46, 2.59, 2.49, 2.65 (Melfort loam, Weyburn sandy loam, Regina clay, Indian Head sandy loam, Asquith loamy sand, Grover et al. 1979)  
 3.28 (soil, measured value, Kenaga 1980; Kenaga & Goring 1980)  
 3.00 (soil, calculated-S as per Kenaga & Goring 1980, Kenaga 1980)  
 2.77 (calculated-MCI  $\chi$ , Bahnick & Doucette 1988)  
 2.28 (Montgomery 1993)  
 3.52 (selected, Lohninger 1994)  
 2.70 (20–25°C, selected, Augustijn-Beckers et al. 1994; Hornsby et al. 1996)  
 3.28 (soil, calculated-MCI  $\chi$ , Sabljic et al. 1995)  
 3.28; 3.21, 2.66 (soil, *cis*-isomer, quoted exptl.; estimated-class-specific model, estimated-general model using molecular descriptors, Gramatica et al. 2000)  
 3.28; 3.21, 2.65 (soil, *trans*-isomer, quoted exptl.; estimated-class-specific model, estimated-general model using molecular descriptors, Gramatica et al. 2000)

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

Volatilization:

Photolysis:  $t_{1/2} = 4$  h, < 1% of 135  $\mu\text{g/mL}$  to degrade in distilled water under > 300 nm light (Ruzo & Casida 1985; quoted, Cessna & Muir 1991).

Oxidation: photooxidation  $t_{1/2} = 0.58$ –5.8 h, based on an estimated rate constant for the vapor-phase reaction with hydroxyl radicals in air (Atkinson 1987; quoted, Howard et al. 1991).

Hydrolysis: neutral hydrolysis rate constant  $k = (1.2 \pm 0.7) \times 10^{-5} \text{ h}^{-1}$  with a calculated first-order  $t_{1/2} = 6.6$  yr at pH 7 (Ellington et al. 1987, 1988);

first-order  $t_{1/2} = 6.6$  yr, based on measured first-order base catalyzed hydrolysis rate constant at pH 7 (Ellington et al. 1987; quoted, Howard et al. 1991)

$t_{1/2} = 2400$  d at pH 2,  $t_{1/2} = 2500$  d at pH 7 and  $t_{1/2} = 32$  d at pH 12 in natural waters (Capel & Larson 1995).

Biodegradation: aqueous aerobic  $t_{1/2} = 252$ –2160 h, based on aerobic soil die-away test data (Anderson & Domsch 1976; Smith 1970; quoted, Howard et al. 1991); aqueous anaerobic  $t_{1/2} = 1008$ –8640 h, based on aerobic soil die-away test data (Anderson & Domsch 1976; Smith 1970; quoted, Howard et al. 1991)

$t_{1/2}(\text{aerobic}) = 11$  d,  $t_{1/2}(\text{anaerobic}) = 42$  d in natural waters (Capel & Larson 1995)

Biotransformation:

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

Half-Lives in the Environment:

Air:  $t_{1/2} = 0.58$ –5.8 h, based on an estimated rate constant for the vapor-phase reaction with hydroxyl radicals in air (Atkinson 1987; quoted, Howard et al. 1991).

Surface water:  $t_{1/2} = 252$ –2160 h, based on aerobic soil die-away test data (Anderson & Domsch 1976; Smith 1970; quoted, Howard et al. 1991)

Biodegradation  $t_{1/2}(\text{aerobic}) = 11$  d,  $t_{1/2}(\text{anaerobic}) = 42$  d, hydrolysis  $t_{1/2} = 2400$  d at pH 2,  $t_{1/2} = 2500$  d at pH 7 and  $t_{1/2} = 32$  d at pH 12 in natural waters (Capel & Larson 1995)



Ground water:  $t_{1/2} = 504\text{--}4320$  h, based on aerobic soil die-away test data (Anderson & Domsch 1976; Smith 1970; quoted, Howard et al. 1991).

Sediment:

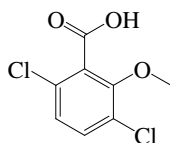
Soil:  $t_{1/2} = 252\text{--}2160$  h, based on aerobic soil die-away test data (Anderson & Domsch 1976; Smith 1970; quoted, Howard et al. 1991; Montgomery 1993);

$t_{1/2} = 30$  d (Hartley & Kidd 1987; quoted, Montgomery 1993);

selected field  $t_{1/2} = 30$  d (Augustijn-Beckers et al. 1994; Hornsby et al. 1996).

Biota:

## 17.1.1.25 Dicamba



Common Name: Dicamba

Synonym: Banex, Banvel, Banvel D, Brush buster, Dianat, MDBA, Mediben

Chemical Name: 3,6-dichloro-2-methoxybenzoic acid; 3,6-dichloro-*o*-anisic acid

Uses: systemic pre-emergent and post-emergent herbicide to control both annual and perennial broadleaf weeds.

CAS Registry No: 1918-00-9

Molecular Formula:  $C_8H_6Cl_2O_3$

Molecular Weight: 221.038

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

115 (Lide 2003)

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

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

1.570 ( $25^{\circ}C$ , Hartley & Kid 1987; Worthing & Hance 1991; Montgomery 1993; Tomlin 1994; Milne 1995)

Molar Volume ( $cm^3/mol$ ):

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

Dissociation Constant  $pK_a$ :

1.94 (Kearney & Kaufman 1975; Spencer 1982; Lee et al. 1993)

1.90 (Cessna & Grover 1978; Weber et al. 1980; Willis & McDowell 1982; Howard 1991; Montgomery 1993; Armbrust 2000)

1.95 (Worthing & Hance 1991; Montgomery 1993; Caux et al. 1993)

1.87 (Tomlin 1994)

1.91 (Hornsby et al. 1996)

Enthalpy of Vaporization,  $\Delta H_v$  (kJ/mol):

77.85 (Rordorf 1989)

Enthalpy of Fusion,  $\Delta H_{fus}$  (kJ/mol):

22.59 (DSC method, Plato & Glasgow 1969)

19.1 (Rordorf 1989)

Entropy of Fusion,  $\Delta S_{fus}$  (J/mol K):

Fugacity Ratio at  $25^{\circ}C$  (assuming  $\Delta S_{fus} = 56$  J/mol K), F: 0.131 (mp at  $115^{\circ}C$ )

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

7900 (Freed 1966; Verschuere 1983)

4500 (Martin & Worthing 1977; quoted, Kenaga 1980; Kenaga & Goring 1980; Khan 1980; Ashton & Crafts 1981; Weber et al. 1980; Hartley & Graham-Bryce 1980)

6500 (Hartley & Kidd 1987; Herbicide Handbook 1989; Caux et al. 1993)

6500 (Worthing & Walker 1987, Worthing & Hance 1991; Montgomery 1993; Tomlin 1994; Milne 1995)

5600 ( $20^{\circ}C$ , selected, Suntio et al. 1988)

4410, 221 (quoted, calculated-group contribution fragmentation method, Kühne et al. 1995)

8310 (selected., Armbrust 2000)

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

0.00454 (Ashton & Crafts 1973; 1981)

0.00267 (Baur & Bovey 1974; Spencer 1976)

0.49 ( $20^{\circ}C$ , Hartley & Graham-Bryce 1980; Khan 1980)

< 0.00013 ( $20$ – $25^{\circ}C$ , Weber et al. 1980; Willis & McDowell 1982)

0.00453 (Herbicide Handbook 1983, 1989; Worthing & Hance 1991)

0.0045 (Hartley & Kidd 1987; Tomlin 1994)

0.50 ( $100^{\circ}C$ , Budavari 1989)

$2.90 \times 10^{-3}$ ,  $6.40 \times 10^{-2}$ , 0.88, 8.60, 63.0 (25, 50, 70, 100,  $125^{\circ}C$ , gas saturation-GC, Rordorf 1989)

$\log (P_s/P_a) = 14.706 - 5139.1/(T/K)$ ; measured range 60.1–110°C (solid, gas saturation-GC, Rordorf 1989)  
 $\log (P_L/P_a) = 11.911 - 4067.0/(T/K)$ ; measured range 115–176°C (liquid, gas saturation-GC, Rordorf 1989)  
 0.50 (20°C, selected, Taylor & Spencer 1990)  
 0.0045 (20°C, Montgomery 1993)

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

0.00012 (20°C, calculated-P/C, Suntio et al. 1988)  
 0.0248 (calculated-P/C, Taylor & Glotfelty 1988)  
 0.0918 (Suntio et al. 1988; quoted, Howard 1991; Majewski & Capel 1995)  
 $2.2 \times 10^{-5}$  (calculated-P/C, Nash 1989)  
 $1.22 \times 10^{-4}$  (20–25°C, calculated-P/C, Montgomery 1993)  
 0.00012, 0.000154 (20, 25°C, quoted, Caux et al. 1993)  
 $4.46 \times 10^{-5}$  (quoted lit., Armbrust 2000)

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

0.477 (Rao & Davidson 1980)  
 2.41 (selected, Dao et al. 1983)  
 2.21 (shake flask, Log P Database, Hansch & Leo 1985, 1987)  
 -1.69 (selected, Gerstl & Helling 1987)  
 3.01 (selected, Travis & Arms 1988)  
 2.46 (Reinert 1989)  
 2.49 (shake flask-HPLC/UV, Jafvert et al. 1990)  
 2.46 (EPA Environmental Fate one-liner database Version 3.04, Lee et al. 1993)  
 2.21 (recommended, Sangster 1993)  
 0.48 (Montgomery 1993)  
 -0.80 (pH 7, Tomlin 1994)  
 2.21 (recommended, Hansch et al. 1995)

Bioconcentration Factor,  $\log \text{BCF}$ :

0.699 (calculated-S, Kenaga 1980)  
 -2.00 (calculated- $K_{oc}$ , Kenaga 1980)  
 -4.58 (beef biotransfer factor  $\log B_b$ , correlated- $K_{ow}$ , Oehler & Ivie 1980)  
 -4.60 (milk biotransfer factor  $\log B_m$ , correlated- $K_{ow}$ , Oehler & Ivie 1980)  
 1.450 (estimated- $K_{ow}$  per Hansch & Leo 1985, Lyman et al. 1982)  
 0.903 (estimated-S per Suntio et al. 1988, Lyman et al. 1982)

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

-0.398 (soil, quoted exptl., Kenaga 1980)  
 1.63 (soil, calculated-S as per Kenaga & Goring 1980, Kenaga 1980)  
 0.342 (av. soils/sediments, Rao & Davidson 1980)  
 -0.40, 2.08 (quoted, calculated-MCI  $\chi$ , Gerstl & Helling 1987)  
 0.34 (soil, screening model calculations, Jury et al. 1987b)  
 2.67 ( $K_{oc} = 470$  reported, Reinert 1989)  
 0.643 (soil, estimated, Shirmohammadi et al. 1989)  
 -1.00 (selected, USDA 1989; quoted, Neary et al. 1993)  
 0.30 (organic carbon, Wauchope et al. 1991)  
 -0.40, 1.62, 0.18, 0.34 (soil, quoted values, Bottoni & Funari 1992)  
 1.50; 1.46 (soil, quoted exptl.; calculated-MCI  $\chi$  and fragment contribution Meylan et al. 1992)  
 -0.40, 0.34 (Montgomery 1993)  
 0.30 (Tomlin 1994)  
 1.50 (quoted or calculated-QSAR MCI  $\chi$ , Sabljic et al. 1995)  
 1.114 (quoted lit., Armbrust 2000)

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

2.74 (organo-clay DODMA140-SAz, sorption isotherm, Zhao et al. 1996)

- 2.57 (organo-clay DODMA-SAz, sorption isotherm-HPLC/UV, Zhao et al. 1996)  
 2.48 (organo-clay HDTMA-SAz, sorption isotherm-HPLC/UV, Zhao et al. 1996)  
 2.59 (organo-clay HDTMA-SWy, sorption isotherm-HPLC/UV, Zhao et al. 1996)

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

##### Volatilization:

Photolysis: aqueous photolysis rate constant  $k = 7.5 \times 10^{-4} \text{ h}^{-1}$  (Armbrust 2000).

Oxidation: photooxidation  $t_{1/2} = 2.4\text{--}6.0 \text{ d}$ , based on estimated rate constant for the vapor-phase reaction with hydroxyl radicals in the atmosphere (Atkinson 1985; quoted, Howard 1991); measured hydroxy radical reaction rate constant for dicamba  $4.8 \times 10^{12} \text{ M}^{-1} / \text{h}$  (Armbrust 2000).

Hydrolysis:  $t_{1/2} > 133 \text{ d}$  for  $2 \mu\text{g mL}^{-1}$  to hydrolyze in dark sterile pond water at  $37\text{--}39^\circ\text{C}$  (Scifres et al. 1973; quoted, Muir 1991);

stable aqueous hydrolysis rates at pH 5, 7, 9 (Armbrust 2000).

Biodegradation:  $t_{1/2} = 60 \text{ d}$  to  $> 160 \text{ d}$  for  $100 \mu\text{g mL}^{-1}$  to degrade in pond sediment/water under lighted conditions at  $20\text{--}30^\circ\text{C}$  (Scifres et al. 1973; quoted, Muir 1991); under lab. conditions using nonsterile sandy loam, silty clay, or heavy clay soil, 50% of applied dicamba degraded within 2 weeks; however in sterilized (via heating) soil, over 90% of applied dicamba was recovered after 4 weeks, suggesting that microbes were responsible for the decomposition (Smith 1973; quoted, Howard 1991);

$t_{1/2} > 25 \text{ d}$  for 5.85 mg of labeled dicamba to plants to degrade following washoff from plants and sands in model ecosystem (derived from data of Yu et al. 1975; Muir 1991);

$k = 0.022 \text{ d}^{-1}$  by soil incubation die-away studies (Rao & Davidson 1980; quoted, Scow 1982);

rate of biodegradation in soil generally increases with temperature and soil moisture (up to 50%) and tends to be faster when the soil is slightly acidic (Herbicide Handbook 1983; quoted, Howard 1991);

aerobic rate constant  $k = 1.60 \times 10^{-3} \text{ h}^{-1}$  (Armbrust 2000).

##### Biotransformation:

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

#### Half-Lives in the Environment:

Air:  $t_{1/2} \sim 2.42 \text{ d}$  for reaction with hydroxyl radicals (estimated, Eisenreich et al. 1981; quoted, Caux et al. 1993)  
 $t_{1/2} = 2.42\text{--}6.0 \text{ d}$ , based on estimated rate constant for the vapor-phase reaction with hydroxyl radicals in the atmosphere (Atkinson 1985; quoted, Howard 1991).

##### Surface water:

Ground water:  $t_{1/2} = 23.5 \text{ d}$  determined under batch conditions at  $28^\circ\text{C}$ ,  $t_{1/2} = 38 \text{ d}$  at  $20^\circ\text{C}$ , and  $t_{1/2} = 151 \text{ d}$  at  $12^\circ\text{C}$  and were all higher than  $t_{1/2} \sim 13.5 \text{ d}$  from the decrease in column effluent concentrations over time (Comfort et al. 1992);

reported  $t_{1/2} = 14\text{--}433, 201 \text{ and } 25 \text{ d}$  (Bottoni & Funari 1992)

$t_{1/2} < 7 \text{ d}$  in surface water (Caux et al. 1993).

##### Sediment:

Soil: estimated persistence of 2 months (Kearney et al. 1969; quoted, Jury et al. 1987a);

$t_{1/2} = 59, 19, \text{ and } 17 \text{ d}$  with disappearance rates:  $k = 0.0117, 0.036 \text{ and } 0.041 \text{ d}^{-1}$  at pH 4.3, 5.3 and 6.5 (Hamaker 1972; quoted, Nash 1988);

persistence of 2 months in soil (Edwards 1973; quoted, Morrill et al. 1982);

degradation  $t_{1/2} = 32 \text{ d}$  and  $17 \text{ d}$  in Quachita Highlands = forest and grassland soil respectively,  $t_{1/2} = 26 \text{ d}$  in

Gross Timbers Forest soil, average  $t_{1/2} = 25 \text{ d}$  in 3 soils (Altom & Stritzke 1973);

first-order  $t_{1/2} \sim 31.5 \text{ d}$  in soil from biodegradation rate constant  $k = 0.022 \text{ d}^{-1}$  by soil incubation die-away studies (Rao & Davidson 1980; quoted, Scow 1982);

nonpersistent in soils with  $t_{1/2} < 20 \text{ d}$  (Willis & McDowell 1982);

mean  $t_{1/2} = 14 \text{ d}$  under lab. conditions from review of persistence literature, while the mean  $t_{1/2} = 8 \text{ d}$  under field conditions (Rao & Davidson 1982; quoted, Howard 1991);

non-persistent with  $t_{1/2} < 20 \text{ d}$  in soil (Willis & McDowell 1982);

$t_{1/2} = 14 \text{ d}$  from screening model calculations (Jury et al. 1987b);

$t_{1/2} < 14 \text{ d}$  under conditions amenable to rapid metabolism (Herbicide Handbook 1989);

selected  $t_{1/2} = 14 \text{ d}$  (Wauchope et al. 1991; quoted, Dowd et al. 1993);

$t_{1/2} < 14\text{--}25 \text{ d}$  (Worthing & Hance 1991; quoted, Montgomery 1993);

reported  $t_{1/2} = 20$  d, 25 d and 14–433 d (Bottoni & Funari 1992);

$t_{1/2} = 4$ –555 d with a mean  $t_{1/2} = 24$  d (Caux et al. 1993);

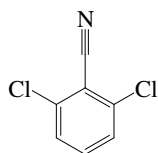
$t_{1/2} < 14$  d (Tomlin 1994).

Biota: biochemical  $t_{1/2} = 14$  d from screening model calculations (Jury et al. 1987b);

average  $t_{1/2} = 25$  d in the forest (USDA 1989; quoted, Neary et al. 1993);

biological  $t_{1/2} = 0.64$  h (Caux et al. 1993).

## 17.1.1.26 Dichlobenil



Common Name: Dichlobenil

Synonym: Barrier 2G, Barrier 50W, Casoron, DBN, DCB, Decabane, Du-Sprex, Dyclomec, NIA 5996, Niagara 5006, Niagara 5996, Norosac

Chemical Name: 2,6-dichlorobenzonitrile

Uses: soil applied herbicide to control many annual and perennial broadleaf weeds.

CAS Registry No: 1194-65-6

Molecular Formula:  $C_7H_3Cl_2N$

Molecular Weight: 172.012

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

144.5 (Lide 2003)

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

270 (Verloop 1972; Khan 1980; Worthing & Hance 1991; Tomlin 1994; Milne 1995)

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

> 1.0 (Milne 1995)

Molar Volume ( $cm^3/mol$ ):

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

Dissociation Constant  $pK_a$ :

Enthalpy of Vaporization,  $\Delta H_v$  ( $kJ/mol$ ):

65.74 (Rordorf 1989)

Enthalpy of Fusion,  $\Delta H_{fus}$  ( $kJ/mol$ ):

25.94 (DSC method, Plato & Glasgow 1969)

34.33 (Verloop 1972)

24.2 (Rordorf 1989)

Entropy of Fusion,  $\Delta S_{fus}$  ( $J/mol K$ ):

Fugacity Ratio at  $25^{\circ}C$  (assuming  $\Delta S_{fus} = 56 J/mol K$ ), F: 0.0672 (mp at  $144.5^{\circ}C$ )

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

18 ( $20^{\circ}C$ , Günther et al. 1968; Weber 1972; Verloop 1972; Spencer 1982; Verschueren 1983)

25 (Günther et al. 1968; Montgomery 1993)

18 (Martin & Worthing 1977; Herbicide Handbook 1978)

18 (Wauchope 1978; Khan 1980; Burkhard & Guth 1981)

18 ( $20^{\circ}C$ , Ashton & Crafts 1981; Hartley & Kidd 1987; Herbicide Handbook 1989)

18 ( $20^{\circ}C$ , Worthing & Walker 1987, Worthing & Hance 1991; Tomlin 1994)

21.2 ( $20$ – $25^{\circ}C$ , selected, Wauchope et al. 1992; Lohninger 1994; Hornsby et al. 1996)

18, 25 ( $20^{\circ}C$ ,  $25^{\circ}C$ , Milne 1995)

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

0.072 ( $20^{\circ}C$ , effusion manometer technique, Barnsley & Rosher 1961)

0.0733 ( $20^{\circ}C$ , Verloop 1972; Khan 1980; Ashton & Crafts 1981; Herbicide Handbook 1989)

0.0667 ( $20^{\circ}C$ , Weber 1972; Worthing & Walker 1987)

0.0004 ( $20^{\circ}C$ , Spencer 1976)

0.0666 ( $20^{\circ}C$ , effusion method, Spencer 1976)

0.0733 ( $20$ – $25^{\circ}C$ , Weber et al. 1980)

0.073 ( $20^{\circ}C$ , Hartley & Kidd 1987)

0.070 ( $20^{\circ}C$ , selected, Suntio et al. 1988)

0.110, 1.80, 20.0, 160, 970 (25, 50, 70, 100,  $125^{\circ}C$ , gas saturation-GC, Rordorf 1989)

$\log(P_s/Pa) = 14.787 - 4698.2/(T/K)$ ; measured range  $32.4$ – $125^{\circ}C$  (solid, gas saturation-GC, Rordorf 1989)

$\log (P_L/P_a) = 11.754 - 3434.1/(T/K)$ ; measured range 32.4–125°C (liquid, gas saturation-GC, Rordorf 1989)  
 0.133 (20–25°C, selected, Wauchope et al. 1992; Hornsby et al. 1996)  
 0.0733 (Montgomery 1993)  
 0.088 (20°C, gas saturation, Tomlin 1994)

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

0.700 (20°C, volatilization rate, Burkhard & Guth 1981)  
 0.669 (20°C, calculated-P/C, Suntio et al. 1988)  
 0.637 (20°C, calculated-P/C, Muir 1991)  
 0.669 (20–25°C, calculated-P/C, Montgomery 1993)

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

2.90 (Rao & Davidson 1980; selected, Suntio et al. 1988, Magee 1991)  
 2.57; 2.65 (RP-HPLC-RT correlation; shake flask, Eadsforth & Moser 1983)  
 3.06 (shake flask, Geyer et al. 1984)  
 2.94 (Hansch & Leo 1985)  
 1.63 (Reinert 1989)  
 2.98 (selected, Dao et al. 1983, Gerstl & Helling 1987)  
 2.90 (shake flask, Log P Database, Hansch & Leo 1987)  
 2.90 (recommended, Sangster 1993)  
 2.70 (Tomlin 1994)  
 2.74 (recommended, Hansch et al. 1995)  
 2.95 (RP-HPLC-RT correlation, Nakamura et al. 2001)  
 2.98 (RP-HPLC-RT correlation using short ODP column, Donovan & Pescatore 2002)

Bioconcentration Factor,  $\log \text{BCF}$ :

1.74 (fish in static water, Kenaga 1975; Kenaga & Goring 1980)  
 2.08 (calculated-S, Kenaga 1980; quoted, Isensee 1991)  
 1.08 (calculated- $K_{oc}$ , Kenaga 1980)  
 1.18–1.60 (fish, Freitag et al. 1982)  
 1.30 (algae, Freitag et al. 1982)  
 1.72 (estimated-S, Lyman et al. 1982; quoted, Howard 1991)  
 2.03–2.32 (Montgomery 1993)

Sorption Partition Coefficient,  $\log K_{oc}$  at 25°C or as indicated:

2.91 (potting soil with 22% organic content, Massini 1961)  
 2.08 (sandy loam with 5% organic content, Massini 1961)  
 2.37 (soil, Hamaker & Thompson 1972–1987)  
 2.95 (soil, calculated-S as per Kenaga & Goring 1980, Kenaga 1980)  
 2.35 (Rao & Davidson 1980)  
 2.94 (soil, estimated-S, Lyman et al. 1982; quoted, Howard 1991)  
 2.37, 1.45 (quoted, calculated-MCI  $\chi$ , Gerstl & Helling 1987)  
 2.96 (Reinert 1989)  
 2.37; 2.31 (reported as  $\log K_{OM}$ ; estimated as  $\log K_{OM}$ , Magee 1991)  
 2.21, 2.57–2.96 (soil, quoted values, Bottoni & Funari 1992)  
 2.60 (soil, 20–25°C, estimated, Wauchope et al. 1992; Hornsby et al. 1996)  
 2.60 (estimated-chemical structure, Lohninger 1994)  
 2.31 (soil, calculated-MCI  $^1\chi$ , Sabljic et al. 1995)

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

Volatilization:  $t_{1/2} \sim 7.4$  d, based on Henry's law constant for a model river 1-m deep with a wind velocity of 3 m/s and flowing at 1 m/s (estimated, Lyman et al. 1982; quoted, Howard 1991);  
 $t_{1/2} \sim 11$  d from 1 m depth of water at 20°C (estimated, Muir 1991).  
 Photolysis: photolytic  $t_{1/2} = 15$  d in water (Tomlin 1994).

Oxidation: photooxidation  $t_{1/2} = 92$  d in air, based on estimation for the vapor-phase reaction with hydroxyl radicals in atmosphere (Atkinson 1987; quoted, Howard 1991).

Hydrolysis:

Biodegradation:  $t_{1/2} \sim 7$  d for 5  $\mu\text{g/mL}$  to biodegrade in sediment suspension at 30°C (Miyazaki et al. 1975; quoted, Muir 1991).

Biotransformation:

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

#### Half-Lives in the Environment:

Air:  $t_{1/2} = 92$  d, based on estimation for the vapor-phase reaction with hydroxyl radicals in atmosphere (Atkinson 1987; quoted, Howard 1991).

Surface water:

Ground water: reported  $t_{1/2} = 44\text{--}360$  d (Bottoni & Funari 1992)

Sediment:  $t_{1/2} \sim 7$  d for 5  $\mu\text{g/mL}$  to biodegrade in sediment suspension at 30°C (Miyazaki et al. 1975; quoted, Muir 1991).

Soil: estimated persistence of 4 months (Kearney et al. 1969; quoted, Jury et al. 1987);

$t_{1/2} = 1\text{--}6$  months in soil depending on soil type (Beynon & Wright 1972; Verloop 1972; quoted, Tomlin 1994);

persistence of 4 months in soil (Edwards 1973; quoted, Morrill et al. 1982);

persistence of 4 months (Wauchope 1978);

$t_{1/2} = 1.5$  to 12 months depending upon soil type (Herbicide Handbook 1989);

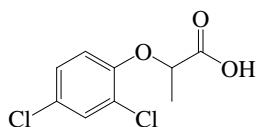
selected  $t_{1/2} = 60$  d (Wauchope et al. 1992; Hornsby et al. 1996);

reported  $t_{1/2} = 45\text{--}360$  d (Bottoni & Funari 1992).

Biota:



## 17.1.1.27 Dichlorprop



Common Name: Dichlorprop

Synonym: Cornox RK, dichloroprop, Dikofag DP, 2,4-DP, Hedonal DP, Polymone

Chemical Name: (±)-2-(2,4-dichlorophenoxy) propanoic acid; (±)-2-(2,4-dichlorophenoxy) propionic acid

Uses: herbicide and growth regulator to control annual broadleaf and grass weeds; also to control aquatic weeds and chemical maintenance of embankments and roadside verges.

CAS Registry No: 120-36-5

Molecular Formula:  $C_9H_8Cl_2O_3$

Molecular Weight: 235.064

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

117.5 (Lide 2003)

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

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

1.64 ( $25^{\circ}C$ , Bailey & White 1965)

1.42 (Herbicide Handbook 1989; Tomlin 1994)

Molar Volume ( $cm^3/mol$ ):

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

165.6 (calculated-density)

Dissociation Constant  $pK_a$ :

2.855 (Cessna & Grover 1978)

2.86 (Wauchope et al. 1992; Hornsby et al. 1996)

3.00 (Tomlin 1994)

Enthalpy of Vaporization,  $\Delta H_v$  ( $kJ/mol$ ):

127.9 (Rordorf 1989)

Enthalpy of Fusion,  $\Delta H_{fus}$  ( $kJ/mol$ ):

34.31 (DSC method, Plato 1972)

30.9 (Rordorf 1989)

Entropy of Fusion,  $\Delta S_{fus}$  ( $J/mol K$ ):

Fugacity Ratio at  $25^{\circ}C$  (assuming  $\Delta S_{fus} = 56 J/mol K$ ),  $F$ : 0.124 (mp at  $117.5^{\circ}C$ )

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

350 ( $20^{\circ}C$ , Woodford & Evans 1963; Spencer 1973)

350 (Martin & Worthing 1977)

350 ( $20^{\circ}C$ , Hartley & Kidd 1987; Worthing & Walker 1987, 1991)

710 ( $28^{\circ}C$ , Herbicide Handbook 1989)

50 (ester,  $20$ – $25^{\circ}C$ , estimated, Wauchope et al. 1992; Lohninger 1994; Hornsby et al. 1996)

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

$4.50 \times 10^{-4}$  ( $20^{\circ}C$ , Hartley & Kidd 1987)

$2.90 \times 10^{-7}$ ,  $4.10 \times 10^{-5}$ ,  $2.8 \times 10^{-3}$ , 0.11, 2.80 ( $25$ ,  $50$ ,  $70$ ,  $100$ ,  $125^{\circ}C$ , gas saturation-GC, Rordorf 1989)

$\log(P_s/Pa) = 21.26 - 8289.2/(T/K)$ ; measured range  $95.7$ – $118^{\circ}C$  (solid, gas saturation-GC, Rordorf 1989)

$\log(P_l/Pa) = 17.174 - 6682.8/(T/K)$ ; measured range  $120$ – $150^{\circ}C$  (liquid, gas saturation-GC, Rordorf 1989)

$4.00 \times 10^{-4}$  ( $20$ – $25^{\circ}C$ , estimated, Wauchope et al. 1992; Hornsby et al. 1996)

$< 1.0 \times 10^{-5}$  ( $20^{\circ}C$ , Tomlin 1994)

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

$2.69 \times 10^{-4}$  (calculated-P/C, this work)

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

- 2.75 (RP-HPLC- $k'$  correlation, Braumann et al. 1983)
- 3.43 (shake flask-GC, Ilchmann et al. 1993)
- 2.06 to -0.22 (pH 4–7, shake flask-LSC, Riise & Salbu 1992)
- 1.77 (Tomlin 1994)
- 3.43 (recommended, Sangster 1993; Hansch et al. 1995)

Bioconcentration Factor,  $\log BCF$ :

- 1.36 (calculated-S, Kenaga 1980)

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

- 2.23 (soil, calculated-S, Kenaga 1980)
- 3.00 (soil, 20–25°C, estimated, Wauchope et al. 1992; Lohninger 1994; Hornsby et al. 1996)
- 2.05, 2.07, 1.70, 1.79, 1.73 (5 soils: soil A 30.4% OC and pH 4.4, soil B 14.6% OC pH 4.1, soil C/loam 3.3% OC pH 5.0, soil D/silty clay 1.3% OC pH 5.1, soil E/sand 1.4% OC pH 5.3, batch equilibrium-sorption isotherms, Riise Salbu 1992)
- 1.08–1.60 (Tomlin 1994)

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

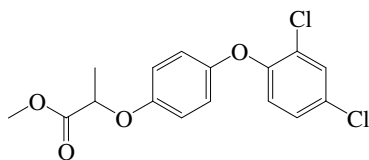
Photolysis: photodegradation  $t_{1/2} = 10$  to 19 d on 3 Spanish natural dry soils;  $t_{1/2} = 22$  to 59 d on 10% peat-amended dry soils; degradation  $t_{1/2} \sim 2$ –6 d on moist soils at field capacity and saturation soils for degradation at 0, 1 and 2 exposures days; and  $t_{1/2} = 16$ –37 d on moist soils at field capacity and saturated soils for degradation at 2, 4 and 10 exposure days (Romero et al. 1998)

## Half-Lives in the Environment:

Soil:  $t_{1/2} = 12$  d and 8 d in Quachita Highlands = forest and grassland soil, respectively,  $t_{1/2} = 10$  d in gross timbers forest soil, average  $t_{1/2} = 10$  d in 3 soils (Altom & Stritzke 1973); selected field  $t_{1/2} = 10$  d (Wauchope et al. 1992; Hornsby et al. 1996);  $t_{1/2} \sim 8$  d in soil (Tomlin 1994)

photodegradation  $t_{1/2} = 10$ –19 d in 3 Spanish natural dry soils,  $t_{1/2} = 22$ –59 d in the 10% peat-amended dry soils; degradation  $t_{1/2} \sim 2$ –6 d on moist soils at field capacity and saturation soils for degradation at 0, 1 and 2 exposures days; and  $t_{1/2} = 16$ –37 d on moist soils at field capacity and saturated soils for degradation at 2, 4 and 10 exposure days (Romero et al. 1998)

## 17.1.1.28 Diclofop-methyl



Common Name: Diclofop-methyl

Synonym: Hoelon, dichlordiphenoprop, Hoegrass, Illoxan

Chemical Name: methyl 2-[4-(2',4'-dichlorophenoxy)-phenoxy]propanoate

Uses: herbicide to control post-emergent wild oats, wild millets, and other annual grass weeds in wheat, barley, rye, red fescue, and broadleaf weeds in crops such as soybeans, sugar cane, fodder beet, flax, legumes, oilseed rape, sunflowers, clover, lucerne, groundnuts, brassicas, carrots, celery, beet root, parsnips, lettuce, spinach, potatoes, tomatoes, fennel, alliums, herbs, etc.

CAS Registry No: 51338-27-3

Molecular Formula:  $C_{16}H_{14}Cl_2O_4$

Molecular Weight: 341.186

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

40 (Lide 2003)

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

175–176 (at 0.1 mmHg, Hartley & Kidd 1987; Herbicide Handbook 1989)

Density ( $g/cm^3$ ):

1.30 (40 $^{\circ}C$ , Hartley & Kidd 1987; Worthing & Walker 1987; Herbicide Handbook 1989)

1.035 (Herbicide Handbook 1989)

Acid Dissociation Constants,  $pK_a$ :

3.1 (Wauchope et al. 1992; Hornsby et al. 1996)

Molar Volume ( $cm^3/mol$ ):

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

329.7 (calculated-density)

Dissociation Constant  $pK_a$ :

3.1 (Wauchope et al. 1992; Hornsby et al. 1996)

Enthalpy of Fusion,  $\Delta H_{fus}$  (kJ/mol):

Entropy of Fusion,  $\Delta S_{fus}$  (J/mol K):

Fugacity Ratio at 25 $^{\circ}C$  (assuming  $\Delta S_{fus} = 56$  J/mol K), F: 0.713 (mp at 40 $^{\circ}C$ )

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

3.0 (22 $^{\circ}C$ , Hartley & Kidd 1987; Worthing & Walker 1987; Worthing & Hance 1991)

3.0 (22 $^{\circ}C$ , Herbicide Handbook 1989)

0.80 (20–25 $^{\circ}C$ , selected, Wauchope et al. 1992; Hornsby et al. 1996)

0.80 (20 $^{\circ}C$ , pH 7, Tomlin 1994)

4.23 (Majewski & Capel 1995)

4.06 (calculated-group contribution method, Kühne et al. 1995)

3.0 (Lohninger 1994; Milne 1995)

0.8 (selected, Halfon et al. 1996)

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

$3.44 \times 10^{-5}$  (20 $^{\circ}C$ , Worthing 1983, 1987; Hartley & Kidd 1987)

$3.40 \times 10^{-5}$  (20 $^{\circ}C$ , Worthing & Walker 1987, Worthing & Hance 1991)

$3.47 \times 10^{-5}$ ,  $1.6 \times 10^{-4}$ ,  $3.87 \times 10^{-3}$  (20 $^{\circ}C$ , 30 $^{\circ}C$ , 54.3 $^{\circ}C$ , Herbicide Handbook 1989)

$5.91 \times 10^{-5}$  (selected, Wauchope et al. 1992; Hornsby et al. 1996)

$2.5 \times 10^{-4}$ ,  $7.7 \times 10^{-3}$  (20 $^{\circ}C$ , 50 $^{\circ}C$ , Tomlin 1994)

$4.80 \times 10^{-5}$  (quoted, Majewski & Capel 1987)

$4.7 \times 10^{-4}$  (selected, Halfon et al. 1996)

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

- 0.00387 (calculated-P/C, Majewski & Capel 1995)  
 0.199 (calculated-P/C, this work)

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

- 4.80 (shake flask, Log P Database, Hansch & Leo 1987)  
 4.601 (Stevens et al. 1988)  
 4.58 (Worthing & Hance 1991)  
 4.60 (shake flask, pH 7, Baker et al. 1992)  
 4.80 (recommended, Sangster 1993)  
 4.5775 (Tomlin 1994)  
 4.80 (recommended, Hansch et al. 1995)  
 5.52 (Pomona-database, Müller & Kördel 1996)  
 4.87 (RP-HPLC-RT correlation using short ODP column, Donovan & Pescatore 2002)

Bioconcentration Factor,  $\log \text{BCF}$  or  $\log K_{\text{B}}$ :

- 2.74 (calculated-S as per Kenaga 1980, this work)

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

- 4.69, 4.20 (Wauchope et al. 1992)  
 4.15–4.39 (soil, quoted values, Bottoni & Funari 1992)  
 4.20 ( $20\text{--}25^\circ\text{C}$ , soil, recommended, Wauchope et al. 1992; Hornsby et al. 1996)  
 4.25 (soil, HPLC-screening method, mean value of different stationary and mobile phases, Kördel et al. 1993, 1995b)  
 4.15–4.39 (soil, Tomlin 1994)  
 4.20 (estimated-chemical structure, Lohninger 1994)  
 4.25; 3.61 (HPLC-screening method; calculated-PCKOC fragment method, Müller & Kördel 1996)  
 5.505, 5.334, 4.122, 4.737, 4.182 (first generation Eurosoils ES-1, ES-2, ES-3, ES-4, ES-5, shake flask/batch equilibrium-HPLC/UV, Gawlik et al. 1998)  
 4.002, 3.731, 3.453, 3.257, 3.715 (second generation Eurosoils ES-1, ES-2, ES-3, ES-4, ES-5, shake flask-batch equilibrium-HPLC/UV and HPLC- $k'$  correlation, Gawlik et al. 2000)

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

Volatilization:

Photolysis:

Oxidation:

Hydrolysis:

Biodegradation: first-order rate constants  $k = -0.0883, -0.225, -0.266 \text{ h}^{-1}$  in nonsterile sediment and  $k = -0.0158, -0.0139, -0.0134 \text{ h}^{-1}$  in sterile sediment by shake-tests at Davis Bayou,  $k = -0.0457, -0.103, -0.120 \text{ h}^{-1}$  in nonsterile water and  $k = -0.00233, -0.00722, -0.00785 \text{ h}^{-1}$  in sterile water by shake-tests at Davis Bayou (Walker et al. 1988)

$t_{1/2} = 10 \text{ d}$  in sandy soils and  $t_{1/2} \sim 30 \text{ d}$  in sandy clay soils under aerobic conditions (Herbicide Handbook 1989)

Biotransformation:

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

## Half-Lives in the Environment:

Air:

Surface water:  $t_{1/2} = 363 \text{ d}$  at  $25^\circ\text{C}$  and pH 5,  $t_{1/2} = 31.7 \text{ d}$  at pH 7 and  $t_{1/2} = 0.52 \text{ d}$  at pH 9 (Tomlin 1994).

Ground water: reported  $t_{1/2} = 6\text{--}9, 23\text{--}38$  and  $150 \text{ d}$  (Bottoni & Funari 1992)

Sediment:

Soil:  $t_{1/2} = 10 \text{ d}$  in sandy soils and  $t_{1/2} \sim 30 \text{ d}$  in sandy clay soils while under anaerobic conditions, results were similar except that the very rapid cleavage of the ester bond by hydrolysis within one hour to propionic acid derivatives was experienced and within 2 d, up to 86% of the parent compound was metabolized into various free acid metabolites and up to 3.7% of phenol metabolites (Herbicide Handbook 1989);

$t_{1/2}$  = 6–9 d, 23–38 d and 150 d (Bottoni & Funari 1992);

selected field  $t_{1/2}$  = 30 d at pH 7.0 (Wauchope et al. 1992; Hornsby et al. 1996)

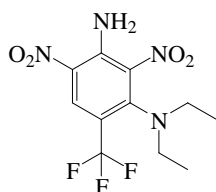
V = 1–57 d and  $t_{1/2}$  = 30–281 d for various soils in field trials (Tomlin 1994).

$t_{1/2}$  = 30 d (selected, Halfon et al. 1996).

Biota:  $t_{1/2}$  = 3–7 d for wheat (Herbicide Handbook 1989)

$t_{1/2}$  = 3 d in sugar beet (Tomlin 1994).

## 17.1.1.29 Dinitramine



Common Name: Dinitramine

Synonym: Cobex, Cobexo

Chemical Name: *N,N*-diethyl-2,6-dinitro-4-(trifluoromethyl)-*m*-phenylenediamine

Uses: herbicide for selective pre-plant soil incorporating control of many annual grass and broadleaf weeds in cotton, soybeans, peas, groundnuts, beans, sunflowers, safflowers, carrots, turnips, fennel, chicory, etc. and in transplanted tomatoes, capsicums, aubergines, and brassicas.

CAS Registry No: 29091-05-2

Molecular Formula:  $C_{11}H_{13}N_4O_4F_3$

Molecular Weight: 322.241

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

98 (Lide 2003)

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

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

1.50 ( $25^{\circ}C$ , Ashton & Crafts 1981; Hartley & Kidd 1987)

Molar Volume ( $cm^3/mol$ ):

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

Dissociation Constant  $pK_a$ :

4.5 (Haag & Yao 1992)

Enthalpy of Fusion,  $\Delta H_{fus}$  ( $kJ/mol$ ):

Entropy of Fusion,  $\Delta S_{fus}$  ( $J/mol K$ ):

Fugacity Ratio at  $25^{\circ}C$  (assuming  $\Delta S_{fus} = 56 J/mol K$ ), F: 0.192 (mp at  $98^{\circ}C$ )

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

- 1.1 (Martin & Worthing 1977; Kenaga 1980; Kenaga & Goring 1980; Khan 1980; Isensee 1991)
- 1.0 (Wauchope 1978; Verschueren 1983)
- 1.0 ( $20^{\circ}C$ , Ashton & Crafts 1981; Hartley & Kidd 1987)
- 1.1 (Worthing & Walker 1987, 1991)
- 1.1 ( $20$ – $25^{\circ}C$ , selected, Augustijn-Beckers et al. 1994; Hornsby et al. 1996)
- 1.0 ( $20^{\circ}C$ , Tomlin 1994; Milne 1995)

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

- 0.00048 (Khan 1980; Ashton & Crafts 1981)
- 0.00048 (Verschueren 1983)
- 0.000479 (Hartley & Kidd 1987; Worthing & Hance 1991; Tomlin 1994)
- 0.00040 ( $20^{\circ}C$ , selected, Suntio et al. 1988)
- 0.00048 ( $20$ – $25^{\circ}C$ , selected, Augustijn-Beckers et al. 1994; Hornsby et al. 1996)

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

- 0.160 ( $20^{\circ}C$ , calculated-P/C, Suntio et al. 1988)

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

- 4.31 (selected, Dao et al. 1983)
- 4.30 (Worthing & Hance 1991; Tomlin 1994)
- 4.30 (Milne 1995)
- 4.30 (recommended, Hansch et al. 1995)
- 3.89 (LOGPSTAR or CLOGP data, Sabljic et al. 1995)

## Bioconcentration Factor, log BCF:

- 2.77 (calculated-S, Kenaga 1980; quoted, Isensee 1991)
- 2.45 (calculated- $K_{OC}$ , Kenaga 1980)

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

- 3.60 (soil, Harvey 1974)
- 3.61 (soil, calculated-S as per Kenaga & Goring 1980, Kenaga 1980)
- 3.60 (20–25°C, estimated, Augustijn-Beckers et al. 1994; Hornsby et al. 1996)
- 3.84 (estimated-chemical structure, Lohninger 1994)
- 3.63 (soil, calculated-MCI  $^1\chi$ , Sabljic et al. 1995)
- 3.63; 3.42 (soil, quoted exptl.; estimated-general model using molecular descriptors, Gramatica et al. 2000)

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

## Volatilization:

Photolysis:  $t_{1/2} < 1$  h in distilled water, river water and ocean water under sunlight (Newsom & Woods 1973; quoted, Cessna & Muir 1991).

## Oxidation:

## Hydrolysis:

Biodegradation:  $t_{1/2} = 22$  d for 0.5  $\mu\text{g/mL}$  to biodegrade in flooded soil with approximately 1 cm of water on top of the soil (Savage 1978; quoted, Muir 1991).

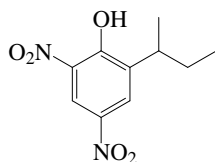
## Biotransformation:

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

## Half-Lives in the Environment:

Soil:  $t_{1/2} = 22$  d for 0.5  $\mu\text{g/mL}$  to biodegrade in flooded soil with approximately 1 cm of water on top of the soil (Savage 1978; quoted, Muir 1991);  
persistence of 3 months in soil (Wauchope 1978);  
selected field  $t_{1/2} = 30$  d (Augustijn-Beckers et al. 1994; Hornsby et al. 1996);  
 $t_{1/2} = 10\text{--}66$  d (Tomlin 1994).

## 17.1.1.30 Dinoseb



Common Name: Dinoseb

Synonym: Anatox, Aretit, Basanite, Butaphene, Caldon, Chemox, Dibutox, Dinitrall, DNBP, DN-289, DNOSAP, DNOSBP, DNSBP, Dow General, Dyanap, Dytap

Chemical Name: 2-*sec*-butyl-4,6-dinitrophenol

Uses: herbicides/insecticides; pre- or post-emergence control of broadleaf weeds in cereals, maize, lucerne, clover, trefoil, grass leys, potatoes, peas, onions, garlics, peas, leeks, soya beans, orchards, groundnuts, strawberries, vineyards and other crops; for control of strawberry runners and raspberry suckers and overwintering forms of insect pests on fruit trees; also used as a desiccant for leguminous seed crops; destruction of potato haulms; as a pre-harvest hop defoliant, etc.

CAS Registry No: 88-85-7

Molecular Formula:  $C_{10}H_{12}N_2O_5$

Molecular Weight: 240.212

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

40 (Lide 2003)

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

362 (estimated, Grain 1982)

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

1.265 ( $45^{\circ}C$ , Hartley & Kidd 1987; Herbicide Handbook 1989; Milne 1995)

Molar Volume ( $cm^3/mol$ ):

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

Dissociation Constant  $pK_a$ :

4.62 (radiometer/pH meter, Cessna & Grover 1978; Hornsby et al. 1996)

4.61 (radiometer/pH meter, Cessna & Grover 1978)

4.62 (Worthing & Walker 1987, 1991)

4.50 (Yao & Haag 1991)

Enthalpy of Fusion,  $\Delta H_{fus}$  (kJ/mol):

Entropy of Fusion,  $\Delta S_{fus}$  (J/mol K):

Fugacity Ratio at  $25^{\circ}C$  (assuming  $\Delta S_{fus} = 56$  J/mol K), F: 0.713 (mp at  $40^{\circ}C$ )

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

50 (Günther 1968; Spencer 1982; Thomas 1982)

52 (Kearney & Kaufman 1975; Khan 1980)

50 (Martin & Worthing 1977; Kenaga 1980)

52 (Ashton & Crafts 1981; Herbicide Handbook 1989)

100 (rm. temp., Worthing & Walker 1983, Worthing & Hance 1991)

52 ( $20^{\circ}C$ , Hartley & Kidd 1987; Milne 1995)

52 ( $20$ – $25^{\circ}C$ , selected, Hornsby et al. 1996)

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

130 ( $151.5^{\circ}C$ , Khan 1980)

133 ( $151.1^{\circ}C$ , Ashton & Crafts 1981)

0.0008, 0.0067 (supercooled liquid, estimated, Grain 1982)

0.0067 (Thomas 1982)

0.0023 ( $30^{\circ}C$ , Spencer 1982)

10 ( $20^{\circ}C$ , selected, Suntio et al. 1988)

0.183 ( $60^{\circ}C$ , Worthing & Hance 1991)

0.0067 ( $20$ – $25^{\circ}C$ , selected, Hornsby et al. 1996)



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

51.1 (20°C, calculated-P/C, Suntio et al. 1988)

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

3.59 (Hansch & Leo 1979)  
 3.69 (calculated, Zitko et al. 1976)  
 3.69 (Hansch & Leo 1985)  
 4.10 (RP-PHLC-RT correlation, Klein et al. 1988)  
 3.14 (shake flask/slow stirring-GC, De Bruijn et al. 1989)  
 3.0, 3.57 (pH 7, pH 2, shake flask, Brooke et al. 1990)  
 3.69 (recommended, Sangster 1993)  
 3.56 (recommended, Hansch et al. 1995)

Bioconcentration Factor,  $\log \text{BCF}$ :

1.83 (calculated-S, Kenaga 1980a; quoted, Howard 1991)  
 0.778 (calculated- $K_{oc}$ , Kenaga 1980)  
 1.51 (measured, Kenaga 1980; quoted, Isensee 1991)

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

2.85 (soil, Thomas 1982)  
 2.09 (soil, Kenaga 1980a; Kenaga & Goring 1980)  
 2.71 (soil, calculated-S as per Kenaga & Goring 1980, Kenaga 1980a)  
 3.82 (HPLC- $k'$  correlation, cyanopropyl column, mobile phase buffered to pH 3, Hodson & Williams 1988)  
 2.68 (estimated as  $\log K_{om}$ , Magee 1991)  
 1.80, 2.04, 2.08 (soil, literature values, Bottoni & Funari 1992)  
 2.70 (selected, Lohninger 1994)  
 2.09 (soil, calculated-MCI  $^1\chi$ , Sabljic et al. 1995)  
 1.48 (soil, 20–25°C, estimated, Hornsby et al. 1996)

Adsorption coefficient,  $K_d$  ( $\text{L}\cdot\text{kg}^{-1}$ ):

6.4, 64 (homoionic  $\text{K}^+$ -kaolinite,  $\text{K}^+$ -montmorillonite clay minerals, Haderlein et al. 1996)

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

Volatilization: initial rate constant  $k = 1.1 \times 10^{-3} \text{ h}^{-1}$  and predicted rate constant  $k = 2.6 \times 10^{-3} \text{ h}^{-1}$  from soil with  $t_{1/2} = 266.5 \text{ h}$  (Thomas 1982).

Photolysis:

Oxidation:

photooxidation  $t_{1/2} = 12.2\text{--}122 \text{ h}$  in air, based on estimated rate constant for the reaction with hydroxyl radical in air (Atkinson 1987; quoted, Howard et al. 1991)

$k(\text{aq.}) = (0.003\text{--}2) \times 10^5 \text{ M}^{-1} \text{ s}^{-1}$  for direct reaction with ozone in water at pH 1.9–5.0 and  $24 \pm 1^\circ\text{C}$ , with  $t_{1/2} = 0.16 \text{ s}$  at pH 7 (Yao & Haag 1991).

$k(\text{calc}) = 4 \times 10^9 \text{ M}^{-1} \text{ s}^{-1}$  for the reaction with hydroxyl radical in aqueous solutions at  $24 \pm 1^\circ\text{C}$  (Haag & Yao 1992).

Hydrolysis:

Biodegradation: aqueous aerobic  $t_{1/2} = 1032\text{--}2952 \text{ h}$ , based on aerobic soil mineralization data for one soil (Doyle et al. 1978; quoted, Howard et al. 1991) and aqueous anaerobic  $t_{1/2} = 96\text{--}360 \text{ h}$ , based on anaerobic soil die-away test data for isopropalin (Gingerich & Zimdahl 1976; quoted, Howard et al. 1991).

Biotransformation:

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

Half-Lives in the Environment:

Air:  $t_{1/2} = 12.2\text{--}122 \text{ h}$ , based on estimated rate constant for the reaction with hydroxyl radical in air (Atkinson 1987; quoted, Howard et al. 1991).

Surface water:  $t_{1/2} = 1032\text{--}2952 \text{ h}$ , based on aerobic soil mineralization data for one soil (Doyle et al. 1978; quoted, Howard et al. 1991);

measured rate constant  $k = (0.003\text{--}2) \times 10^5 \text{ M}^{-1} \text{ s}^{-1}$  for direct reaction with ozone in water at pH 1.9–5.0 and  $24 \pm 1^\circ\text{C}$ , with  $t_{1/2} = 0.16 \text{ s}$  at pH 7 (Yao & Haag 1991).

Ground water:  $t_{1/2} = 96\text{--}5904 \text{ h}$ , based on estimated unacclimated aqueous aerobic and anaerobic biodegradation half-lives (Howard et al. 1991)

reported  $t_{1/2} = 30 \text{ d}$  (Bottoni & Funari 1992)

Sediment:

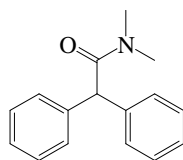
Soil:  $t_{1/2} = 1032\text{--}2952 \text{ h}$ , based on aerobic soil mineralization data for one soil (Doyle et al. 1978; quoted, Howard et al. 1991);

reported  $t_{1/2} = 30 \text{ d}$  (Bottoni & Funari 1992);

field  $t_{1/2} = 30 \text{ d}$  at  $20\text{--}25^\circ\text{C}$  (estimated, Hornsby et al. 1996).

Biota:

## 17.1.1.31 Diphenamid



Common Name: Diphenamid

Synonym: Difenamide, Dimid, Dymid, Enide, Fenam, Rideon

Chemical Name: *N,N*-dimethyldiphenylacetamide; *N,N*-dimethyl- $\alpha$ -phenyl-benzeneacetamide

Uses: herbicide for pre-emergence control of annual grasses and some broadleaf weeds in cotton, sweet potatoes, tomatoes, vegetables, capsicums, okra, soybeans, groundnuts, tobacco, pome fruit, stone fruit, citrus fruit, bush fruit, strawberries, forestry nurseries, and ornamental plants, shrubs, and trees.

CAS Registry No: 957-51-7

Molecular Formula:  $C_{16}H_{17}NO$

Molecular Weight: 239.312

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

135 (Lide 2003)

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

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

1.17 ( $23.3^{\circ}C$ , Hartley & Kidd 1987; Tomlin 1994; Milne 1995)

Molar Volume ( $cm^3/mol$ ):

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

Dissociation Constant  $pK_a$ :

Enthalpy of Fusion,  $\Delta H_{fus}$  ( $kJ/mol$ ):

27.405 (DSC method, Plato & Glasgow 1969)

Entropy of Fusion,  $\Delta S_{fus}$  ( $J/mol K$ ):

Fugacity Ratio at  $25^{\circ}C$  (assuming  $\Delta S_{fus} = 56 J/mol K$ ), F: 0.0833 (mp at  $135^{\circ}C$ )

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

240 (Melnikov 1971)

260 ( $27^{\circ}C$  Spencer 1973, 1982; Khan 1980; Worthing & Walker 1987)

260 (Martin & Worthing 1977; Weber et al. 1980; Kenaga 1980)

260 ( $27^{\circ}C$ , Hartley & Kidd 1987; Herbicide Handbook 1989; Tomlin 1994)

280 ( $20$ – $25^{\circ}C$ , selected, Hornsby et al. 1996)

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

$< 1.33 \times 10^{-4}$  (Weber et al. 1980)

negligible ( $20^{\circ}C$ , Hartley & Kidd 1987; Tomlin 1994)

$4.0 \times 10^{-6}$  ( $20$ – $25^{\circ}C$ , selected, Hornsby et al. 1996)

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

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

Bioconcentration Factor,  $\log BCF$ :

1.43 (calculated-S, Kenaga 1980)

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

2.32 (soil, calculated-S, Kenaga 1980)

2.32 (selected, Lohninger 1994)

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

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

Photolysis:  $t_{1/2} = 2.25$  h in distilled water (Tanaka et al. 1981; quoted, Cessna & Muir 1991);

Half-Lives in the Environment:

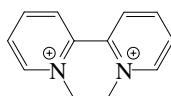
Soil: estimated persistence of 8 months (Kearney et al. 1969; Edwards 1973; quoted, Morrill et al. 1982; Jury et al. 1987);

persistence under warm damp conditions is ca. 3–6 months (Herbicide Handbook 1989; Tomlin 1994)

field  $t_{1/2} = 30$  d at 20–25°C (selected, Hornsby et al. 1996).

Biota:

## 17.1.1.32 Diquat



Common Name: Diquat

Synonym: Aquacide, Deiquat, Dextrone, Ortho, Pathclear, Preeglone, Reglone, Weedol, Weedtrine-D

Chemical Name: 1,1'-ethylene-2,2'-dipyridine

Uses: nonselective contact herbicide to control broadleaf weeds in fruit and vegetable crops.

CAS Registry No: 2764-72-9

Molecular Formula:  $C_{12}H_{14}N_2$

Molecular Weight: 186.236

Melting Point ( $^{\circ}C$ ): 335–340 (Spencer 1982)

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

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

1.22–1.27 (Ashton & Crafts 1981; Herbicide Handbook 1989; Montgomery 1993; Tomlin 1994)

Molar Volume ( $cm^3/mol$ ):

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

149.6 (calculated-density)

Dissociation Constant  $pK_a$ :

Enthalpy of Fusion,  $\Delta H_{fus}$  ( $kJ/mol$ ):

Entropy of Fusion,  $\Delta S_{fus}$  ( $J/mol\ K$ ):

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

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

700000 (Khan 1980; Spencer 1982)

670000 (Weber et al. 1980)

700000 (Verschuereen 1983)

700000 (Worthing & Hance 1991; Tomlin 1994)

700000 (Montgomery 1993)

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

< 0.00533 (Agrochemicals Handbook 1983)

<  $1.3 \times 10^{-5}$  (Worthing & Hance 1991; Tomlin 1994)

<  $1.3 \times 10^{-5}$  ( $20^{\circ}C$ , Montgomery 1993)

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

<  $6.38 \times 10^{-9}$  ( $20$ – $25^{\circ}C$ , calculated-P/C, Montgomery 1993)

<  $3.42 \times 10^{-9}$  (calculated-P/C, this work)

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

–3.05 (Garten & Trabalka 1983)

2.78 (Reinert 1989)

–4.60 ( $20^{\circ}C$ , Worthing & Hance 1991; Tomlin 1994)

–4.60 (Montgomery 1993)

Bioconcentration Factor,  $\log BCF$ :

–2.84 (calculated-S as per Kenaga 1980, this work)

–5.92 (calculated- $\log K_{ow}$  as per Mackay 1982, this work)

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

2.84 (Reinert 1989)

0.420 (calculated, Montgomery 1993)

0.425 (calculated-S as per Kenaga 1980, this work)

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

## Volatilization:

Photolysis:  $t_{1/2} = 192$  h for 10  $\mu\text{g/mL}$  to degrade in distilled water under 240–260 nm light (Funderburk et al. 1960; quoted, Cessna & Muir 1991);

$t_{1/2} < 5$  wk for 4  $\mu\text{g/mL}$  to degrade in distilled water under sunlight (Slade & Smith 1967; quoted, Cessna & Muir 1991);

dry diquat photodecomposed by UV light with  $t_{1/2} = 48$  h (Funderburk & Bozarth 1967; quoted, Montgomery 1993);

$t_{1/2} \sim 48$  h when associated with aerosols (Howard 1991);

$t_{1/2} = 3$  wk for 3% of 5  $\mu\text{g/mL}$  to degrade in distilled water under sunlight (Smith & Grove 1969; quoted, Cessna & Muir 1991).

## Oxidation:

$k(\text{aq.}) = 5.9 \times 10^9 \text{ M}^{-1} \text{ s}^{-1}$  for the reaction (Fenton with reference to acetophenone) with hydroxyl radical in aqueous solutions at pH 3.1 and at  $24 \pm 1^\circ\text{C}$  (Buxton et al. 1988; quoted, Faust & Hoigné 1990; Haag & Yao 1992)

$k(\text{aq.}) = (0.6 \pm 0.2) \text{ M}^{-1} \text{ s}^{-1}$  for direct reaction with ozone in water at pH 3.1 and  $22^\circ\text{C}$ , with a half-life of 15 h at pH 7 (Yao & Haag 1991).

$k(\text{aq.}) = (8.0 \pm 1.8) \times 10^8 \text{ M}^{-1} \text{ s}^{-1}$  for the reaction (Fenton with reference to acetophenone) with hydroxyl radical in aqueous solutions at pH 3.1 and at  $24 \pm 1^\circ\text{C}$  (Haag & Yao 1992).

Hydrolysis:  $t_{1/2} = 74$  d under simulated sunlight at pH 7 (Montgomery 1993; Tomlin 1994).

Biodegradation:  $t_{1/2} \sim 50$  d to biodegrade in lake water (Hiltibran 1972; quoted, Muir 1991);

$t_{1/2} > 158$  d for 1.5  $\mu\text{g/mL}$  of infested sediment-water microcosm to biodegrade in sediment and  $t_{1/2} \sim 2$  d in water both at  $25^\circ\text{C}$  (derived from Simsiman & Chesters 1976; Muir 1991).

## Biotransformation:

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

## Half-Lives in the Environment:

## Air:

Surface water:  $t_{1/2} \sim 50$  d to biodegrade in lake water (Hiltibran 1972; quoted, Muir 1991);

$t_{1/2} \sim 2$  d of  $^{14}\text{C}$ -diquat in water of a weed-infested simulated lake impoundment containing Lake Mendota sediment, the rapid disappearance is attributed to adsorption by sediments, suspended particulate matter and aquatic plants (shake flask-scintillation spectrometry, Simsiman & Chesters 1976)

measured rate constant  $k = (0.6 \pm 0.2) \text{ M}^{-1} \text{ s}^{-1}$  for direct reaction with ozone in water at pH 3.1 and  $22^\circ\text{C}$ , with  $t_{1/2} = 15$  h at pH 7 (Yao & Haag 1991).

## Ground water:

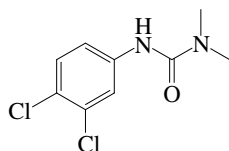
Sediment: Slow microbial degradation due to tight bonding of adsorbed Diquat to the clay minerals on the sediment (shake flask-liquid scintillation spectrometry, Simsiman & Chesters 1976)

$t_{1/2} > 158$  d for 1.5  $\mu\text{g/mL}$  of infested sediment-water microcosm to biodegrade (derived from results of Simsiman & Chesters 1976; Muir 1991).

## Soil:

## Biota:

## 17.1.1.33 Diuron



Common Name: Diuron

Synonym: AF 101, Cekiuron, Crisuron, Dailon, DCMU, Diater, dichlorofonidim, Di-on, Direx, DMU, Drexel, Duran, Dynex, Herbatox, Karmex, Marmer, NA 2767, Telvar, Unidron, Urox D, Vonduron

Chemical Name: 3-(3,4-dichlorophenyl)-1,1-dimethylurea; *N'*-(3,4-dichlorophenyl)-*N,N*-dimethylurea

Uses: pre-emergence herbicide in soils to control germinating broadleaf grasses and weeds in crops such as apples, cotton, grapes, pears, pineapple, and alfalfa; also used as sugar cane flowering depressant.

CAS Registry No: 330-54-1

Molecular Formula:  $C_9H_{10}Cl_2N_2O$

Molecular Weight: 233.093

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

158 (Lide 2003)

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

180 (decomposes, Montgomery 1993)

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

Molar Volume ( $cm^3/mol$ ):

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

188.0 (modified Le Bas method at normal boiling point, Spurlock & Biggar 1994a)

Dissociation Constant  $pK_a$ :

-1 to -2 (Montgomery 1993)

Enthalpy of Vaporization,  $\Delta H_v$  (kJ/mol):

66.0 (Rordorf 1989)

Enthalpy of Fusion,  $\Delta H_{fus}$  (kJ/mol):

33.89 (DSC method, Plato & Glasgow 1969)

27.3 (Rordorf 1989)

Entropy of Fusion,  $\Delta S_{fus}$  (J/mol K):

Fugacity Ratio at  $25^{\circ}C$  (assuming  $\Delta S_{fus} = 56$  J/mol K), F: 0.0496 (mp at  $158^{\circ}C$ )

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

42.0 (Günther et al. 1968; Melnikov 1971; Spencer 1973, 1982; Khan 1980; Ashton & Crafts 1981)

42.0 ( $20^{\circ}C$ , Weber 1972; Weber et al. 1980)

37.3 (shake flask-UV, Freed et al. 1976; Freed 1976)

42.0 (Martin & Worthing 1977; Hartley & Kidd 1987; Worthing & Walker 1987, Worthing & Hance 1991; Herbicide Handbook 1989; Tomlin 1994; Milne 1995)

42.4 (shake flask, Briggs 1981)

22.0 (shake flask-HPLC, Ellgehausen et al. 1981)

38.7 (generator column-HPLC/RI, Swann et al. 1983)

120 (RP-HPLC-RT correlation, Swann et al. 1983)

19.6, 40.1, 53.4 (4, 25,  $40^{\circ}C$ , shake flask-liquid scintillation spectrometer LSS, Madhun et al. 1986)

42.0 ( $20$ – $25^{\circ}C$ , selected, Wauchope et al. 1992; Hornsby et al. 1996)

40.0 ( $20^{\circ}C$ , Montgomery 1993)

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

$1.6 \times 10^{-5}$  (estimated, Nex & Swezey 1954)

$3.8 \times 10^{-6}$  ( $20^{\circ}C$ , Johnson & Julin 1974)

$4.1 \times 10^{-4}$  ( $50^{\circ}C$ , Khan 1980; Ashton & Crafts 1981)

$< 1.3 \times 10^{-4}$  ( $20$ – $25^{\circ}C$ , Weber et al. 1980)

$2.5 \times 10^{-4}$  (Thomas 1982)

- $2.1 \times 10^{-5}$  (Jury et al. 1983; quoted, Taylor & Glotfelty 1988; Taylor & Spencer 1990)
- $3.6 \times 10^{-4}$  (Jury et al. 1983; quoted, Howard 1991)
- $2.7 \times 10^{-4}$  (selected, Nkedi-Kizza et al. 1985)
- $4.1 \times 10^{-4}$  (50°C, Hartley & Kidd 1987; Worthing & Hance 1991; Herbicide Handbook 1989)
- $2.0 \times 10^{-4}$  (20°C, selected, Suntio et al. 1988)
- $5.30 \times 10^{-4}$ ,  $1.0 \times 10^{-2}$ , 0.130, 1.20, 79 (25, 50, 70, 100, 125°C, gas saturation-GC, Rordorf 1989)
- $\log (P_s/Pa) = 13.339 - 4953.8/(T/K)$ ; measured range 36.2–90.2°C (solid, gas saturation-GC, Rordorf 1989)
- $\log (P_L/Pa) = 9.800335 - 3445.24/(T/K)$ ; measured range not specified (liquid, gas saturation-GC, Rordorf 1989)
- $9.2 \times 10^{-6}$  (20–25°C, selected, Wauchope et al. 1992; Hornsby et al. 1996)
- $1.1 \times 10^{-6}$  (Tomlin 1994)

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

- $1.4 \times 10^{-4}$  (calculated-P/C, Jury et al. 1984, 1987a,b; Jury & Ghodrati 1989)
- $1.2 \times 10^{-4}$  (20°C, calculated-P/C, Suntio et al. 1988)
- $1.3 \times 10^{-4}$  (calculated-P/C, Taylor & Glotfelty 1988)
- 0.274 (calculated-P/C, Howard 1991)
- $2.1 \times 10^{-5}$  (20°C, calculated-P/C, Muir 1991)
- $1.5 \times 10^{-4}$  (20–25°C, calculated-P/C, Montgomery 1993)

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

- 2.60 (calculated-f const., Rekker 1977)
- 2.81 (Rao & Davidson 1980)
- 2.68 (shake flask-UV, Briggs 1981)
- 2.89 (shake flask-HPLC, Ellgehausen et al. 1981)
- 2.60 (Elgar 1983)
- 2.77 (Hansch & Leo 1985)
- 2.69, 2.65, 2.63 (4, 25, 40°C, shake flask-liquid scintillation spectrometer LSS, Madhun et al. 1986)
- 2.86 (shake flask, Mitsutake et al. 1986)
- 1.97–2.81 (Montgomery 1993)
- 2.78 (recommended, Sangster 1993)
- 2.45 (RP-HPLC-RT correlation, Sicbaldi & Finizio 1993)
- 2.80 (Aquasol Database 1994; quoted, Pinsuwan et al. 1995)
- 2.81 (shake flask, Spurlock & Biggar 1994a)
- $2.85 \pm 1.70$  (Tomlin 1994)
- 2.58, 2.73 (shake flask-UV, RP-HPLC- $k'$  correlation, Liu & Qian 1995)
- 2.68 (recommended, Hansch et al. 1995)
- 2.45 (RP-HPLC-RT correlation, Finizio et al. 1997)

Bioconcentration Factor,  $\log \text{BCF}$ :

- 1.40 (measured, Isensee 1976)
- 1.88 (calculated-S, Kenaga 1980)
- 1.34 (calculated- $K_{oc}$ , Kenaga 1980)
- 2.16 (*Pimephales promelas*, Call et al. 1987)
- 2.41, 2.48 (cuticle/water: tomato, pepper, Chaumat et al. 1991)
- 2.41, 2.51 (cuticle/water: box tree, laurel, Chaumat et al. 1991)
- 2.55, 2.28 (cuticle/water: pear, ivy, Chaumat et al. 1991)
- 1.18, 1.64 (cuticle/water: cleavers, vanilla, Chaumat et al. 1991)
- 2.45, 2.48 (cuticle/water: tomato, pepper, Evelyne et al. 1992)

Bioaccumulation Factor,  $\log \text{BF}$ :

- −1.70 (adipose tissue in both male & female Albino rats, Hodge et al. 1967)

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

- 2.60 (soil, Hamaker & Thompson 1972; Farmer 1976; Hance 1976)



- 2.75 (soil, calculated-S as per Kenaga & Goring 1977, Kenaga 1980)
- 2.59 (average of 3 soils, HPLC-RT correlation, McCall et al. 1980)
- 2.15–2.52 (Peck et al. 1980)
- 2.21 (soil, converted from reported  $K_{OM}$  multiplied 1.724, Briggs 1981)
- 3.06, 2.41 (estimated-S, solubility and mp, Karickhoff 1981)
- 1.58, 2.42 (estimated- $K_{OW}$ , Karickhoff 1981)
- 2.58 (average of 84 soils, Rao & Davidson 1982)
- 2.18 (soil, Thomas 1982)
- 2.83 (Webster soil, Nkedi-Kizza 1983)
- 2.49 (soil slurry method, Swann et al. 1983)
- 2.48 (RP-HPLC-RT correlation, Swann et al. 1983)
- 3.03, 2.94 (4°C, 25°C, Semiahmoo soil, batch equilibrium method-LSS, Madhun et al. 1986)
- 2.82, 2.68 (4°C, 25°C, Adkins soil, batch equilibrium method-LSS, Madhun et al. 1986)
- 2.86, 2.44, 2.48; 2.81, 2.74, 2.44 (estimated- $K_{OW}$ ; solubility, Madhun et al. 1986)
- 2.50 (calculated-MCI  $\chi$ , Gerstl & Helling 1987)
- 2.58 (soil, screening model calculations, Jury et al. 1987a,b; Jury & Ghodrati 1989)
- 2.35, 2.57 (2 subsurface soils from Oklahoma, Bouchard & Wood 1988)
- 2.94, 2.68 (mucky peat soil, loam sand soil, quoted, Howard 1991)
- 2.18, 2.48–2.49, 2.59, 2.66 (soil, quoted values, Bottoni & funari 1992)
- 2.68 (soil, 20–25°C, selected, Wauchope et al. 1992; Hornsby et al. 1996)
- 2.21–2.87 (Montgomery 1993)
- 2.68 (selected, Lohninger 1994)
- 2.60 (Tomlin 1994)
- 2.70 (calculated- $K_{OW}$ , Liu & Qian 1995)
- 2.40 (soil, calculated-MCI  $^1\chi$ , Sabljic et al. 1995)
- 3.07, 2.37, 2.82, 2.51, 2.96 (calculated- $K_{OW}$ ; HPLC-screening method with different LC-columns, Szabo et al. 1999)
- 2.48, 2.42 (soil, estimated-class-specific model, estimated-general model using molecular descriptors, Gramatica et al. 2000)
- 2.44, 2.43, 2.57 (soils: organic carbon  $OC \geq 0.1\%$ ,  $OC \geq 0.5\%$ ,  $0.1 \leq OC < 0.5\%$ , average, Delle Site 2001)
- 2.78<sup>c</sup> (sediment: organic carbon  $OC \geq 0.5\%$ , average, Delle Site 2001)

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

- Volatilization:  $2.5 \times 10^{-3} \text{ h}^{-1}$  (initial) and  $5.3 \times 10^{-4} \text{ h}^{-1}$  (predicted) from soil with  $t_{1/2} = 1307 \text{ h}$  (Thomas 1982); the calculated  $t_{1/2} = 1918 \text{ d}$  due to volatilization from soil when incorporated into 1 cm of soil (Jury et al. 1983; quoted, Howard 1991).
- Photolysis:  $t_{1/2} = 2.25 \text{ h}$  for 80–84% of 40  $\mu\text{g/mL}$  to degrade in distilled water under 300 nm light (Tanaka et al. 1981; quoted, Cessna & Muir 1991); in surface waters should be photolyzed within a few days (Howard 1991).
- Oxidation: photooxidation  $t_{1/2} = 0.12 \text{ d}$  in air, based on estimation for the vapor-phase reaction with hydroxyl radical in the atmosphere (Atkinson 1987; quoted, Howard 1991).
- Hydrolysis:  $t_{1/2} > 4$  months for 4660  $\mu\text{g/mL}$  to hydrolyze in phosphate buffer at pH 5–9 and 20°C (El-Dib & Aly 1976; quoted, Muir 1991).
- Biodegradation:  $t_{1/2} = 328 \text{ d}$  for a 100 d leaching and screening test in 0–10 cm depth of soil (Rao & Davidson 1980; quoted, Jury et al. 1983, 1984, 1987a);
- $t_{1/2} = 3\text{--}10 \text{ d}$  for 40  $\mu\text{g/mL}$  to biodegrade in pond sediment of anaerobic media at 30°C (Attaway et al. 1982a quoted, Muir 1991);
- $t_{1/2} < 17 \text{ d}$  for 40  $\mu\text{g/mL}$  to biodegrade in pond sediment at 30°C (Attaway et al. 1982b; quoted, Muir 1991);
- 67–99% will be degraded in 10 wk under aerobic conditions by mixed cultures isolated from pond water and sediments forming 6–7 products (Ellis & Camper 1982; quoted, Howard 1991; Muir 1991);
- $t_{1/2} < 70 \text{ d}$  at 30°C (Ellis & Camper 1982; quoted, Muir 1991; Montgomery 1993);
- $t_{1/2} \sim 5 \text{ d}$  for 0.22  $\mu\text{g/mL}$  to biodegrade in pond sediment of anaerobic media (Stepp et al. 1985; quoted, Muir 1991);
- $t_{1/2}(\text{aerobic}) \sim 20 \text{ d}$  for 0.0005–10  $\mu\text{g/mL}$  to biodegrade in filtered sewage water at 20°C (Wang et al. 1985; quoted, Muir 1991).

Biotransformation: ~ 7% of a selection of 90 strains of micromycetes mostly isolated from soil-soil fungi, depleted over 50% of diuron (20 mg/L) in 5-d experiment (Vroumsia et al. 1996)

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

#### Half-Lives in the Environment:

Air:  $t_{1/2}$  = 0.12 d, based on estimation for the vapor-phase reaction with hydroxyl radical in the atmosphere (Atkinson 1987; quoted, Howard 1991).

Surface water: should be photolyzed within a few days (Howard 1991).

Ground water: reported half-lives or persistence,  $t_{1/2}$  = 20–70, 90–180, 200, and 328 d (Bottoni & Funari 1992)

Sediment:  $t_{1/2}$  = 3–10 d for 40 µg/mL to biodegrade in pond sediment of anaerobic media at 30°C (Attaway et al. 1982a; quoted, Muir 1991);

$t_{1/2}$  < 17 d for 40 µg/mL to biodegrade in pond sediment at 30°C (Attaway et al. 1982b);

$t_{1/2}$  ~ 5 d for 0.22 µg/mL to biodegrade in pond sediment of anaerobic media (Stepp et al. 1985)

Soil: estimated persistence of 10 months in soil (Kearney et al. 1969; quoted, Jury et al. 1987);

persistence of 8 months in soil (Edwards 1973; quoted, Morrill et al. 1982);

$t_{1/2}$  = 7.0 months at 15°C and  $t_{1/2}$  = 5.5 months at 30°C in soils (Freed & Haque 1973);

persistence of 10 months (Wauchope 1978);

rate constant  $k$  = 0.0031 d<sup>-1</sup> with  $t_{1/2}$  = 328 d under field conditions (Rao & Davidson 1980);

calculated  $t_{1/2}$  = 1918 d due to volatilization from soil when incorporated into 1 cm of soil (Jury et al. 1983; quoted, Howard 1991);

$t_{1/2}$  ~ 200–4000 d in loamy sand and peat at 25–35°C as follows (Madhum & Freed 1987):

$t_{1/2}$  = 705, 414, and 225 d at 25, 30, and 35°C, respectively, at herbicide concn at 5 µg/kg, while  $t_{1/2}$  = 1392, 630, and 406 d at 25, 30, and 35°C, respectively, at herbicide concn at 100 µg/kg in an Adkins loamy sand; however, the half-lives were considerable higher in peat.  $t_{1/2}$  = 3991, 2164, and 1165 d at 25, 30, and 35°C, respectively, at herbicide concn at 5 µg/kg while  $t_{1/2}$  = 3416, 1832, and 896 d at 25, 30, and 35°C, respectively, at herbicide concn at 100 µg/kg in a Semiahoo mucky peat (Madhun & Freed 1987)

$t_{1/2}$  = 328 d from screening model calculations (Jury et al. 1987a,b; Jury & Ghodrati 1989);

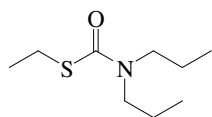
reported  $t_{1/2}$  = 20–70 d, 90–180 d, 200 d and 328 d (Bottoni & Funari 1992);

$t_{1/2}$  = 75–102 d in 0–40 cm soil cores taken, from cultivated field,  $t_{1/2}$  = 55–65 d from meadow and  $t_{1/2}$  = 29–35 d from gravel track (Hassink et al. 1994);

selected field  $t_{1/2}$  = 90 d (Wauchope et al. 1992; Hornsby et al. 1996).

Biota: biochemical  $t_{1/2}$  = 328 d from screening model calculations (Jury et al. 1987a,b; Jury & Ghodrati 1989).

## 17.1.1.34 EPTC



Common Name: EPTC

Synonym: Eptam, Eradicane, FDA 1541, R 1608, Torbin

Chemical Name: carbamic acid, dipropylthio-, *S*-ethyl ester; *S*-ethyldipropyl(thiocarbamate); *S*-ethyldipropylcarbamo-thioate

Uses: selective systemic herbicide for pre-emergence control of perennial and annual grasses, broadleaf weeds.

CAS Registry No: 759-94-4

Molecular Formula:  $C_9H_{19}NOS$

Molecular Weight: 189.318

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

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

235.0 (Khan 1980; Herbicide Handbook 1989)

127.0 (at 20 mmHg, Hartley & Kidd 1987; Budavari 1989; Worthing & Hance 1991; Montgomery 1993; Tomlin 1994; Milne 1995)

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

0.9546 ( $30^{\circ}C$ , Spencer 1982; Hartley & Kidd 1987; Montgomery 1993; Tomlin 1994; Milne 1995)

0.960 ( $25^{\circ}C$ , Herbicide Handbook 1989; Montgomery 1993)

Molar Volume ( $cm^3/mol$ ):

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

Dissociation Constant  $pK_a$ :

Enthalpy of Fusion,  $\Delta H_{fus}$  (kJ/mol):

Entropy of Fusion,  $\Delta S_{fus}$  (J/mol K):

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

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

375 (shake flask-GC, Freed et al. 1967)

365 (Martin & Worthing 1977)

370 ( $20^{\circ}C$ , Khan 1980; Ashton & Crafts 1981; Herbicide Handbook 1989)

370–375 (Weber et al. 1980)

375 ( $20^{\circ}C$ , Spencer 1982)

370 (Beste & Humburg 1983; Jury et al. 1983, 1984)

375 (Hartley & Kidd 1987; Montgomery 1993; Tomlin 1994)

375 ( $24^{\circ}C$ , Worthing & Walker 1987, Worthing & Hance 1991)

365 ( $20^{\circ}C$ , Budavari 1989; Milne 1995)

344 ( $20$ – $25^{\circ}C$ , selected, Wauchope et al. 1992; Hornsby et al. 1996; Lohninger 1994)

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

4.666 (extrapolated, Patchett et al. 1964)

20.66 (Bailey & White 1965)

1.84 ( $20^{\circ}C$ , effusion method, Hamaker & Kerlinger 1971)

2.16, 2.63, 3.69, 8.266 (23, 24, 28,  $40^{\circ}C$ , Hamaker 1972)

4.532 (Khan 1980; Ashton & Crafts 1981; Herbicide Handbook 1989)

2.62 ( $20^{\circ}C$ , volatilization rate, Burkhard & Guth 1981)

2.80 (Patchett et al. 1983)

0.612 ( $20^{\circ}C$ , GC-RT correlation, Kim 1985)

4.70 (Hartley & Kidd 1987)

2.00 ( $20^{\circ}C$ , selected, Suntio et al. 1988)

4.532 ( $35^{\circ}C$ , Budavari 1989)

4.50 (Worthing & Hance 1991)

- 4.532 (20–25°C, selected, Wauchope et al. 1992; Hornsby et al. 1996)  
 4.532 (20°C, Montgomery 1993)  
 0.00001 (Tomlin 1994)

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

- 1.32 (20°C, volatilization rate, Burkhard & Guth 1981)  
 1.463 (calculated-P/C, Jury et al. 1983, 1984, 1987a,b; Jury & Ghodrati 1989)  
 1.02 (20°C, calculated-P/C, Suntio et al. 1988)  
 1.463 (calculated-P/C, Taylor & Glotfelty 1988)  
 1.013 (20–25°C, calculated-P/C, Montgomery 1993)  
 1.023 (calculated-P/C, this work)

Octanol/Water Partition Coefficient, log K<sub>OW</sub>:

- 1.76 (selected, Dao et al. 1983)  
 3.21 (shake flask, Log P Database, Hansch & Leo 1987)  
 3.20 (Worthing & Hance 1991; Montgomery 1993; Tomlin 1994; Milne 1995)  
 3.21 (recommended, Sangster 1993)  
 3.21 (recommended, Hansch et al. 1995)  
 3.45 (RP-HPLC-RT correlation, Finizio et al. 1997)

Bioconcentration Factor, log BCF:

- 1.34 (calculated-S, Kenaga 1980; quoted, Isensee 1991)  
 1.08 (calculated-K<sub>OC</sub>, Kenaga 1980)

Sorption Partition Coefficient, log K<sub>OC</sub>:

- 2.38 (soil, Hamaker & Thompson 1972)  
 2.45 (soil, Hamaker & Thompson 1972)  
 2.23 (soil, calculated-S as per Kenaga & Goring 1980, Kenaga 1980)  
 2.58 (soil, screening model calculations, Jury et al. 1987a,b; Jury & Ghodrati 1989)  
 2.23–2.38, 2.45 (quoted values, Bottoni & Funari 1992)  
 2.30 (soil, 20–25°C, selected, Wauchope et al. 1992)  
 2.38 (Montgomery 1993)  
 2.30 (selected, Lohninger 1994)  
 2.45 (selected, Wienhold & Gish 1994)  
 2.38 (soil, calculated-MCI <sup>1</sup>χ, Sabljic et al. 1995)  
 2.23, 1.98 (soil, estimated-class specific model, estimated-general model using molecular descriptors, Gramatica et al. 2000)  
 2.03, 2.00 (soils: organic carbon OC ≥ 0.1%, OC ≥ 0.5%, average, Delle Site 2001)

Environmental Fate Rate Constants, k, or Half-Lives, t<sub>1/2</sub>:

Volatilization: t<sub>1/2</sub> = 3.7 d (Jury et al. 1983).

Photolysis: rate constant k = 5.2 × 10<sup>-3</sup> s<sup>-1</sup> for a light intensity corresponding to a 12-h average NO<sub>2</sub> photolysis rate with a black lamp spectral distribution (Kwok et al. 1992);

photodegradation t<sub>1/2</sub> = 14.0 and 18.5 min in water solution under irradiation with UV light at 254 nm (Abu-Qare & Duncan 2002).

Oxidation: second order rate constants k<sub>OH</sub> = (3.10–3.40) × 10<sup>-11</sup> cm<sup>3</sup> molecule<sup>-1</sup> s<sup>-1</sup> for gas-phase reaction with OH radical, k<sub>NO<sub>3</sub></sub> = 0.92 × 10<sup>-14</sup> cm<sup>3</sup> molecule<sup>-1</sup> s<sup>-1</sup> with NO<sub>3</sub> radical and k<sub>O<sub>3</sub></sub> < 1.3 × 10<sup>-19</sup> cm<sup>3</sup> molecule<sup>-1</sup> s<sup>-1</sup> with O<sub>3</sub> at 298 K (Kwok et al. 1992);

calculated lifetime of 6 h for the vapor-phase reaction with OH radical in the troposphere (Atkinson et al. 1992; Kwok et al. 1992).

Hydrolysis:

Biodegradation: t<sub>1/2</sub> = 30 d for a 100 d leaching and screening test in 0–10 cm depth of soil (Nash 1980; quoted, Jury et al. 1983, 1984, 1987a; quoted, Grover 1991).

Biotransformation:

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

Half-Lives in the Environment:

Air: calculated tropospheric lifetimes are: > 8 h due to photolysis, 5.8 d due to reaction with OH radical, 5.0 d with  $\text{NO}_3$  radical and > 125 d with  $\text{O}_3$  (Kwok et al. 1992);

calculated lifetime of 6 h for the vapor-phase reaction with OH radical in the troposphere (Atkinson et al. 1992; Kwok et al. 1992).

Surface water:  $t_{1/2} = 14.0$  and 18 min for elimination in water under irradiation with UV light at 254 nm (Abu-Qare & Duncan 2002).

Ground water: reported half-lives or persistence,  $t_{1/2} = 7$  and 30 d (Bottoni & Funari 1992)

Sediment:

Soil: estimated persistence of 4 months in soil (Kearney et al. 1969; quoted, Jury et al. 1987a);

$t_{1/2} = 30$  d from screening model calculations (Jury et al. 1987a,b; Jury & Ghodrati 1989);

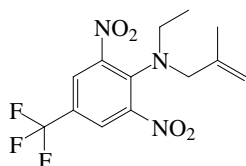
$t_{1/2} \sim 1$  wk in moist loam soil at 21 to 27°C (Herbicide Handbook 1974, 1989);

reported  $t_{1/2} = 7, 30$  d (Bottoni & Funari 1992);

selected field  $t_{1/2} = 6$  d (Wauchope et al. 1992; quoted, Richards & Baker 1993; Hornsby et al. 1996).

Biota: biochemical  $t_{1/2} = 30$  d from screening model calculations (Jury et al. 1987a,b; Jury & Ghodrati 1989)

## 17.1.1.35 Ethalfluralin



Common Name: Ethalfluralin

Synonym: Benzenamine, Somilan, Sonalan, Sonalen

Chemical Name: *N*-ethyl-*N*-(2-methyl-2-propenyl)-2,6-dinitro-(trifluoromethyl)-benzenamine

CAS Registry No: 55283-68-6

Uses: herbicide

Molecular Formula:  $C_{13}H_{14}F_3N_3O_4$

Molecular Weight: 333.263

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

57 (Lide 2003)

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

256 (decomposes, Hartley & Kidd 1987; Tomlin 1994; Milne 1995)

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

1.32 (Ashton & Crafts 1981; Herbicide Handbook 1989)

Molar Volume ( $cm^3/mol$ ):

Dissociation Constant  $pK_a$ :

Enthalpy of Fusion,  $\Delta H_{fus}$  ( $kJ/mol$ ):

Entropy of Fusion,  $\Delta S_{fus}$  ( $J/mol K$ ):

Fugacity Ratio at  $25^{\circ}C$  (assuming  $\Delta S_{fus} = 56 J/mol K$ ),  $F$ : 0.485 (mp at  $57^{\circ}C$ )

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

0.21 (Ashton & Crafts 1981)

0.20 (pH 7, Spencer; Hartley & Kidd 1987; Worthing & Walker 1987)

0.30 (pH 7, Herbicide Handbook 1989)

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

0.30 (pH 7, Tomlin 1994; Milne 1995)

0.40 (Majewski & Capel 1995)

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

$1.10 \times 10^{-4}$  (Worthing & Walker 1983, 1987; Hartley & Kidd 1987)

0.0109 (Spencer 1982; Herbicide Handbook 1989)

0.0117 (selected, Wauchope et al. 1992; Hornsby et al. 1996)

0.0117 (Tomlin 1994)

$2.22 \times 10^{-4}$  ( $20$ – $25^{\circ}C$ , Majewski & Capel 1995)

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

0.183 (calculated-P/C, Majewski & Capel 1995)

13 (calculated-P/C, Wolt 1997)

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

5.11 (pH 7, Tomlin 1994; Milne 1995)

4.92 (quoted values; selected, Wolt 1997)

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

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

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

- 3.60 (selected, soil, Wauchope et al. 1992; Hornsby et al. 1996)
- 3.60–3.90 (soil, Tomlin 1994)
- 3.61–3.92 (soil, Wolt 1997)

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

## Volatilization:

Photolysis:  $t_{1/2} = 6.3$  h in aqueous phase and  $t_{1/2} = 2$  h in vapor phase (Tomlin 1994);

Aqueous photolysis  $t_{1/2} = 6.3$  h in pH 5 sterile buffer solution; soil photolysis  $t_{1/2} = 14.2$  d in air-dry sandy loam soil when exposed to a xenon light source; air photolysis  $t_{1/2} = 2$  h when exposed to a light source simulating summer sunlight at 34°C (Wolt 1997).

## Oxidation:

Hydrolysis: no hydrolysis after 33 d at pH 3, 6 and 9 (51°C, Tomlin 1994); stable in sterile, buffered solutions across a range of pH (Wolt 1997).

## Biodegradation:

Biotransformation:  $t_{1/2} = 45$  d for aerobic metabolism in sandy loam soils and  $t_{1/2} = 14$  d for more rapid metabolism anaerobically in the same soil (quoted, Tomlin 1994; Wolt 1997).

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

## Half-Lives in the Environment:

Air: air photolysis  $t_{1/2} = 2$  h when exposed to a light source simulating summer sunlight at 34°C (Wolt 1997).

Surface water: water photolysis  $t_{1/2} = 6.3$  h in pH 5 sterile buffer solution;  $t_{1/2} = 2$  d for dissipation from the water column in a pond water-sediment system under outdoor conditions (Wolt 1997).

## Ground water:

Sediment:  $t_{1/2} = 38$  h in anaerobic pond water sediment system (Wolt 1997).

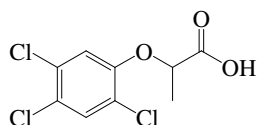
Soil: reported field  $t_{1/2} = 30$ –60 d, 60 d, 25–46 d; recommended  $t_{1/2} = 60$  d (Wauchope et al. 1992; Hornsby et al. 1996);

$t_{1/2} = 45$  d for aerobic metabolism in sandy loam soils and  $t_{1/2} = 14$  d for more rapid metabolism anaerobically in the same soil (Tomlin 1994);

terrestrial field dissipation  $t_{1/2} = 4$ –146 d,  $t_{1/2} = 45$  d in moist aerobic soil,  $t_{1/2} = 14$  d in anaerobic soil shifted to anaerobic conditions (Wolt 1997).

## Biota:

## 17.1.1.36 Fenoprop



Common Name: Fenoprop

Synonym: Silvex, 2,4,5-TP, Kuron, Kurosal, Fruitone T

Chemical Name: 2-(2,4,5-trichlorophenoxy) propionic acid

CAS Registry No: 93-72-1

Uses: herbicide/growth regulator

Molecular Formula:  $C_9H_7Cl_3O_3$

Molecular Weight: 269.509

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

181.6 (Lide 2003)

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

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

Molar Volume ( $cm^3/mol$ ):

Dissociation Constant  $pK_a$ :

2.84 (Worthing 1983, 1987; Augustijn-Beckers et al. 1994)

Enthalpy of Vaporization,  $\Delta H_v$  (kJ/mol):

75.75 (Rordorf 1989)

Enthalpy of Fusion,  $\Delta H_{fus}$  (kJ/mol):

44.6 (Rordorf 1989)

Entropy of Fusion,  $\Delta S_{fus}$  (J/mol K):

Fugacity Ratio at  $25^{\circ}C$  (assuming  $\Delta S_{fus} = 56$  J/mol K), F: 0.0291 (mp at  $181.6^{\circ}C$ )

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

140 (Kenaga & Goring 1980, Kenaga 1980a,b, Spencer 1982)

140 (Worthing & Walker 1983, 1987; Budavari 1989)

200 (Verschuere 1983)

176 (Hartley & Kidd 1987)

12.0 (calculated-MCI  $\chi$ , Patil 1994)

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

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

$2.30 \times 10^{-3}$ ,  $4.40 \times 10^{-2}$ , 0.55, 4.90, 34.0 ( $25$ ,  $50$ ,  $70$ ,  $100$ ,  $125^{\circ}C$ , gas saturation-GC, Rordorf 1989)

$\log(P_s/Pa) = 13.953 - 4948/(T/K)$ ; measured range  $85.4$ – $181^{\circ}C$  (gas saturation-GC, Rordorf 1989)

$\log(P_l/Pa) = 11.727 - 3956.9/(T/K)$ ; measured range  $181$ – $211^{\circ}C$  (gas saturation-GC, Rordorf 1989)

$< 1.33 \times 10^{-6}$  (estimated, Augustijn-Beckers et al. 1994; Hornsby et al. 1996)

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

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

2.44 (Kenaga 1980a)

3.86 (estimated, Garten & Trabalka 1983)

3.13 (counter-current chromatography, Ilchmann et al. 1993)

2.75 (calculated-MCI  $\chi$ , Patil 1994)

3.80 (selected, Hansch et al. 1995)

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

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

1.76 (calculated, Kenaga 1980a)

1.58, 2.23 (calculated-solubility,  $K_{ow}$ , Kenaga 1980b)



- 1.76 (fish, flowing water, Garten & Grabalka 1983)  
2.35 (Isensee 1991)

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

- 3.41 (soil, Kenaga & Goring 1980)  
2.46 (calculated- $K_{OW}$ , Kenaga 1980b)  
1.91 (soil: calculated-MCI  $\chi$ , Meylan et al. 1992)  
2.48 (soil, selected, Augustijn-Beckers et al. 1994; Hornsby et al. 1996)  
3.28 (soil, calculated-MCI  $\chi$ , Sabljic et al. 1995)

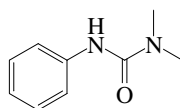
Environmental Fate Rate Constants, k, or Half-Lives,  $t_{1/2}$ :

Biodegradation:  $t_{1/2} > 205$  d for ring cleavage in soil suspensions (Verschueren 1983)

Half-Lives in the Environment:

Soil: persistence 47–205 d in soil (Alexander et al. 1961)  
degradation  $t_{1/2} = 21$  d and 14 d in Quachita Highlands' forest and grassland soil respectively,  $t_{1/2} = 15$  d in  
gross timbers forest soil, average  $t_{1/2} = 17$  d in 3 soils (Altom & Stritzke 1973);  
 $t_{1/2} = 5$ –11 d in a microagroecosystem study (Nash 1983);  
 $t_{1/2} > 205$  d for ring cleavage in soil suspensions (Verschueren 1983);  
field  $t_{1/2} = 21$  d (Augustijn-Beckers et al. 1994; Hornsby et al. 1996)

## 17.1.1.37 Fenuron



Common Name: Fenuron

Synonym: Dozer, Dybar, Falisilvan, Fenidim, Fenulon, Urab

Chemical Name: 1,1-dimethyl-3-phenylurea; *N,N*-dimethyl-*N'*-phenylurea

Uses: herbicide to control woody plants and deep-rooted perennial weeds, often used in combination with chlorpropham to extend its weed control spectrum and range of crops.

CAS Registry No: 101-42-8

Molecular Formula:  $C_9H_{12}N_2O$

Molecular Weight: 164.203

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

132 (Lide 2003)

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

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

1.13 ( $25^{\circ}C$ , Hartley & Kidd 1987)

1.08 (Worthing & Hance 1991; Tomlin 1994)

Molar Volume ( $cm^3/mol$ ):

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

159.0 (modified Le Bas method, Spurlock & Biggar 1994a)

Dissociation Constant  $pK_a$ :

Enthalpy of Fusion,  $\Delta H_{fus}$  (kJ/mol):

24.267 (DSC method, Plato & Glasgow 1969)

Entropy of Fusion,  $\Delta S_{fus}$  (J/mol K):

Fugacity Ratio at  $25^{\circ}C$  (assuming  $\Delta S_{fus} = 56$  J/mol K), F: 0.0892 (mp at  $132^{\circ}C$ )

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

2600 (Freed 1966)

2400 (Günther et al. 1968)

3850 (Martin & Worthing 1977; Kenaga 1980; Kenaga & Goring 1980; Verschueren 1983)

3850 (Khan 1980; Weber et al. 1980; Ashton & Crafts 1981; Willis & McDowell 1982)

3700 (shake flask-HPLC, Ellgehausen et al. 1981)

3850 (Hartley & Kidd 1987; Worthing & Walker 1987; Worthing & Hance 1991; Tomlin 1994)

3000 ( $20^{\circ}C$ , selected, Suntio et al. 1988)

3900 (Spurlock 1992; Spurlock & Biggar 1994b)

3850 ( $20$ – $25^{\circ}C$ , selected, Augustijn-Beckers et al. 1994; Hornsby et al. 1996)

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

0.0213 ( $60^{\circ}C$ , Khan 1980; Verschueren 1983)

0.0210 ( $60^{\circ}C$ , Hartley & Kidd 1987)

0.0050 ( $20^{\circ}C$ , selected, Suntio et al. 1988)

0.0210 ( $60^{\circ}C$ , Worthing & Hance 1991; Tomlin 1994)

0.0267 ( $20$ – $25^{\circ}C$ , selected, Augustijn-Beckers et al. 1994; Hornsby et al. 1996)

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

0.00027 ( $20^{\circ}C$ , calculated-P/C, Suntio et al. 1988)

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

0.98 (shake flask-UV, Hansch & Anderson 1967)

1.00 (Leo et al. 1971)

1.00 (shake flask-UV, Lord et al. 1980)

0.96	(shake flask-UV, Briggs 1981; Karickhoff 1981)
0.88	(shake flask-HPLC, Ellgehausen et al. 1981)
0.62	(HPLC- $k'$ correlation, McDuffie 1981)
0.70	(Elgar 1983)
1.18	(RP-HPLC- $k'$ correlation, Braumann et al. 1983)
1.00	(shake flask-HPLC, Spurlock & Biggar 1994a)
0.98	(recommended, Sangster 1993)
1.18	(RP-HPLC-RT correlation, Sicbaldi & Finizio 1993)
0.98	(recommended, Hansch et al. 1995)
1.18	(RP-HPLC-RT correlation, Finizio et al. 1997)

#### Bioconcentration Factor, log BCF:

0.778	(calculated-S, Kenaga 1980)
0.0	(calculated- $K_{OC}$ , Kenaga 1980)
1.34	(earthworms, Lord et al. 1980)
0.699, 0.602	(cuticle/water: tomato, pepper, Evelyne et al. 1992)

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

1.43	(soil, Hamaker & Thompson 1972)
1.67	(soil, calculated-S as per Kenaga & Goring 1980, Kenaga 1980)
0.88	(reported as log $K_{OM}$ , Briggs 1981)
0.61	(estimated- $K_{OW}$ , Karickhoff 1981)
1.80, 1.86	(estimated-S, Karickhoff 1981)
0.72, 0.84	(estimated-S and mp, Karickhoff 1981)
1.74	(calculated-MCI $\chi$ , Gerstl & Helling 1987)
1.62	(20–25°C, selected, Augustijn-Beckers et al. 1994; Hornsby et al. 1996)
1.40	(soil, calculated-MCI $^1\chi$ , Sabljic et al. 1995)
1.40; 1.40, 1.70	(soil, quoted obs.; estimated-class-specific model, estimated-general model using molecular descriptors, Gramatica et al. 2000)
1.42, 1.41	(soils: organic carbon OC $\geq$ 0.1%, OC $\geq$ 0.5%, average, Delle Site 2001)

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

Biodegradation: aerobic  $t_{1/2} \geq 10$  d for 0.01  $\mu\text{g/mL}$  to biodegrade in river water (Eichelberger & Lichtenberg 1971; quoted, Muir 1991).

#### Half-Lives in the Environment:

##### Air:

Surface water: aerobic  $t_{1/2} \geq 10$  d for 0.01  $\mu\text{g/mL}$  to biodegrade in river water (Eichelberger & Lichtenberg 1971; quoted, Muir 1991);  
persistence of up to 4 weeks in river water (Eichelberger & Lichtenberg 1971).

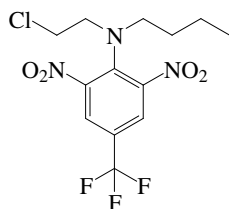
##### Ground water:

##### Sediment:

Soil:  $t_{1/2} = 4.5$  months at 15°C and 2.2 months at 30°C in soils (Freed & Haque 1973);  
persistence of 8 months in soil (Edwards 1973; quoted, Morrill et al. 1982);  
selected field  $t_{1/2} = 60$  d (Augustijn-Beckers et al. 1994; Hornsby et al. 1996).

##### Biota:

## 17.1.1.38 Fluchloralin



Common Name: Fluchloralin

Synonym: BAS-392H, Basalin

Chemical Name: *N*-(2-chloroethyl)-2,6-dinitro-*N*-propyl-4-(trifluoromethyl)benzenamine; *N*-(2-chloroethyl) $\alpha,\alpha,\alpha$ -trifluoro-2,6-dinitro-*N*-propyl-*p*-toluidine

Uses: herbicide for pre-plant or pre-emergence control of annual grass and broadleaf weeds in cotton, groundnuts, jute, potatoes, rice soybeans, and sunflowers, etc.

CAS Registry No: 33245-39-5

Molecular Formula:  $C_{12}H_{13}ClF_3N_3O_4$

Molecular Weight: 355.697

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

42 (Lide 2003)

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

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

Molar Volume ( $cm^3/mol$ ):

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

Dissociation Constant  $pK_a$ :

Enthalpy of Fusion,  $\Delta H_{fus}$  (kJ/mol):

Entropy of Fusion,  $\Delta S_{fus}$  (J/mol K):

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

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

1.00	( $20^{\circ}C$ , Weber 1972; Ashton & Crafts 1981)
1.00	(Edwards 1977)
< 1.0	(Martin & Worthing 1977; Herbicide Handbook 1978, 1989)
0.70	( $20^{\circ}C$ , Spencer 1982)
< 1.0	(Worthing & Walker 1987, 1991; Tomlin 1994)
10	(Budavari 1989; Milne 1995)
0.90	( $20$ – $25^{\circ}C$ , selected, Augustijn-Beckers et al. 1994; Hornsby et al. 1996)
0.50	(selected, Lohninger 1994)

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

0.0033	( $20^{\circ}C$ , Weber 1972; Worthing & Walker 1987)
0.373	( $20^{\circ}C$ , Ashton & Crafts 1981)
0.0008, 0.0033, 0.0133, 0.533	( $20, 30, 40, 50^{\circ}C$ , gas saturation, Spencer 1982)
0.0035	(Herbicide Handbook 1983; quoted, Nash 1988)
0.0037, 0.0033	( $20^{\circ}C, 30^{\circ}C$ , Herbicide Handbook 1989)
0.004	( $20^{\circ}C$ , Worthing & Hance 1991; Tomlin 1994)
0.004	( $20$ – $25^{\circ}C$ , selected, Augustijn-Beckers et al. 1994; Hornsby et al. 1996)

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

1.174	( $20^{\circ}C$ , calculated-P/C, Muir 1991)
1.343	calculated-P/C, this work)

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

4.63	(selected, Magee 1991)
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4.70 (CLOGPSTAR or CLOGP data, Sabljic et al. 1995)

Bioconcentration Factor, log BCF:

> 2.79, 2.40 (calculated-S, calculated- $K_{OC}$ , Kenaga 1980)

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

3.56 (soil, Harvey 1974)

3.60 (soil, Kenaga 1980)

> 3.64 (soil, calculated-S as per Kenaga & Goring 1980, Kenaga 1980)

4.25 (calculated-MCI  $\chi$ , Bahnick & Doucette 1988)

3.56; 3.58 (reported as log  $K_{OM}$ , estimated as log  $K_{OM}$ , Magee 1991)

3.48 (20–25°C, estimated, Augustijn-Beckers et al. 1994; Hornsby et al. 1996)

3.80 (estimated-chemical structure, Lohninger 1994)

3.55 (soil, calculated-MCI  $\chi$ , Sabljic et al. 1995)

3.55; 4.02 (soil, quoted obs.; estimated-general model using molecular descriptors, Gramatica et al. 2000)

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

Volatilization: estimated  $t_{1/2} \sim 1$  d from 1 m depth of water (20°C, Muir 1991).

Photolysis:  $t_{1/2} = 13$  d for 84% of 5  $\mu\text{g/mL}$  to degrade in distilled water under sunlight (Nilles & Zabik 1974; quoted, Cessna & Muir 1991);

$t_{1/2} = 8$  h for 50% of 2000  $\mu\text{g/mL}$  to degrade in methanol under sunlight (Plimmer & Klingebiel 1974; quoted, Cessna & Muir 1991).

Oxidation:

Hydrolysis:

Biodegradation:  $t_{1/2} = 8$  d for 0.5  $\mu\text{g/mL}$  to biodegrade in soil at 20–42°C (Savage 1978; quoted, Muir 1991);

$t_{1/2} = 3.6$  wk for 2.0  $\mu\text{g/mL}$  to biodegrade in soil at 25°C (Brewer et al. 1982; quoted, Muir 1991).

Biotransformation:

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

Half-Lives in the Environment:

Soil:  $t_{1/2} = 8$  d for 0.5  $\mu\text{g/mL}$  to biodegrade in soil at 20–42°C (Savage 1978; quoted, Muir 1991);

$t_{1/2} = 1.5$  d on Bosket silt loam,  $t_{1/2} = 4$  d on Sharkey clay for the first 3 to 5 days when sprayed onto soil surface, rate of loss much slower for the remainder of the 7- or 12-d sampling period with  $t_{1/2} = 13$  d on Bosket silt loam,  $t_{1/2} = 8$  d on Sharkey clay (Savage & Jordon 1980)

measured dissipation rate  $k = 0.099\text{--}0.13$   $\text{d}^{-1}$  (derived from Savage & Jordan 1980, Nash 1988);

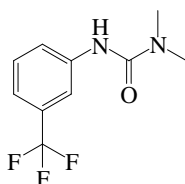
field studies,  $t_{1/2} = 12.2$  wk - 1978 first study;  $t_{1/2} = 13.0$  wk -1978 second study;  $t_{1/2} = 17.6$  wk -1979, in a Crowley silt loam at Stuttgart, Arkansas (Brewer et al. 1982)

Laboratory studies:  $t_{1/2} = 28.7$  wk at 4°C, 10.5 wk at 25°C for soils of field capacity moisture (27% w/w for Crowley silt loam) and  $t_{1/2} = 20.8$  wk at 4°C,  $t_{1/2} = 8.4$  wk at 25°C for flooded soil of Crowley silt loam;  $t_{1/2} = 29.3$  wk at 4°C,  $t_{1/2} = 10.5$  wk at 25°C for soil of field capacity moisture (34% w/w for Sharkey silty clay) and  $t_{1/2} = 20.8$  wk at 4°C and  $t_{1/2} = 4.3$  wk at 25°C for flooded soil, Sharkey silty clay (Brewer et al. 1982);

$t_{1/2} = 3.6$  wk for 2.0  $\mu\text{g/mL}$  to biodegrade in soil at 25°C (derived from Brewer et al. 1982, Muir 1991); estimated dissipation rate  $k = 0.29$ , and  $0.120$   $\text{d}^{-1}$  (Nash 1988);

estimated field  $t_{1/2} \sim 60$  d (Augustijn-Beckers et al. 1994; Hornsby et al. 1996).

## 17.1.1.39 Fluometuron



Common Name: Fluometuron

Synonym: CIBA 2059, Cotoran, Cottonex, Higalcoton, Lanex, Meturon, Pakhtaran

Chemical Name: 1,1-dimethyl-3-( $\alpha,\alpha,\alpha$ -trifluoro-*m*-tolyl)urea; N,N-dimethyl-N'-[3-(trifluoromethyl)phenyl]urea

Uses: herbicide to control many annual broadleaf weeds in sugar cane and cotton.

CAS Registry No: 2164-17-2

Molecular Formula:  $C_{10}H_{11}F_3N_2O$

Molecular Weight: 232.201

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

163–164.5 (Hartley & Kidd 1987; Herbicide Handbook 1989; Worthing & Hance 1991; Montgomery 1993; Tomlin 1994; Milne 1995)

164 (Lide 2003)

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

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

1.390 (Hartley & Kidd 1987; Worthing & Hance 1991; Montgomery 1993; Tomlin 1994; Milne 1995)

Molar Volume ( $cm^3/mol$ ):

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

167.1 (calculated-density)

Dissociation Constant  $pK_a$ :

–1.00 (Sangster 1993)

Enthalpy of Fusion,  $\Delta H_{fus}$  ( $kJ/mol$ ):

29.706 (DSC method, Plato 1972)

Entropy of Fusion,  $\Delta S_{fus}$  ( $J/mol K$ ):

Fugacity Ratio at  $25^{\circ}C$  (assuming  $\Delta S_{fus} = 56 J/mol K$ ), F: 0.0433 (mp at  $164^{\circ}C$ )

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

90 (Melnikov 1971; Spencer 1973, 1982; quoted, Wauchope 1978; Khan 1980; Weber et al. 1980)

90 ( $20^{\circ}C$ , Martin & Worthing 1977; Herbicide Handbook 1978,89)

106 (shake flask-UV, Briggs 1981)

90 (Herbicide Handbook 1983)

105 ( $20^{\circ}C$ , Hartley & Kidd 1987; Worthing & Walker 1987, 1991)

110 ( $20$ – $25^{\circ}C$ , selected, Wauchope et al. 1992; Hornsby et al. 1996)

80 (Montgomery 1993)

110 (Tomlin 1994)

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

$6.70 \times 10^{-5}$  ( $20$ – $25^{\circ}C$ , Weber et al. 1980)

$6.70 \times 10^{-5}$  (Herbicide Handbook 1983)

$6.70 \times 10^{-5}$  ( $20^{\circ}C$ , Hartley & Kidd 1987; Herbicide Handbook 1989; Montgomery 1993)

$6.60 \times 10^{-5}$  ( $20^{\circ}C$ , Worthing & Hance 1991)

$1.25 \times 10^{-4}$  ( $20$ – $25^{\circ}C$ , selected, Wauchope et al. 1992; Hornsby et al. 1996)

$1.25 \times 10^{-4}$  (Tomlin 1994)

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

$< 0.283$  ( $20$ – $25^{\circ}C$ , calculated-P/C, Montgomery 1993)

$1.73 \times 10^{-4}$  (calculated-P/C, this work)

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

1.34	(Briggs 1969)
2.42	(shake flask-UV, Briggs 1981)
1.88	(shake flask-UV, pH 5, Barak et al. 1983)
2.40	(selected, Gerstl & Helling 1987)
2.23	(Worthing & Hance 1991; Tomlin 1994; Milne 1995)
2.23, 2.38	(Montgomery 1993)
2.03	(RP-HPLC-RT correlation, Sicbaldi & Finizio 1993)
2.20	(recommended, Sangster 1993)
2.42	(recommended, Hansch et al. 1995)
2.03	(RP-HPLC-RT correlation, Finizio et al. 1997)

## Bioconcentration Factor, log BCF:

1.67	(calculated-S, Kenaga 1980)
0.954	(calculated- $K_{oc}$ , Kenaga 1980)

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

2.24	(soil, Abernethy & Davidson 1971; Davidson & McDougal 1973; Savage & Wauchope 1974; Carringer et al. 1975; Wood & Davidson 1975)
2.30	(soil, Kenaga 1980)
2.57	(soil, calculated-S as per Kenaga & Goring 1980, Kenaga 1980)
1.82	(soil, converted from reported $K_{om}$ multiplied by 1.724, Briggs 1981)
2.30	(calculated-MCI $\chi$ , Gerstl & Helling 1987)
2.00	(soil, 20–25°C, selected, Wauchope et al. 1992; Hornsby et al. 1996)
1.46–2.08	(Montgomery 1993)
2.00	(estimated-chemical structure, Lohninger 1994)
1.49–2.07	(Tomlin 1994)
2.00	(soil, calculated-MCI $\chi$ , Sabljic et al. 1995)
2.33; 2.66., 2.03, 2.64, 2.36, 1.94	(quoted lit., calculated- $K_{ow}$ ; HPLC-screening method with different LC-columns, Szabo et al. 1999)
2.14, 2.51	(soil, estimated-class-specific model, estimated-general model using molecular descriptors, Gramatica et al. 2000)

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

## Volatilization:

Photolysis:  $t_{1/2} = (11 \pm 2 \text{ h})$  in 10 ppm aqueous solutions under summer sunlight of 9.1 h/d exposure and  $t_{1/2} = (33 \pm 16) \text{ h}$  under spring sunlight of 3.7 h/d exposure (Burkhard et al. 1975).

## Oxidation:

Hydrolysis:  $t_{1/2} = 1.6 \text{ yr}$  at 20°C and pH 1,  $t_{1/2} = 2.4 \text{ yr}$  at pH 5, and  $t_{1/2} = 2.8 \text{ yr}$  at pH 9 (Montgomery 1993).

## Biodegradation:

## Biotransformation:

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

## Half-Lives in the Environment:

## Air:

Surface water:  $t_{1/2} = 730\text{--}1010 \text{ d}$  at pH 5–9 and 20°C in aqueous solutions (Herbicide Handbook 1989).

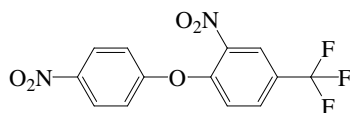
## Ground water:

## Sediment:

Soil: measured dissipation rate  $k = 0.023\text{--}0.043 \text{ d}^{-1}$  (Horowitz & Herzlinger 1974: quoted, Nash 1988); estimated dissipation rate  $k = 0.0012$ , and  $0.011 \text{ d}^{-1}$  (Nash 1988); persistence of 4 months in soil (Wauchope 1978); selected field  $t_{1/2} = 85 \text{ d}$  (Wauchope et al. 1992; Hornsby et al. 1996); soil  $t_{1/2} = 30 \text{ d}$  (Pait et al. 1992); median  $t_{1/2} \sim 30 \text{ d}$  in soil (Herbicide Handbook 1989; Tomlin 1994).

## Biota:

## 17.1.1.40 Fluorodifen



Common Name: Fluorodifen

Synonym: Preforan, Soyex

Chemical Name: 4-nitrophenyl  $\alpha,\alpha,\alpha$ -trifluoro-2-nitro-*p*-tolyl ether

Uses: herbicide.

CAS Registry No: 15457-05-3

Molecular Formula:  $C_{13}H_7F_3N_2O_5$

Molecular Weight: 328.200

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

94 (Spencer 1982; Milne 1995; Lide 2003)

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

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

Molar Volume ( $cm^3/mol$ ):

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

Dissociation Constant  $pK_a$ :

Enthalpy of Fusion,  $\Delta H_{fus}$  (kJ/mol):

Entropy of Fusion,  $\Delta S_{fus}$  (J/mol K):

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

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

2.0 ( $20^{\circ}C$ , Spencer 1973, 1982)

< 2.0 (Weber et al. 1980)

2.0 (shake flask-HPLC, Ellgehausen et al. 1981)

2.0 ( $20^{\circ}C$ , Worthing & Walker 1987, Worthing & Hance 1991)

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

$9.33 \times 10^{-6}$  ( $20^{\circ}C$ , Spencer 1982)

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

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

3.30 (shake flask-HPLC, Ellgehausen et al. 1980; Geyer et al. 1991)

4.40 ( $20 \pm 2^{\circ}C$ , shake flask-UV, Briggs 1981)

3.65 (shake flask-HPLC, Ellgehausen et al. 1981)

3.60 (HPLC-RT correlation, Nandihalli et al. 1993)

3.65 (recommended, Sangster 1993)

3.65 (recommended, Hansch et al. 1995)

Bioconcentration Factor,  $\log BCF$ :

2.019 (algae,  $\log BF$ -bioaccumulation factor, Ellgehausen et al. 1980)

2.386 (catfish,  $\log BF$ -bioaccumulation factor, Ellgehausen et al. 1980)

1.178 (daphnids,  $\log BF$ -bioaccumulation factor, Ellgehausen et al. 1980)

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

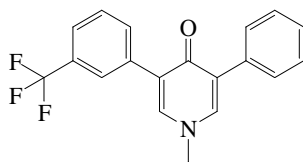
3.13 (calculated-MCI  $\chi$ , Gerstl & Helling 1987)

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

Half-Lives in the Environment:



## 17.1.1.41 Fluridone



Common Name: Fluridone

Synonym: Brake, EL-171, Fluridon, Pride, Sonar

Chemical Name: 1-methyl-3-phenyl-5-[3-(trifluoromethyl)phenyl] 4(1H)-pyridinone; 1-methyl-3-phenyl-5-( $\alpha,\alpha,\alpha$ -trifluorom-tolyl)-4-pyridone

Uses: herbicide to control annual grass and broadleaf weeds and certain perennial species in cotton; also used to control aquatic weeds and plants in lakes, ponds, ditches, etc.

CAS Registry No: 59756-60-4

Molecular Formula:  $C_{19}H_{14}F_3NO$

Molecular Weight: 329.315

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

155 (Lide 2003)

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

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

Molar Volume ( $cm^3/mol$ ):

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

Dissociation Constant:

12.3 ( $pK_b$ , Wauchope et al. 1992)

Enthalpy of Fusion,  $\Delta H_{fus}$  (kJ/mol):

Entropy of Fusion,  $\Delta S_{fus}$  (J/mol K):

Fugacity Ratio at  $25^{\circ}C$  (assuming  $\Delta S_{fus} = 56$  J/mol K), F: 0.0530 (mp at  $155^{\circ}C$ )

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

12.0 ( $20^{\circ}C$ , Weber 1972; Worthing & Walker 1987)  
12.0 (Kenaga 1980)  
12.0 (Herbicide Handbook 1983, 1989; Budavari 1989; Milne 1995)  
12.0 (Hartley & Kidd 1987; Worthing & Walker 1987, Worthing & Hance 1991)  
10.0 ( $20-25^{\circ}C$ , selected, Wauchope et al. 1992; Hornsby et al. 1996)  
10.0 (selected, Lohninger 1994)

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

$1.31 \times 10^{-5}$  ( $20^{\circ}C$ , Weber 1972; Worthing & Walker 1987)  
 $1.00 \times 10^{-5}$  (Herbicide Handbook 1983)  
0.013 (Hartley & Kidd 1987; Worthing & Hance 1991)  
 $1.33 \times 10^{-5}$  (Herbicide Handbook 1989)  
 $1.33 \times 10^{-5}$  ( $20-25^{\circ}C$ , selected, Wauchope et al. 1992; Hornsby et al. 1996)  
 $1.30 \times 10^{-5}$  (Tomlin 1994)

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

$3.59 \times 10^{-4}$  ( $20^{\circ}C$ , calculated-P/C, Muir 1991)

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

1.87 (Reinert 1989)  
1.87 (Worthing & Hance 1991; Tomlin 1994; Milne 1995)  
2.98 (shake flask, Takahashi et al. 1993; quoted, Sangster 1993)  
3.16 (LOGPSTAR or CLOGP data, Sabljic et al. 1995)

## Bioconcentration Factor, log BCF:

- 2.18 (calculated-S, Kenaga 1980; quoted, Isensee 1991)  
 0.778 (measured, West et al. 1983; quoted, Isensee 1991)

Sorption Partition Coefficient, log  $K_{OC}$  at 25°C or as indicated:

- 1.60 (soil, Kenaga 1980)  
 2.97–3.39 (pond sediment, Muir et al. 1980)  
 3.36, 2.95 (lake and river sediment, Muir et al. 1980)  
 2.94 (Reinert 1989)  
 2.90, 3.81, 3.03 (Norfolk sand pH 6.0, Norfolk with montmorillonite pH 5.9, Norfolk sand with added organic matter pH 5.3, Reinert 1989)  
 3.43, 2.57, 2.43 (California soil at pH 6, 7, 7.3, Reinert 1989)  
 3.00 (20–25°C, selected, Wauchope et al. 1992; Hornsby et al. 1996)  
 3.00 (selected, Lohninger 1994)  
 2.85 (soil, calculated-MCI  $\chi$ , Sabljic et al. 1995)

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

Volatilization: estimated  $t_{1/2}$  = 10,000 d from 1 m depth of water at 20°C (Muir 1991).

Photolysis:  $t_{1/2}$  ~ 23 h to degrade in distilled water under > 290 nm light (West et al. 1979; quoted, Cessna & Muir 1991);

$t_{1/2}$  ~ 6 h for 5 µg/mL to degrade in nonsterile pond water under sunlight (Muir & Grift 1982; quoted, Cessna & Muir 1991);

$t_{1/2}$  = 27 d for 85% of 10 µg/mL to degrade in distilled water and for 85% of 10 µg/mL to degrade in lake water at pH 8.4 both under sunlight (Sanders & Mosier 1983; quoted, Cessna & Muir 1991; Howard et al. 1991)

resistance to decomposition by UV light with  $t_{1/2}$  = 23 h in deionized water (Herbicide Handbook 1989).

Oxidation: photooxidation  $t_{1/2}$  = 0.359–3.20 h, based on estimated rate constant for reaction with hydroxyl radicals (Atkinson 1987; quoted, Howard et al. 1991) and ozone (Atkinson & Carter 1984; quoted, Howard et al. 1991).

Hydrolysis:  $t_{1/2}$  > 113 d for 1 µg/mL to hydrolyze in pond water at 4°C (Ghassemi et al. 1981; quoted, Muir 1991);  $t_{1/2}$  = 23 h in water (Tomlin 1994).

Biodegradation: aqueous aerobic  $t_{1/2}$  = 44–192 d, based on soil die-away test data and field study soil persistence (Banks et al. 1979; quoted, Howard et al. 1991);

$t_{1/2}$  = 12 months for 5 µg/mL to biodegrade in static sediment and water, and  $t_{1/2}$  ~ 9 months in aerobic and anaerobic sediment and water all at 25°C (Muir & Grift 1982; quoted, Muir 1991);

aqueous anaerobic  $t_{1/2}$  = 176 d to 2.1 yr, based on estimated unacclimated aqueous aerobic biodegradation half-life (Howard et al. 1991);

microbial degradation  $t_{1/2}$  > 343 d at pH 7.3 with 2.6% organic matter in a silt loam soil (Tomlin 1994).

## Biotransformation:

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

$k_1$  = 0.9–1.3 h<sup>-1</sup> (*Chironomus tentans* larvae in pond sediment-water system, 96-h exposure, calculated by using first-order kinetic and concn factors, Muir et al. 1983)

$k_1$  = 0.70–5.6 h<sup>-1</sup> (*Chironomus tentans* larvae in river sediment-water system, 96-h exposure, calculated by using first-order kinetic and concn factors, Muir et al. 1983)

$k_1$  = 1.7–3.40 h<sup>-1</sup> (*Chironomus tentans* larvae in sediment (sand)-water system, 96-h exposure, calculated by using first-order kinetic and concn factors, Muir et al. 1983)

$k_1$  = 1.7–2.1 h<sup>-1</sup> (*Chironomus tentans* larvae in sediment (sand)-water system, 96-h exposure, calculated by using initial uptake data of 0–12 h, Muir et al. 1983)

$k_2$  = 0.052 h<sup>-1</sup> (*Chironomus tentans* larvae in pond sediment-water system, calculated by concentration decay curve, Muir et al. 1983)

$k_2$  = 0.118 h<sup>-1</sup> (*Chironomus tentans* larvae in river water system, calculated by concentration decay curve, Muir et al. 1983)

$k_2$  = 0.055 h<sup>-1</sup> (*Chironomus tentans* larvae in river sediment-water system, calculated by concentration decay curve, Muir et al. 1983)

$k_2 = 0.041 \text{ h}^{-1}$  (*Chironomus tentans* larvae in sediment (sand)-water system, calculated by concentration decay curve, Muir et al. 1983)

#### Half-Lives in the Environment:

Air:  $t_{1/2} = 0.359\text{--}3.20 \text{ h}$ , based on estimated rate constant for reaction with hydroxyl radicals (Atkinson 1987; quoted, Howard et al. 1991) and ozone (Atkinson & Carter 1984; quoted, Howard et al. 1991).

Surface water:  $t_{1/2} \sim 21 \text{ d}$  in water (Hartley & Kidd 1987);

$t_{1/2} = 288\text{--}864 \text{ h}$ , based on estimated photolysis half-life in water (Howard et al. 1991);

anaerobic  $t_{1/2} = 9 \text{ months}$  and aerobic  $t_{1/2} \sim 20 \text{ d}$  (Tomlin 1994).

Ground water:  $t_{1/2} = 2112\text{--}9216 \text{ h}$ , based on estimated unacclimated aqueous aerobic biodegradation half-life (Howard et al. 1991).

Sediment:  $t_{1/2} = 12 \text{ months}$  for  $5 \mu\text{g/mL}$  to biodegrade in static sediment and water, and  $t_{1/2} \sim 9 \text{ months}$  in aerobic and anaerobic sediment and water all at  $25^\circ\text{C}$  (Muir & Grift 1982; quoted, Muir 1991).

Soil: measured dissipation rate  $k = 0.0041 \text{ d}^{-1}$  (Banks et al. 1979; quoted, Nash 1988) with estimated  $t_{1/2} = 44\text{--}192 \text{ d}$  (Banks et al. 1979; quoted, Howard et al. 1991);

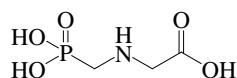
estimated dissipation rate  $k = 0.0067 \text{ and } 0.025 \text{ d}^{-1}$  (Nash 1988);

selected field  $t_{1/2} = 21 \text{ d}$  (Wauchope et al. 1992; Hornsby et al. 1996);

$t_{1/2} \sim 90 \text{ d}$  in the hydrosol (Tomlin 1994).

Biota: elimination  $t_{1/2} = 13.2 \text{ h}$  in pond sediment-water,  $t_{1/2} = 5.9 \text{ h}$  in river water,  $t_{1/2} = 12.5 \text{ h}$  in river sediment-water,  $t_{1/2} = 16.9$  in sand-water systems (*Chironomus tentans* larvae, Muir et al. 1983)

## 17.1.1.42 Glyphosate



Common Name: Glyphosate

Synonym: Mon-0573, 0468, 2139; Polado, Roundup

Chemical Name: *N*-(phosphoromethyl)glycine

Uses: nonselective, post-emergent, broad spectrum herbicide to control annual and perennial grasses, sedges, broadleaf, and emerged aquatic weeds; also used to control insects on fruit trees.

CAS Registry No: 1071-83-6

Molecular Formula:  $C_3H_8NO_3P$

Molecular Weight: 169.074

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

230 (dec., Montgomery 1993; Milne 1995; Lide 2003)

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

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

1.74 (Herbicide Handbook 1989; Montgomery 1993)

Molar Volume ( $cm^3/mol$ ):

Dissociation Constant  $pK_a$ :

5.70 (Worthing & Hance 1991)

2.60, 5.90, 10.40 ( $pK_1$ ,  $pK_2$ ,  $pK_3$ , Yao & Haag 1991; Haag & Yao 1992)

2.32, 5.86, 10.86 ( $pK_1$ ,  $pK_2$ ,  $pK_3$ , Montgomery 1993; Hornsby et al. 1996)

Enthalpy of Fusion,  $\Delta H_{fus}$  (kJ/mol):

Entropy of Fusion,  $\Delta S_{fus}$  (J/mol K):

Fugacity Ratio at  $25^{\circ}C$  (assuming  $\Delta S_{fus} = 56$  J/mol K), F: 0.0097 (mp at  $230^{\circ}C$ )

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

10000 (Spencer 1973, 1982; Herbicide Handbook 1978; Ashton & Crafts 1981)

12000 (Martin & Worthing 1977; Worthing & Walker 1987, Worthing & Hance 1991; Tomlin 1994)

15700 (Herbicide Handbook 1989)

12000 (Budavari 1989; Montgomery 1993; Milne 1995)

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

$2.59 \times 10^{-5}$  ( $45^{\circ}C$ , Herbicide Handbook 1989)

$4.00 \times 10^{-5}$  (Worthing & Hance 1991)

0.001 (Montgomery 1993; quoted, Majewski & Capel 1995)

negligible (Tomlin 1994)

0.0 (selected, Halfon et al. 1996)

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

$1.41 \times 10^{-5}$  (calculated-P/C, Montgomery 1993)

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

-1.70 (shake flask, pH 5.3, Martin & Edgington 1981)

-4.10 (shake flask, pH 2.5, Stevens et al. 1988)

-3.25 (Reinert 1989)

-4.59 (Worthing & Hance 1991)

-1.60 (Montgomery 1993)

-4.10, -1.70 (pH 2.5, pH 5.3, quoted, Sangster 1993)

-1.70 (pH 5.3, selected, Hansch et al. 1995)

0.94 (RP-HPLC-RT correlation, Finizio et al. 1997)

## Bioconcentration Factor, log BCF:

0.477	(calculated-S, Kenaga 1980; quoted, Isensee 1991)
2.26	(calculated- $K_{OC}$ , Kenaga 1980)

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

3.42	(soil, Sprankle et al. 1975; Hance 1976; Nomura & Hilton 1977)
1.40	(soil, calculated-S as per Kenaga & Goring 1980, Kenaga 1980)
1.22	(selected, USDA 1989; quoted, Neary et al. 1993)
-0.43	(Reinert 1989)
3.69, 3.53, 3.42	(3 agricultural soils: Houston clay loam at pH 7.5, Muskingum silt loam at pH 5.8, Sassafras sandy loam at pH 5.6, Reinert 1989)
4.38	(organic carbon, Wauchope et al. 1991)
3.43–3.69	(Montgomery 1993)

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

## Volatilization:

Photolysis:  $t_{1/2} = 48$  h for 0% of 168  $\mu\text{g/mL}$  to degrade in distilled water under  $> 290$  nm light (Rueppel et al. 1977; quoted, Cessna & Muir 1991);  
 $t_{1/2} = 9$  wk for  $> 90\%$  of 2  $\mu\text{g/mL}$  to degrade in distilled water under sunlight (Lund-Høie & Friestad 1986; quoted, Cessna & Muir 1991);  
 $t_{1/2} = 4.0$  d and 3–4 wk for aqueous solutions of 1.0 and 2000 ppm under indoor UV light (Lund-Høie & Friestad 1986; quoted, Montgomery 1993).

## Oxidation:

$k(\text{aq.}) = 7.3 \times 10^8 \text{ M}^{-1} \text{ s}^{-1}$  for the reaction (photo-Fenton with reference to glycolic acid) with hydroxyl radical in aqueous solutions at pH 3.8 and at  $24 \pm 1^\circ\text{C}$  (Buxton et al. 1988; quoted, Faust & Hoigné 1990; Haag & Yao 1992)  
 $k(\text{aq.}) = (0.027\text{--}8.2) \times 10^3 \text{ M}^{-1} \text{ s}^{-1}$  for direct reaction with ozone in water at pH 1.8–7.0 and  $22 \pm 2^\circ\text{C}$ , with a half-life of 4.0 s at pH 7 (Yao & Haag 1991).  
 $k(\text{aq.}) = (1.8 \pm 0.5) \times 10^8 \text{ M}^{-1} \text{ s}^{-1}$  for the reaction (photo-Fenton with reference to glycolic acid) with hydroxyl radical in aqueous solutions at pH 3.8 and at  $24 \pm 1^\circ\text{C}$  (Haag & Yao 1992).

Hydrolysis:  $t_{1/2} = 7$  d for 10  $\mu\text{g/mL}$  to hydrolyze in sterile water + soil (Rueppel et al. 1977; quoted, Muir 1991);  
 $t_{1/2} = 32$  d for 25 and 250  $\mu\text{g/mL}$  to hydrolyze in sterile distilled water at pH 3, 6 and 9 in the dark at 5 and  $35^\circ\text{C}$  (Ghassemi et al. 1981; quoted, Muir 1991)

Biodegradation:  $t_{1/2} < 28$  d for 10  $\mu\text{g/mL}$  to biodegrade in soil-water suspension (Rueppel et al. 1977; quoted, Muir 1991);

$t_{1/2} > 9$  wk for 2  $\mu\text{g/mL}$  to biodegrade in polluted lake water (Rueppel et al. 1977; quoted, Muir 1991);  
rate constant  $k = 0.1 \text{ d}^{-1}$  from soil incubation die-away studies (Rao & Davidson 1980; quoted, Scow 1982);  
 $t_{1/2} = 70$  d in pond water at pH 7.2,  $t_{1/2} = 63$  d in swamp water at pH 6.3 and  $t_{1/2} = 49$  d in Sphagnum bog water at pH 4.2 (Ghassemi et al. 1981; quoted, Muir 1991).

## Biotransformation:

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

## Half-Lives in the Environment:

## Air:

Surface water:  $t_{1/2} > 9$  wk for 2  $\mu\text{g/mL}$  to biodegrade in polluted lake water (Rueppel et al. 1977; quoted, Muir 1991);  
 $t_{1/2} = 70$  d in pond water at pH 7.2,  $t_{1/2} = 63$  d in swamp water at pH 6.3 and  $t_{1/2} = 49$  d in Sphagnum bog water at pH 4.2 (Ghassemi et al. 1981; quoted, Muir 1991);  
measured rate constant  $k = (0.027 - 8.2) \times 10^3 \text{ M}^{-1} \text{ s}^{-1}$  for direct reaction with ozone in water at pH 1.8–7.0 and  $22 \pm 2^\circ\text{C}$ , with  $t_{1/2} = 4.0$  s at pH 7 (Yao & Haag 1991).

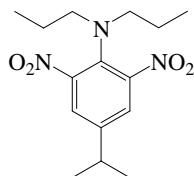
## Ground water:

## Sediment:

Soil:  $t_{1/2} < 28$  d for 10  $\mu\text{g/mL}$  to biodegrade in soil-water suspension (Rueppel et al. 1977; quoted, Muir 1991); estimated first-order  $t_{1/2} = 7$  d from biodegradation rate constant  $k = 0.1 \text{ d}^{-1}$  from soil incubation die-away studies (Rao & Davidson 1980; quoted, Scow 1982); moderately persistent in soil with  $t_{1/2} = 20\text{--}100$  d (Willis & McDowell 1982); average  $t_{1/2} < 60$  d (Hartley & Kidd 1987; Herbicide Handbook 1989; quoted, Montgomery 1993); selected  $t_{1/2} = 47$  d (Wauchope et al. 1991; quoted, Dowd et al. 1993; Halfon et al. 1996).

Biota: average  $t_{1/2} = 60$  d in the forest (USDA 1989; quoted, Neary et al. 1993).

## 17.1.1.43 Isopropalin



Common Name: Isopropalin

Synonym: EL 179, Isopropaline, Isopropalin solution, Paarlan

Chemical Name: 4-(1-methylethyl)-2,6-dinitro-*N,N*-dipropylaniline; 4-(1-methylethyl)-2,6-dinitro-*N,N*-dipropylbenzenamine; 2,6-dinitro-*N,N*-dipropylcumidine

Uses: herbicide used pre-planting and incorporated with soil preparation to control broadleaf weeds and grasses in transplanted tobacco, and in direct-seeded tomatoes and capsicums.

CAS Registry No: 33820-53-0

Molecular Formula:  $C_{15}H_{23}N_3O_4$

Molecular Weight: 309.362

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

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

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

Molar Volume ( $cm^3/mol$ ):

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

Dissociation Constant  $pK_a$ :

Enthalpy of Fusion,  $\Delta H_{fus}$  (kJ/mol):

Entropy of Fusion,  $\Delta S_{fus}$  (J/mol K):

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

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

0.11	(Martin & Worthing 1977; Herbicide Handbook 1978)
1.10	(Ashton & Crafts 1981)
0.10	(Spencer 1982; Hartley & Kidd 1987; Budavari 1989; Milne 1955)
0.10	(Worthing & Walker 1987, Worthing & Hance 1991)
0.08	(Herbicide Handbook 1989)
0.10	(20– $25^{\circ}C$ , selected, Wauchope et al. 1992; Hornsby et al. 1996)
0.02	(predicted-AQUAFAC, Lee et al. 1996)

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

0.0019	( $30^{\circ}C$ , Ashton & Crafts 1981)
0.0019	( $30^{\circ}C$ , Hartley & Kidd 1987)
0.0040	( $25.6^{\circ}C$ , Herbicide Handbook 1989)
0.0012	(20– $25^{\circ}C$ , selected, Wauchope et al. 1992; Hornsby et al. 1996)

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

5.34	(calculated-P/C, this work)
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Octanol/Water Partition Coefficient,  $\log K_{ow}$ :

Bioconcentration Factor,  $\log BCF$ :

3.50	(calculated-S, Kenaga 1980; quoted, Isensee 1991)
3.88	(calculated- $K_{oc}$ , Kenaga 1980)

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

4.88	(soil, Harvey 1974)
4.17	(soil, calculated-S as per Kenaga & Goring 1980, Kenaga 1980)
4.17–4.88	(soil, quoted values, Bottoni & Funari 1992)

- 4.00 (20–25°C, selected, Wauchope et al. 1992; Hornsby et al. 1996)  
 4.00 (selected, Lohninger 1994)  
 3.50 (soil, estimated-general model using molecular descriptors, Gramatica et al. 2000)

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

##### Volatilization:

Photolysis: atmosphere photolysis  $t_{1/2} = 288\text{--}864$  h, based on observed photolysis on soil TLC plates under summer sunlight (Helling 1976; quoted, Howard et al. 1991) and adjusted for relative winter sunlight intensity (Lyman et al. 1982; quoted, Howard et al. 1991); aqueous photolysis  $t_{1/2} = 288\text{--}864$  h, based on observed photolysis on soil TLC plates under summer sunlight (Helling 1976; quoted, Howard et al. 1991) and adjusted for relative winter sunlight intensity (Lyman et al. 1982; quoted, Howard et al. 1991).

Oxidation: photooxidation  $t_{1/2} = 0.743\text{--}74.3$  h in air, based on estimated rate constant for the vapor-phase reaction with hydroxyl radicals in air (Atkinson 1987; quoted, Howard et al. 1991).

##### Hydrolysis:

Abiotic Transformation: Degradation by abiotic reductive transformations:

$k = 1.71 \text{ M}^{-1} \text{ s}^{-1}$  in  $\text{H}_2\text{S}$  with (mecapto)juglone (hydroquinone moiety, an abiotic reductant found in natural systems) solution at pH 6.65 (Wang & Arnold 2003)

Aqueous solutions with surface-bound Fe(II) species and their first-order rate constants as:

$k = 0.94 \times 10^{-3} \text{ h}^{-1}$  at pH 6.5,  $k = 0.36 \times 10^{-2} \text{ h}^{-1}$  at pH 7.0,  $k = 0.057 \text{ h}^{-1}$  at pH 7.4, and  $k = 1.76 \text{ h}^{-1}$  at pH 7.8 for aqueous ferrous ion system;

$k = 0.297 \text{ h}^{-1}$  at pH 6.5,  $k = 0.586 \text{ h}^{-1}$  at pH 6.7,  $k = 1.28 \text{ h}^{-1}$  at pH 7.0, and  $k = 6.90 \text{ h}^{-1}$  at pH 7.3 for Fe(II)/goethite system;

$k = 9.91 \times 10^{-3} \text{ h}^{-1}$  at pH 6.5,  $k = 8.45 \times 10^{-3} \text{ h}^{-1}$  at pH 7.0,  $k = 7.45 \times 10^{-3} \text{ h}^{-1}$  at pH 7.4 and  $k = 6.96 \times 10^{-2} \text{ h}^{-1}$  at pH 7.8 for Fe(II)/clay system, all with total dissolved Fe(II) = 1 mM (Wang & Arnold 2003)

##### Biodegradation:

$t_{1/2}(\text{aq. aerobic}) = 408\text{--}2520$  h, based on aerobic soil die-away test data for one soil at 15°C and 30°C (Gingerich & Zimdahl 1976; quoted, Howard et al. 1991)

$t_{1/2}(\text{aq. anaerobic}) = 96\text{--}360$  h, based on anaerobic soil die-away test that tested one soil (Gingerich & Zimdahl 1976; quoted, Howard et al. 1991)

##### Biotransformation:

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

#### Half-Lives in the Environment:

Air:  $t_{1/2} = 0.743\text{--}74.3$  h, based on estimated rate constant for the vapor-phase reaction with hydroxyl radicals in air (Atkinson 1987; quoted, Howard et al. 1991).

Surface water:  $t_{1/2} = 288\text{--}864$  h, based on observed photolysis on soil TLC plates under summer sunlight (Helling 1976; quoted, Howard et al. 1991) and adjusted for relative winter sunlight intensity (Lyman et al. 1982; quoted, Howard et al. 1991).

Ground water:  $t_{1/2} = 96\text{--}5040$  h, based on estimated unacclimated aqueous aerobic and anaerobic degradation half-lives (Howard et al. 1991)  
 reported  $t_{1/2} < 180$  d (Bottoni & Funari 1992)

##### Sediment:

Soil:  $t_{1/2} = 408\text{--}2520$  h, based on aerobic soil die-away test data for one soil at 15°C and 30°C (Gingerich & Zimdahl 1976; quoted, Howard et al. 1991);

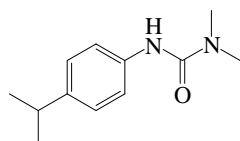
selected field  $t_{1/2} = 100$  d (Wauchope et al. 1992; Hornsby et al. 1996);

$t_{1/2} < 180$  d (Bottoni & Funari 1992).

##### Biota:



## 17.1.1.44 Isoproturon



Common Name: Isoproturon

Synonym: Alon, Arelon, CGA 18731, Gramion, Graminon, Hoe 16410, Hytane, IP 50, IP flo, Tolkan

Chemical Name: 3-(4-isopropylphenyl)-1,1-dimethylurea; 3-*p*-cumenyl-1,1-dimethylurea

Uses: herbicide used for pre- and post-emergence control of annual grasses and broadleaf weeds in spring and winter wheat (except durum wheat), spring and winter barley, winter rye, and triticale.

CAS Registry No: 34123-59-6

Molecular Formula: C<sub>12</sub>H<sub>18</sub>N<sub>2</sub>O

Molecular Weight: 206.284

Melting Point (°C):

155–156 (Worthing & Hance 1991)

158 (Tomlin 1994)

Boiling Point (°C):

Density (g/cm<sup>3</sup> at 20°C):

1.16 (Hartley & Kidd 1987; Tomlin 1994)

Molar Volume (cm<sup>3</sup>/mol):

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

Dissociation Constant pK<sub>a</sub>:

Enthalpy of Fusion, ΔH<sub>fus</sub> (kJ/mol):

Entropy of Fusion, ΔS<sub>fus</sub> (J/mol K):

Fugacity Ratio at 25°C (assuming ΔS<sub>fus</sub> = 56 J/mol K), F:

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

60 (Martin & Worthing 1977)

70 (20°C, Spencer 1982)

72 (20°C, Hartley & Kidd 1987)

55 (Worthing & Walker 1987, Worthing & Hance 1991)

55.9 (Chaumat et al. 1991)

65 (22°C, Tomlin 1994; quoted, Otto et al. 1997)

65 (20°C, selected, Traub-Eberhard et al. 1994)

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

3.3 × 10<sup>-6</sup> (20°C, Spencer 1982; Hartley & Kidd 1987)

3.3 × 10<sup>-6</sup> (20°C, Worthing & Hance 1991)

3.3 × 10<sup>-6</sup>, 3.15 × 10<sup>-2</sup>, 0.172 (20, 77, 150°C, Tomlin 1994)

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

1.05 × 10<sup>-5</sup> (calculated-P/C, Otto et al. 1997)

1.24 × 10<sup>-5</sup> (calculated-P/C, this work)

Octanol/Water Partition Coefficient, log K<sub>ow</sub> at 25°C or as indicated:

2.87 (shake flask, Log P Database, Hansch & Leo 1987)

2.25 (Worthing & Hance 1991)

2.30 (shake flask, pH 7, Baker et al. 1992)

2.537 (calculated, Evelyne et al. 1992)

2.30 (Behrendt & Bruggemann 1993)

2.87 (recommended, Sangster 1993)

2.87 (recommended, Hansch et al. 1995)

- 2.50 (pH 7, 22°C, Tomlin 1994)  
 2.40 (quoted Pomona-database, Müller & Kördel 1996)

Bioconcentration Factor, log BCF:

- 1.79 (calculated-S, Kenaga 1980)  
 1.76, 1.82 (cuticle/water: tomato, pepper; Chaumat et al. 1991)  
 1.71, 1.90 (cuticle/water: box tree, pear; Chaumat et al. 1991)  
 1.52, 1.20 (cuticle/water: ivy, vanilla; Chaumat et al. 1991)  
 1.76, 1.82 (cuticle/water: tomato, pepper; Evelyne et al. 1992)

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

- 2.66 (soil, calculated-S, Kenaga 1980)  
 1.86 (soil, HPLC-screening method, mean value of different stationary and mobile phases, Kördel et al. 1993)  
 2.11 (soil, quoted from Kördel et al. 1993, Traub-Eberhard et al. 1994)  
 1.86; 2.40 (HPLC-screening method; calculated-PCKOC fragment method, Müller & Kördel 1996)  
 2.57, 1.71, 1.78, 1.73, 2.34 (first generation Eurosoils ES-1, ES-2, ES-3, ES-4, ES-5, shake flask/batch equilibrium-HPLC/UV, Gawlik et al. 1998, 1999)  
 1.86, 2.31; 2.81, 2.24, 2.83, 2.35, 1.93 (quoted lit., calculated- $K_{OW}$ ; HPLC-screening method with different LC-columns, Szabo et al. 1999)  
 2.155, 1.918, 1.790, 1.719, 2.367 (second generation Eurosoils ES-1, ES-2, ES-3, ES-4, ES-5, shake flask/batch equilibrium-HPLC/UV and HPLC- $k'$  correlation, Gawlik et al. 1999)  
 2.155, 1.918, 1.790, 1.719, 2.367 (second generation Eurosoils ES-1, ES-2, ES-3, ES-4, ES-5, shake flask/batch equilibrium-HPLC/UV and HPLC- $k'$  correlation, Gawlik et al. 2000)  
 1.78, 2.10 (Kishon river sediments, sorption isotherm, Chefetz et al. 2004)

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

Volatilization:

Photolysis: atmosphere photolysis  $t_{1/2} = 288\text{--}864$  h, based on observed photolysis on soil TLC plates under summer sunlight (Helling 1976; quoted, Howard et al. 1991) and adjusted for relative winter sunlight intensity (Lyman et al. 1982; quoted, Howard et al. 1991);

aqueous photolysis  $t_{1/2} = 288\text{--}864$  h, based on observed photolysis on soil TLC plates under summer sunlight (Helling 1976; quoted, Howard et al. 1991) and adjusted for relative winter sunlight intensity (Lyman et al. 1982; quoted, Howard et al. 1991);

$t_{1/2} = 1.5$  h for 215  $\mu\text{g/mL}$  to degrade in distilled water under 254 nm light (Kulshrestha & Mukerjee 1986; quoted, Cessna & Muir 1991).

Oxidation: photooxidation  $t_{1/2} = 0.743\text{--}74.3$  h in air, based on estimated rate constant for the vapor-phase reaction with hydroxyl radicals in air (Atkinson 1987; quoted, Howard et al. 1991).

Hydrolysis:

Biodegradation: aqueous aerobic  $t_{1/2} = 408\text{--}2520$  h, based on aerobic soil die-away test data for one soil at 15°C and 30°C (Gingerich & Zimdahl 1976; quoted, Howard et al. 1991); aqueous anaerobic  $t_{1/2} = 96\text{--}360$  h, based on anaerobic soil die-away test which tested one soil (Gingerich & Zimdahl 1976; quoted, Howard et al. 1991)

Biotransformation: ~ 11% of a selection of 90 strains of micromycetes mostly isolated from soil-soil fungi, depleted over 50% of isoproturon (100 mg/L) in 5-d experiment (Vroumsia et al. 1996)

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

Half-Lives in the Environment:

Air:  $t_{1/2} = 0.743\text{--}74.3$  h, based on estimated rate constant for the vapor-phase reaction with hydroxyl radicals in air (Atkinson 1987; quoted, Howard et al. 1991).

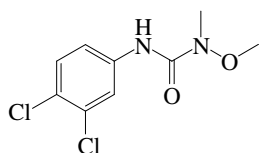
Surface water:  $t_{1/2} = 288\text{--}864$  h, based on observed photolysis on soil TLC plates under summer sunlight (Helling 1976; quoted, Howard et al. 1991) and adjusted for relative winter sunlight intensity (Lyman et al. 1982; quoted, Howard et al. 1991).

Groundwater:  $t_{1/2} = 96\text{--}5040$  h, based on estimated unacclimated aqueous aerobic and anaerobic degradation half-lives (Howard et al. 1991)  
 reported half-lives or persistence,  $t_{1/2} = 12\text{--}29$  and  $60\text{--}120$  d (Bottoni & Funari 1992)

## Sediment:

Soil:  $t_{1/2} = 408\text{--}2520$  h, based on aerobic soil die-away test data for one soil at 15°C and 30°C (Gingerich & Zimdahl 1976; quoted, Howard et al. 1991);  
reported  $t_{1/2} = 12\text{--}29$  d and 60–120 d (Bottoni & Funari 1992);  
 $t_{1/2} = 15\text{--}21$  d in sandy loam,  $t_{1/2} = 11$  d in silt loam at 20°C (Traub-Eberhard et al. 1994)  
Degradation and mineralization  $t_{1/2} = 16$  d, 24 d and 34 d for pelosol, brown calcareous soil and brown acid soil, respectively, over 120 days under controlled laboratory conditions (Pieuchot et al. 1996)  
estimated  $t_{1/2} \sim 14.6$  d under conventional tillage,  $t_{1/2} = 7.99$  d under ridge tillage and  $t_{1/2} = 12.17$  d with no tillage (Otto et al. 1997).

## 17.1.1.45 Linuron



Common Name: Linuron

Synonym: Afalon, Cephalon, Garnitan, Herbicide 326, Hoe 2810, Linex 4L, Linorox, Linurex, Lorox, Methoxydiuron, Premalin, Scarclex, Sinuron

Chemical Name: 3-(3,4-dichlorophenyl)-1-methoxy-1-methylurea; *N'*-(3,4-dichlorophenyl)-*N*-methoxy-*N*-methylurea

Uses: selective pre-emergence and post-emergence herbicide used on a wide variety of food crops to control many annual broadleaf and grass weeds.

CAS Registry No: 330-55-2

Molecular Formula:  $C_9H_{10}Cl_2N_2O_2$

Molecular Weight: 249.093

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

93 (Lide 2003)

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

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

Molar Volume ( $cm^3/mol$ ):

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

Dissociation Constant  $pK_a$ :

Enthalpy of Vaporization,  $\Delta H_v$  (kJ/mol):

90.23 (Rordorf 1989)

Enthalpy of Fusion,  $\Delta H_{fus}$  (kJ/mol):

28.66 (DSC method, Plato & Glasgow 1969)

25.9 (Rordorf 1989)

Entropy of Fusion,  $\Delta S_{fus}$  (J/mol K):

Fugacity Ratio at  $25^{\circ}C$  (assuming  $\Delta S_{fus} = 56$  J/mol K), F: 0.215 (mp at  $93^{\circ}C$ )

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

75 (Woodford & Evans 1963; Bailey & White 1965; Hartley & Graham-Bryce 1980; Kenaga 1980; Kenaga & Goring 1980; Beste & Humburg 1983)

75 (Melnikov 1971; Spencer 1973, 1982; Wauchope 1978; Khan 1980; Weber et al. 1980; Ashton & Crafts 1981; Briggs 1981)

75 (Martin & Worthing 1977; Worthing & Walker 1983, 1987; Herbicide Handbook 1978, 1989)

81 (Hartley & Kidd 1987; Milne 1995)

81 ( $24^{\circ}C$ , Worthing & Hance 1991)

75 ( $20$ – $25^{\circ}C$ , selected, Wauchope et al. 1992; Hornsby et al. 1996)

75–81 (Montgomery 1993)

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

0.00147 ( $20^{\circ}C$ , Quellette & King 1977)

0.0012 ( $20^{\circ}C$ , Hartley & Graham-Bryce 1980)

0.002 ( $24^{\circ}C$ , Khan 1980)

0.002 ( $20$ – $25^{\circ}C$ , Weber et al. 1980)

0.002 ( $24^{\circ}C$ , Hartley & Kidd 1987; Worthing & Hance 1991; Montgomery 1993)

0.0014 ( $20^{\circ}C$ , selected, Suntio et al. 1988)

$3.50 \times 10^{-4}$ ,  $1.10 \times 10^{-2}$ , 0.22, 2.90, 28.0 (25, 50, 70, 100,  $125^{\circ}C$ , gas saturation-GC, Rordorf 1989)

$\log(P_s/Pa) = 16.074 - 5824.2/(T/K)$ ; measured range  $40.5$ – $92^{\circ}C$  (solid, gas saturation-GC, Rordorf 1989)

$\log(P_L/Pa) = 12.989 - 4713.7/(T/K)$ ; measured range  $92.7$ – $160^{\circ}C$  (liquid, gas saturation-GC, Rordorf 1989)

0.0011 ( $20^{\circ}C$ , selected, Taylor & Spencer 1990)

0.0023 ( $20$ – $25^{\circ}C$ , selected, Wauchope et al. 1992; Hornsby et al. 1996)

0.0027 (selected, Halfon et al. 1996)

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

0.0054 ( $20^\circ\text{C}$ , calculated-P/C, Suntio et al. 1988)  
 0.004 (Taylor & Glotfelty 1988)  
 0.0062 ( $20\text{--}25^\circ\text{C}$ , calculated-P/C, Montgomery 1993)  
 0.00465 (calculated-P/C, this work)

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

2.19 (Briggs 1969)  
 3.20 (shake flask-UV, Erkell & Walum 1979)  
 2.76 (shake flask-UV, Briggs 1981)  
 3.11 (shake flask, Mitsutake et al. 1986)  
 2.48 (selected, Gerstl & Helling 1987)  
 3.00 (Worthing & Hance 1991; Milne 1995)  
 2.19, 3.00 (Montgomery 1993)  
 2.75 (RP-HPLC-RT correlation, Sicbaldi & Finizio 1993)  
 3.20 (recommended, Sangster 1993)  
 3.20 (recommended, Hansch et al. 1995)  
 3.18 (Pomona-database, Müller & Kördel 1996)  
 2.75 (RP-HPLC-RT correlation, Finizio et al. 1997)  
 2.72 (RP-HPLC-RT correlation, Yu et al. 1997)

Bioconcentration Factor,  $\log \text{BCF}$ :

1.73 (calculated-S, Kenaga 1980; quoted, Isensee 1991)  
 1.68 (calculated- $K_{\text{OC}}$ , Kenaga 1980)  
 1.73 (calculated, Pait et al. 1992)

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

2.91 (soil, Hamaker & Thompson 1972)  
 2.61 (soil, calculated-S as per Kenaga & Goring 1980, Kenaga 1980)  
 2.93 (average soils/sediments, Rao & Davidson 1980)  
 2.43 (soil, converted form reported  $K_{\text{OM}}$  multiplied by 1.724, Briggs 1981)  
 2.93, 2.80, 1.80 (estimated-S, calculated-S and mp, calculated- $K_{\text{OW}}$ , Karickhoff 1981)  
 3.83 (Means & Wijayarathne 1982)  
 2.99, 2.58; 2.62, 2.80 (estimated- $K_{\text{OW}}$ , S, Madhun et al. 1986)  
 2.76, 2.64 (quoted, calculated-MCI  $\chi$ , Gerstl & Helling 1987)  
 2.94 (screening model calculations, Jury et al. 1987b)  
 2.61–2.91, 2.83, 2.93 (soil, quoted values, Bottoni & Funari 1992)  
 2.60 (soil,  $20\text{--}25^\circ\text{C}$ , selected, Wauchope et al. 1992;)  
 2.70–2.78 (Montgomery 1993)  
 2.59 (soil, HPLC-screening method, mean value from different stationary and mobile phases, Kördel et al. 1993, 1995a)  
 2.59 (soil, HPLC-screening method, Kördel et al. 1993, 1995b)  
 2.70 (soil, calculated-MCI  $^1\chi$ , Sabljic et al. 1995)  
 2.59; 2.54 (HPLC-screening method; calculated-PCKOC fragment method, Müller & Kördel 1996)  
 3.28, 2.39, 2.46, 2.29, 3.12 (first generation Eurosoils ES-1, ES2, ES-3, ES-4, ES-5, shake flask/batch equilibrium-HPLC/UV, Gawlik et al. 1998, 1999)  
 2.884, 2.58, 2.45, 1.33, 3.18 (second generation Eurosoils ES-1, ES2, ES-3, ES-4, ES-5, shake flask/batch equilibrium-HPLC/UV, Gawlik et al. 1999)  
 2.884, 2.578, 2.450, 2.336, 3.183 (second generation Eurosoils ES-1, ES-2, ES-3, ES-4, ES-5, shake flask/batch equilibrium-HPLC/UV and HPLC- $k'$  correlation, Gawlik et al. 2000)  
 2.70; 2.55, 2.61 (soil, quoted obs.; estimated-class-specific model, estimated-general model using molecular descriptors, Gramatica et al. 2000)  
 2.65, 2.64 (soils: organic carbon  $\text{OC} \geq 0.1\%$ ,  $\text{OC} \geq 0.5\%$ , average, Delle Site 2001)

2.78 (average values for sediment OC  $\geq 0.5\%$ , Delle Site 2001)

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

##### Volatilization:

Photolysis:  $t_{1/2} = 2$  months for 31% of  $55 \mu\text{g mL}^{-1}$  to degrade in distilled water under sunlight (Rosen et al. 1969; quoted, Cessna & Muir 1991);

$t_{1/2} = 2.25$  h for 67–75% of  $75 \mu\text{g mL}^{-1}$  to degrade in distilled water under 300 nm light (Tanaka et al. 1981; quoted, Cessna & Muir 1991);

atmosphere photolysis  $t_{1/2} = 1344\text{--}4032$  h, based on measured rate constant for summer sunlight photolysis in distilled water (Rosen et al. 1969; quoted, Howard et al. 1991) and adjusted to relative winter sunlight intensity (Lyman et al. 1982; quoted, Howard et al. 1991); aqueous photolysis  $t_{1/2} = 1344\text{--}4032$  h, based on measured rate constant for summer sunlight photolysis in distilled water (Rosen et al. 1969; quoted, Howard et al. 1991) and adjusted to relative winter sunlight intensity (Lyman et al. 1982; quoted, Howard et al. 1991).

Oxidation: photooxidation  $t_{1/2} = 0.49\text{--}4.90$  h in air, based on an estimated rate constant for the vapor-phase reaction with hydroxyl radicals in air (Atkinson 1987; quoted, Howard et al. 1991).

Hydrolysis:  $t_{1/2} > 4$  months for  $4980 \mu\text{g mL}^{-1}$  to hydrolyze in phosphate buffer at pH 5–9 and  $20^\circ\text{C}$  (El-dib & Aly 1976; quoted, Muir 1991).

Biodegradation:  $t_{1/2} = 78$  d in soil (Moyer et al. 1972; quoted, Means et al. 1983),

$t_{1/2} = 87$  d in soil (Hance 1974; quoted, Means et al. 1983),

$t_{1/2} = 58$  and  $180$  d in soil (Urosol & Hance 1974; quoted, Means et al. 1983);

aqueous aerobic  $t_{1/2} = 672\text{--}4272$  h, based on soil die-away test data (Walker 1978; Walker & Zimdahl 1981; quoted, Howard et al. 1991);

rate constant  $k = 0.0096 \text{ d}^{-1}$  by soil incubation die-away studies (Rao & Davidson 1980; quoted, Scow 1982);

aerobic  $t_{1/2} \sim 40$  d for  $1 \mu\text{g mL}^{-1}$  to biodegrade in lake sediment and  $t_{1/2} \sim 60$  d for  $4 \mu\text{g mL}^{-1}$  to biodegrade in lake sediment and water (Huber & Gemes 1981; quoted, Muir 1991);

aerobic  $t_{1/2} \sim 20$  d for  $0.22 \mu\text{g mL}^{-1}$  to biodegrade in pond sediment plus aerobic salts medium of  $34 \text{ g L}^{-1}$  (Stepp et al. 1985; quoted, Muir 1991);

aqueous anaerobic  $t_{1/2} = 2688\text{--}17088$  h, based on estimated unacclimated aqueous aerobic biodegradation half-life (Howard et al. 1991)

degradation rate constant  $k = (3.48 \pm 0.156) \times 10^{-2} \text{ d}^{-1}$  with  $t_{1/2} = 19.9$  d in control soil and  $k = (23.2 \pm 2.07) \times 10^{-2} \text{ d}^{-1}$  with  $t_{1/2} = 2.99$  d in pretreated soil in the field;  $k = (3.73 \pm 0.208) \times 10^{-2} \text{ d}^{-1}$  with  $t_{1/2} = 18.6$  d in control soil and  $k = (18.8 \pm 2.76) \times 10^{-2} \text{ d}^{-1}$  with  $t_{1/2} = 3.68$  d in pretreated soil once only in the laboratory (Walker & Welch 1991)

##### Biotransformation:

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

#### Half-Lives in the Environment:

Air:  $t_{1/2} = 0.49\text{--}4.90$  h, based on an estimated rate constant for the vapor-phase reaction with hydroxyl radicals in air (Atkinson 1987; quoted, Howard et al. 1991).

Surface water:  $t_{1/2} = 672\text{--}4272$  h, based on estimated unacclimated aqueous aerobic biodegradation half-life (Howard et al. 1991).

Ground water:  $t_{1/2} = 1344\text{--}8544$  h, based on estimated unacclimated aqueous aerobic biodegradation half-life (Howard et al. 1991)

reported half-lives or persistence,  $t_{1/2} = 38\text{--}69$  and  $75$  d (Bottoni & Funari 1992).

Sediment: degradation  $t_{1/2} = 12$  d in estuarine sediment ( $12^\circ/\infty$ ) system (Cunningham et al. 1981; quoted, Means et al. 1983);

degradation  $t_{1/2} = 6$  d in estuarine sediment ( $18^\circ/\infty$ ) system (Means et al. 1983).

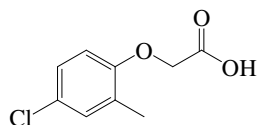
Soil: estimated persistence of 4 months (Kearney et al. 1969; Edwards 1973; quoted, Morrill et al. 1982; Jury et al. 1987a);

$t_{1/2} = 672\text{--}4272$  h, based on soil die-away test data (Walker 1978; Walker & Zimdahl 1981; quoted, Howard et al. 1991);

persistence of 4 months (Wauchope 1978);

correlated  $t_{1/2} = 57$  d at pH 5.1–5.8,  $t_{1/2} = 22$  d at pH 6.3–7.0 and  $t_{1/2} = 19$  d at pH 7.7–8.2 (Boddington Barn soil, Hance 1979) and  $t_{1/2} = 67$  d at pH 4.6–5.2,  $t_{1/2} = 53$  d at pH 5.3–6.1, and  $t_{1/2} \sim 20$  d at pH 6.3–8.0 (Triangle soil, Hance 1979);  
estimated first-order  $t_{1/2} = 72$  d from biodegradation rate constant  $k = 0.0096 \text{ d}^{-1}$  by soil incubation die-away studies (Rao & Davidson 1980; quoted, Scow 1982);  
decomposition  $t_{1/2} = 11$  d in fresh soil and  $t_{1/2} = 12$  d in air dried soil both in polyethylene bags,  $t_{1/2} = 49$  d in undisturbed cores and  $t_{1/2} = 40$  d in perfusion (Hance & Haynes 1981);  
moderately persistent in soil with  $t_{1/2} = 20$ –100 d (Willis & McDowell 1982);  
 $t_{1/2} = 2$  to 5 months under field conditions (Hartley & Kidd 1987; Herbicide Handbook 1989; quoted, Montgomery 1993);  
 $t_{1/2} = 75$  d from screening model calculations (Jury 1987b);  
 $t_{1/2} = 60, 35, 35, 30$  d in plots treated, i.e., repeated application of pesticide, for the first, second, third and fourth time, respectively, in the field; in the laboratory  $t_{1/2}$  reduced from 19 d to 3–7 d in a single pretreatment in moist soil at 20°C (Walker & Welch 1991)  
reported  $t_{1/2} = 38$ –69 d and 75 d (Bottoni & Funari 1992);  
selected field  $t_{1/2} = 60$  d (Wauchope et al. 1992; quoted, Richards & Baker 1993; quoted, Halfon et al. 1996; Hornsby et al. 1996);  
soil  $t_{1/2} = 60$  d (Pait et al. 1992);  
soil  $t_{1/2} = 29$ –67 d (Di Guardo et al. 1994).  
Biota: biochemical  $t_{1/2} = 75$  d from screening model calculations (Jury et al. 1987b).

## 17.1.1.46 MCPA



Common Name: MCPA

Synonym: Agritox, Agroxohe, Agroxone, Anicon Kombi, Bordermaster, Chiptox, Chwastox, Cornox, Ded-weed, Dicopur-M, Dicotex, Dikotes, Emcepan, Empal, Hedapur M 52, Hederax M, Herbicide M, Hedonal, Hormotuho, Kilsem, Krezone, Legumex DB, Leuna M, Leyspray, Linormone, MCP, metaxon, Methoxone, Netazol, Okultin M, Phenoxyline Plus, Raphone, Razol dock killer, Rhomenc, Rhonox, Shamrox, Seppic MMD, Trasan, Ustinex, Vacate, Verdone, Weedar, Weed-rhap, Zelan

Chemical Name: (4-chloro-2-methylphenoxy)acetic acid; 4-chloro-*o*-tolylxyacetic acid

Uses: systemic post-emergence herbicide to control annual and perennial weeds in cereals, rice, flax, vines, peas, potatoes, asparagus, grassland and turf.

CAS Registry No: 94-74-6

Molecular Formula:  $C_9H_9ClO_3$

Molecular Weight: 200.618

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

120 (Montgomery 1993; Milne 1995; Lide 2003)

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

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

1.56 ( $25^{\circ}C$ , Que Hee et al. 1981; Herbicide Handbook 1989; Montgomery 1993)

Molar Volume ( $cm^3/mol$ ):

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

Dissociation Constant  $pK_a$ :

3.05 (potentiometric titration, Nelson & Faust 1969)

3.125 (Cessna & Grover 1978)

3.07 (Worthing & Hance 1991)

3.05–3.13 (Montgomery 1993)

3.12 (Hornsby et al. 1996)

Enthalpy of Fusion,  $\Delta H_{fus}$  (kJ/mol):

Entropy of Fusion,  $\Delta S_{fus}$  (J/mol K):

Fugacity Ratio at  $25^{\circ}C$  (assuming  $\Delta S_{fus} = 56$  J/mol K), F: 0.117 (mp at  $120^{\circ}C$ )

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

1605 (shake flask-UV, Leopold et al. 1960)

1605 (Bailey & White 1965)

< 1000 (Khan 1980)

630 ( $20^{\circ}C$ , Melnikov 1971)

825 (Martin & Worthing 1977; Weber et al. 1980; Milne 1995)

1500 (selected, Seiber et al. 1986)

825 (room temp., Hartley & Kidd 1987; Worthing & Hance 1991)

817 (selected, Gerstl & Helling 1987)

835 (room temp., Worthing & Walker 1987)

730–825 (Montgomery 1993)

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

$7.9 \times 10^{-4}$  (measured-volatilization rate, Seiber et al. 1986)

$2.0 \times 10^{-4}$  ( $20^{\circ}C$ , Hartley & Kidd 1987)

$2.0 \times 10^{-4}$  ( $21^{\circ}C$ , Worthing & Walker 1987, 1991)

$2.3 \times 10^{-5}$  ( $20^{\circ}C$ , Tomlin 1994)

$2.0 \times 10^{-4}$  ( $20^{\circ}C$ , Milne 1995)

$2.0 \times 10^{-4}$  (selected, Halfon et al. 1996)



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

- $1.0 \times 10^{-4}$  (calculated-P/C, Seiber et al. 1986)
- $4.86 \times 10^{-4}$  (calculated-P/C as per Worthing & Walker 1987, Majewski & Capel 1995)
- $< 0.010$  (estimated, Mabury & Crosby 1996)
- $2.5 \times 10^{-4}$  (calculated-P/C, this work)

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

- 2.69 (selected, Dao et al. 1983)
- 2.30 (RP-HPLC- $k'$  correlation, Braumann et al. 1983)
- 1.41 (selected, Gerstl & Helling 1987)
- 0.57 (shake flask-UV, pH 7, Stevens et al. 1988)
- 3.25 (countercurrent LC, Ilchmann et al. 1993)
- 1.37-1.43 (calculated, Montgomery 1993)
- 0.57, 3.25 (quoted, Sangster 1993)
- 2.68 (MedChem Master file or ClogP program, Sabljic et al. 1995)

Bioconcentration Factor,  $\log \text{BCF}$ :

- 1.15 (calculated-S, Kenaga 1980)

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

- 2.04 (soil, calculated-S, Kenaga 1980; quoted, Bottoni & Funari 1992)
- 1.95 (calculated-MCI  $\chi$ , Gerstl & Helling 1987)
- 2.03-2.07 (calculated, Montgomery 1993)
- 1.73 (calculated-QSAR MCI  $^1\chi$ , Sabljic et al. 1995)
- 2.49; 1.58., 3.27, 3.17, 1.85, 2.19 (calculated- $K_{\text{OW}}$ ; HPLC-screening method with different LC-columns, Szabo et al. 1999)

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

Volatilization:  $k = 9.78 \times 10^{-7} \text{ h}^{-1}$  at pH 3.5 (Seiber et al. 1986).

Photolysis:  $t_{1/2} = 71 \text{ h}$  for  $< 10\%$  of  $50 \mu\text{g mL}^{-1}$  to degrade in NaOH solution at pH 9.8 under  $> 290 \text{ nm}$  light (Soderquist & Crosby 1975; quoted, Cessna & Muir 1991);

$t_{1/2} = 245 \text{ h}$  for 17-98.5% of  $9 \mu\text{g mL}^{-1}$  to degrade in distilled water under sunlight (Draper & Crosby 1984; quoted, Cessna & Muir 1991);

$t_{1/2} = 4.6 \text{ d}$  for  $14,700 \mu\text{g mL}^{-1}$  to degrade in droplets of spray solution suspended in air under sunlight (Freiberg & Crosby 1986; quoted, Cessna & Muir 1991).

Oxidation: degradation by ozone in dilute aqueous solutions (Benoit-Guyod et al. 1986) as follows:-

$t_{1/2} = 9.4 \text{ min}$  - dark with  $\text{O}_3$  in air;  $t_{1/2} = 8.4 \text{ min}$  - light with  $\text{O}_3$  in air,  $t_{1/2} = 500 \text{ min}$  - light, air only, at initial pH of 3.55; MCPA concn of  $224 \mu\text{M L}^{-1}$ , ozone input at  $246 \mu\text{M h}^{-1}$ ;

$t_{1/2} = 10.4 \text{ min}$  - dark with  $\text{O}_3$  in air;  $t_{1/2} = 9.0 \text{ min}$  - light with  $\text{O}_3$  in air, at initial pH of 8.0,

$t_{1/2} = 11.5 \text{ min}$  - dark with  $\text{O}_3$  in air;  $t_{1/2} = 11.3 \text{ min}$  - light with  $\text{O}_3$  in air, at initial pH of 7.0,

$t_{1/2} = 8.4 \text{ min}$  - dark with  $\text{O}_3$  in air;  $t_{1/2} = 9.4 \text{ min}$  - light with  $\text{O}_3$  in air, at initial pH of 7.0,

$t_{1/2} = 4.2 \text{ min}$  - dark with  $\text{O}_3$  in air;  $t_{1/2} = 4.2 \text{ min}$  - light with  $\text{O}_3$  in air,  $t_{1/2} = 150 \text{ min}$  - light, air only, at initial pH of 8.0; MCPA concn of  $5 \mu\text{M L}^{-1}$ , ozone input at  $246 \mu\text{M h}^{-1}$ ;

$t_{1/2} = 176 \text{ min}$  - dark with  $\text{O}_3$  in air;  $t_{1/2} = 63 \text{ min}$  - light with  $\text{O}_3$  in air, at initial pH of 8.0, MCPA concn of  $224 \mu\text{M L}^{-1}$ , ozone input at  $4.6 \mu\text{M h}^{-1}$ ;

$t_{1/2} = 300 \text{ min}$  - dark with  $\text{O}_3$  in air;  $t_{1/2} = 162 \text{ min}$  - light with  $\text{O}_3$  in air, at initial pH of 8.0; MCPA concn of  $224 \mu\text{M L}^{-1}$ , ozone input at  $0.2 \mu\text{M h}^{-1}$  (Benoit-Guyod et al. 1986).

measured rate constant  $k_{\text{OH}}(\text{aq.}) = 1.70 \times 10^9 \text{ M}^{-1} \text{ s}^{-1}$  for reaction with hydroxyl radical, in irradiated field water both in the laboratory and sunlit rice paddies (Mabury & Crosby 1996).

Hydrolysis:

Biodegradation:  $t_{1/2} > 168 \text{ h}$  for  $1 \mu\text{g mL}^{-1}$  to degrade in activated sludge (Schmidt 1975; quoted, Muir 1991);

aerobic  $t_{1/2} \sim 9 \text{ d}$  for  $1 \mu\text{g mL}^{-1}$  to degrade in natural water in absence of sunlight (Soderquist & Crosby 1975; quoted, Muir 1991);

$t_{1/2} > 12 \text{ d}$  for  $0.045\text{--}0.156 \mu\text{g mL}^{-1}$  to degrade in water after application to model crop and washoff (Virtanen et al. 1979; quoted, Muir 1991);

$t_{1/2} = 15\text{--}25$  d for  $10\text{ }\mu\text{g mL}^{-1}$  to degrade in flooded soils (Duah-Yentumi & Kuwatsuka 1980; quoted, Muir 1991);

first order microbial degradation  $k = 0.01393\text{ d}^{-1}$  with  $t_{1/2} = 50$  d at room temp,  $k = 0.01687\text{ d}^{-1}$  with  $t_{1/2} = 41$  d at  $35^{\circ}\text{C}$  in sandy clay soil from Finland;  $k = 0.02999\text{ d}^{-1}$  with  $t_{1/2} = 23$  d at room temp,  $k = 0.03397\text{ d}^{-1}$  with  $t_{1/2} = 20$  d at  $35^{\circ}\text{C}$  in sandy loam soil from Bangladesh (Sattar & Paasivirta 1980)

$t_{1/2} > 25$  d for  $10\text{ }\mu\text{g mL}^{-1}$  to degrade in flooded soils (Ursin 1985; quoted, Muir 1991).

Biotransformation:

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

#### Half-Lives in the Environment:

Air:

Surface water: dissipation  $t_{1/2} \sim 4$  d in rice field;  $t_{1/2} = 17$  d in dilute aqueous solution under laboratory irradiation (Soderquist & Crosby 1975);

degradation  $t_{1/2} = 4.2\text{--}300$  min by ozone and light ( $\text{UV} > 300\text{ nm}$ ) in dilute aqueous solution, depending on pH, concn of MCPA and ozone (shake flask-GC, Benoit-Guyod et al. 1986)

degraded rapidly with  $t_{1/2} = 9$  d in rice paddy water held under darkened conditions (Muir 1991)

field dissipation  $t_{1/2} = 28.8$  h in water (Mabury & Crosby 1996)

Ground water: reported  $t_{1/2} < 7$  and  $t_{1/2} = 20\text{--}25$  d (Bottoni & Funari 1992)

Sediment:  $t_{1/2} = 80$  to  $400$  d of MCPA at low concentrations in marine sediments (Muir 1991).

Soil: degradation  $t_{1/2} = 50$  d at room temp.,  $t_{1/2} = 41$  d at  $35^{\circ}\text{C}$  in Finland sandy clay soil; degradation  $t_{1/2} = 23$  d at room temp.,  $t_{1/2} = 20$  d at  $35^{\circ}\text{C}$  in Bangladesh loam soil from first-order rate constant obtained by linear regression (Sattar & Paasivirta 1980);

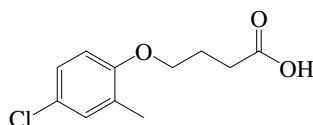
persistence of 3 months in soil (Edwards 1973; quoted, Morrill et al. 1982);

$t_{1/2} = 25$  d in flooded soils (Muir 1991);

$t_{1/2} = 15$  d (selected, Halfon et al. 1996).

Biota:

## 17.1.1.47 MCPB



Common Name: MCPB

Synonym: Bexane, Can-Trol, Legumex, Thistrol, Thitrol, Triflex, Tropotox

Chemical Name: 4-(4-chloro-2-methylphenoxy)butanoic acid; 4-(4-chloro-2-methylphenoxy)-butyric acid

Uses: herbicide for post-emergence control of annual and perennial broadleaf weeds in cereals, clovers, sainfoin, groundnuts, peas, etc. and also used to control broadleaf and woody weeds in forestry.

CAS Registry No: 94-81-5

Molecular Formula:  $C_{11}H_{13}ClO_3$

Molecular Weight: 228.672

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

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

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

> 280 (Tomlin 1994)

Density ( $g/cm^3$  at  $22^{\circ}C$ ):

1.254 (Tomlin 1994)

Molar Volume ( $cm^3/mol$ ):

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

Dissociation Constant  $pK_a$ :

4.80 (potentiometric titration, Nelson & Faust 1969)

4.84 (Worthing & Hance 1991; Tomlin 1994)

Enthalpy of Fusion,  $\Delta H_{fus}$  ( $kJ/mol$ ):

34.31 (DSC method, Plato 1972)

Entropy of Fusion,  $\Delta S_{fus}$  ( $J/mol K$ ):

Fugacity Ratio at  $25^{\circ}C$  (assuming  $\Delta S_{fus} = 56 J/mol K$ ), F: 0.184 (mp at  $100^{\circ}C$ )

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

41 (shake flask-UV, Leopold et al. 1960)

44 (rm. temp., Melnikov 1971)

44 (Bailey & White 1965; Martin & Worthing 1977; Hartley & Kidd 1987)

44 (rm. temp., Worthing & Walker 1987, Worthing & Hance 1991; Tomlin 1994; Milne 1995)

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

$5.77 \times 10^{-5}$ ,  $9.83 \times 10^{-5}$  (20,  $25^{\circ}C$ , Tomlin 1994)

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

$3.22 \times 10^{-4}$  (calculated-P/C, this work)

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

4.60 (selected, Dao et al. 1983)

3.53 (RP-HPLC- $k'$  correlation, Braumann et al. 1983)

3.473 (countercurrent LC, Ilchmann et al. 1993)

2.79 (Tomlin 1994)

3.43 (selected, Hansch et al. 1995)

Bioconcentration Factor,  $\log BCF$ :

1.86 (calculated-S, Kenaga 1980)

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

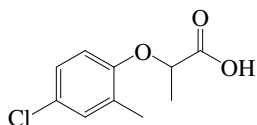
2.73 (soil, calculated-S, Kenaga 1980)

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

Half-Lives in the Environment:

Soil: duration of residual activity in soil is ca. 3–4 months (Hartley & Kidd 1987; Tomlin 1994).

## 17.1.1.48 Mecoprop



Common Name: Mecoprop

Synonym: Compitox, Duplosan, Hedonal, Iso-Cornox, Kilprop, MCPP, Mecopex, Mepro, Methoxone, Propal

Chemical Name: (±)-2-(4-chloro-2-methylphenoxy)propanoic acid; (±)-2-(4-chloro-*o*-tolyl-oxy)propionic acid

Uses: herbicide for post-emergence control of broadleaf weeds in wheat, barley, rye, herbage seed crops, grassland, and under fruit trees and vines, etc.

CAS Registry No: 7085-19-0

Molecular Formula: C<sub>10</sub>H<sub>11</sub>ClO<sub>3</sub>

Molecular Weight: 214.645

Melting Point (°C):

94–95 (Hartley & Kidd 1987; Herbicide Handbook 1989; Worthing & Hance 1991)

Boiling Point (°C):

Density (g/cm<sup>3</sup> at 20°C):

Molar Volume (cm<sup>3</sup>/mol):

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

Dissociation Constant pK<sub>a</sub>:

3.75 (Bailey & White 1965; quoted, Que Hee et al. 1981)

3.105 (Cessna & Grover 1978)

3.78 (Worthing & Hance 1991)

3.11 (Armbrust 2000)

Enthalpy of Fusion, ΔH<sub>fus</sub> (kJ/mol):

28.87 (DSC method, Plato 1972)

Entropy of Fusion, ΔS<sub>fus</sub> (J/mol K):

Fugacity Ratio at 25°C (assuming ΔS<sub>fus</sub> = 56 J/mol K), F:

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

895 (Martin 1961; Bailey & White 1965)

891 (Bailey & White 1965)

620 (20°C, Melnikov 1971; Ashton & Crafts 1981; Herbicide Handbook 1989)

620 (Martin & Worthing 1977)

620 (20°C, Hartley & Kidd 1987; Worthing & Walker 1987, Worthing & Hance 1991)

734 (Tomlin 1994)

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

< 1.0 × 10<sup>-5</sup> (20°C, Hartley & Kidd 1987)

3.10 × 10<sup>-4</sup> (20°C, Worthing & Hance 1991)

0.0 (selected, Halfon et al. 1996)

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

7.43 × 10<sup>-5</sup> (calculated-P/C, this work)

1.11 × 10<sup>-5</sup> (quoted lit., Armbrust 2000)

Octanol/Water Partition Coefficient, log K<sub>ow</sub>:

3.94 (selected, Dao et al. 1983)

2.83 (RP-HPLC-*k'* correlation, Braumann et al. 1983)

0.10 (Worthing & Hance 1991)

0.09; 3.126 (quoted; countercurrent LC, Ilchmann et al. 1993)

3.13 (recommended, Hansch et al. 1995)

## Bioconcentration Factor, log BCF:

1.20 (calculated-S, Kenaga 1980)

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

2.11 (soil, calculated, Kenaga 1980, quoted, Bottoni & Funari 1992)

1.30 (selected, Lohninger 1994)

1.30 (quoted lit., Armbrust 2000)

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

## Volatilization:

Photolysis: photodegradation  $t_{1/2} < 10$  -15 d on 3 Spanish natural dry soils;  $t_{1/2} = 15$ –50 d on 10% peat-amended dry soils; degradation  $t_{1/2} \sim 2$ –5.5 d on moist soils at field capacity and saturated soils for degradation at 0,1 and 2 exposures days; and  $t_{1/2} = 13$ –32 d on moist soils at field capacity and saturated soils for degradation at 2,4 and 10 exposure days (Romero et al. 1998)

Oxidation: photooxidation  $t_{1/2} = 3.8$ –37.8 h in air, based on an estimated rate constant for the vapor-phase reaction with hydroxyl radicals in air (Atkinson 1987; quoted, Howard et al. 1991).

Hydrolysis: stable aqueous hydrolysis rate at pH 5, 7, pH 9; measured hydroxy radical rate constant for mecoprop  $k = 9.0 \times 10^{12} \text{ M}^{-1} \text{ h}^{-1}$  (Armbrust 2000)

Biodegradation: aqueous aerobic  $t_{1/2} = 168$ –240 h, based on aerobic soil grab sample data (Kirkland & Fryer 1972; Smith & Hayden 1981; quoted, Howard et al. 1991); aqueous anaerobic  $t_{1/2} = 672$ –4320 h, based on anaerobic digest or sludge data (Battersby & Wilson 1989; quoted, Howard et al. 1991); aerobic rate constant,  $k = 2.89 \times 10^{-3} \text{ h}^{-1}$  (Armbrust 2000).

## Biotransformation:

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

## Half-Lives in the Environment:

Air:  $t_{1/2} = 3.8$ –37.8 h, based on an estimated rate constant for the vapor-phase reaction with hydroxyl radicals in air (Atkinson 1987; quoted, Howard et al. 1991).

Surface water:  $t_{1/2} = 168$ –240 h, based on estimated aqueous aerobic biodegradation half-life (Howard et al. 1991).

Groundwater:  $t_{1/2} = 336$ –4320 h, based on estimated aqueous aerobic and anaerobic biodegradation half-lives (Howard et al. 1991)  
reported  $t_{1/2} = 8$  d (Bottoni & Funari 1992).

## Sediment:

Soil:  $t_{1/2} = 168$ –240 h, based on aerobic soil grab sample data (Kirkland & Fryer 1972; Smith & Hayden 1981; quoted, Howard et al. 1991);

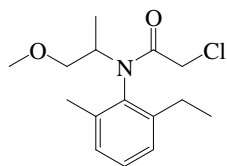
reported  $t_{1/2} = 8$  d (Bottoni & Funari 1992);

$t_{1/2} = 21$  d (selected, Halfon et al. 1996)

photodegradation  $t_{1/2} < 10$  -15 d on 3 Spanish natural dry soils;  $t_{1/2} = 15$ –50 d on 10% peat-amended dry soils; degradation  $t_{1/2} \sim 2$ –5.5 d on moist soils at field capacity and saturated soils for degradation at 0,1 and 2 exposures days; and  $t_{1/2} = 13$ –32 d on moist soils at field capacity and saturated soils for degradation at 2,4 and 10 exposure days (Romero et al. 1998).

## Biota:

## 17.1.1.49 Metolachlor



Common Name: Metolachlor

Synonym: Bicep, CGA 24705, Codal, Cortoran multi, Dual, Metetilachlor, Milocep, Ontrack 8E, Pennant, Primagram, Primextra

Chemical Name: 2-chloro-6'-ethyl-*N*-(2-methoxy-1-methylethyl)acet-*o*-toluidide; 2-chloro-*N*-(2-ethyl-6-methylphenyl)-*N*-(2-methoxy-1-methylethyl)acetamide

Uses: pre-emergence herbicide to control most annual grasses and weeds in beans, chickpeas, corn, cotton, milo, okra, peanuts, peas, potatoes, sunflower, soybeans and some ornamentals.

CAS Registry No: 51218-45-2

Molecular Formula: C<sub>15</sub>H<sub>22</sub>ClNO<sub>2</sub>

Molecular Weight: 283.795

Melting Point (°C): liquid

Boiling Point (°C):

100 (at 0.001 mmHg, Herbicide Handbook 1989; Budavari 1989; Worthing & Hance 1991; Montgomery 1993; Milne 1995)

Density (g/cm<sup>3</sup> at 20°C):

1.12 (Hartley & Kidd 1987; Worthing & Hance 1991; Montgomery 1993; Milne 1995)

1.085 (Herbicide Handbook 1989)

Molar Volume (cm<sup>3</sup>/mol):

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

258.0 (calculated-density)

Dissociation Constant pK<sub>a</sub>:

Enthalpy of Fusion, ΔH<sub>fus</sub> (kJ/mol):

Entropy of Fusion, ΔS<sub>fus</sub> (J/mol K):

Fugacity Ratio at 25°C (assuming ΔS<sub>fus</sub> = 56 J/mol K), F: 1.0

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

530 (Martin & Worthing 1977)

440 (selected, Ellgehausen et al. 1980)

520 (20°C, Ashton & Crafts 1981; Spencer 1982)

530 (shake flask-HPLC, Ellgehausen et al. 1981)

530 (20°C, Hartley & Kidd 1987; Herbicide Handbook 1989; Budavari 1989; Montgomery 1993)

530 (Hartley & Graham-Bryce 1980; Beste & Humburg 1983)

530 (20°C, Worthing & Walker 1987, Worthing & Hance 1991; Majewski & Capel 1995; Milne 1995)

488 (Tomlin 1994)

530 (20–25°C, selected, Hornsby et al. 1996)

531, 505 (supercooled liquid S<sub>L</sub>: literature derived value LDV, final adjust value FAV, Muir et al. 2004)

Vapor Pressure (Pa at 25°C or as indicated and reported temperature dependence equations):

0.00170 (20°C, Hartley & Graham-Bryce 1980)

0.00173 (20°C, Ashton & Crafts 1981)

0.00173 (20°C, volatilization rate, Burkhard & Guth 1981)

0.00170 (20°C, Hartley & Kidd 1987)

0.00170 (20°C, Worthing & Walker 1987, Worthing & Hance 1991)

0.00173 (20°C, Herbicide Handbook 1989; Budavari 1989; Montgomery 1993)

4.20 × 10<sup>-3</sup>, 6.60 × 10<sup>-2</sup>, 0.70, 5.40, 33.0 (25, 50, 70, 100, 125°C, gas saturation-GC, Rordorf 1989)

log (P<sub>L</sub>/Pa) = 13.115 – 4619.7/(T/K); measured range 32.5–140°C (gas saturation-GC, Rordorf 1989)

0.00420 (Tomlin 1994)

- 0.0023 (liquid  $P_L$ , GC-RT correlation; Donovan 1996)  
 0.00418 (selected, Halfon et al. 1996)  
 0.00418 (20–25°C, selected, Hornsby et al. 1996)  
 0.00239, 0.0024 (supercooled liquid  $P_L$ : literature derived value LDV, final adjust value FAV, Muir et al. 2004)

Henry's Law Constant ( $\text{Pa}\cdot\text{m}^3/\text{mol}$  at 25°C or as indicated. Additional data at other temperatures designated \* are compiled at the end of this section):

- 0.00092 (Hartley & Graham-Bryce 1980)  
 0.00093 (20°C, volatilization rate, Burkhard & Guth 1981)  
 0.00091 (20°C, calculated-P/C as per Worthing & Walker 1987)  
 0.00093 (20°C, calculated-P/C, Montgomery 1993)  
 0.00082 (20°C, calculated-P/C, Majewski & Capel 1995)  
 0.00244 (calculated-P/C, Otto et al. 1997)  
 0.00782 (20°C, distilled water, wetted wall column-GC, Rice et al. 1997b)  
 0.00110 (calculated-P/C, this work)  
 0.00238\* (20°C, gas stripping-GC/MS, measured range 283.05–299.45 K, Feigenbrugel et al. 2004)  
 $H'/(M \text{ atm}^{-1}) = (3.0 \pm 0.4) \times 10^{-11} \exp[(10200 \pm 1000)/(T/K)]$ ; temp range 283–310 K (Arrhenius eq., gas stripping-GC/MS, Feigenbrugel et al. 2004)  
 0.0014, 0.0014 (literature derived value LDV, final adjust value FAV, Muir et al. 2004)

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

- 3.13 (shake flask-HPLC, Ellgehausen et al. 1980; Geyer et al. 1991)  
 3.28 (shake flask-HPLC, Ellgehausen et al. 1981)  
 3.45 (Worthing & Hance 1991)  
 2.93, 3.45 (Montgomery 1993)  
 3.13, 3.28 (quoted, Sangster et al. 1993)  
 2.90 (Tomlin 1994)  
 3.45 (Milne 1995)  
 3.31, 2.95 (selected, calculated-f const., Pinsuwan et al. 1995)  
 3.13 (recommended, Hansch et al. 1995)  
 2.60 (RP-HPLC-RT correlation using short ODP column, Donovan & Pescatore 2002)  
 3.10 (literature derived value LDV, Muir et al. 2004)

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

- 9.37 (final adjust value FAV, Muir et al. 2004)

Bioconcentration Factor,  $\log BCF$ :

- 1.813 (log BF-bioaccumulation of algae, Ellgehausen et al. 1980)  
 0.733 (log BF-bioaccumulation of daphnids, Ellgehausen et al. 1980; quoted, Geyer et al. 1991)  
 0.851 (log BF-bioaccumulation of catfish, Ellgehausen et al. 1980)  
 1.26 (calculated-S, Kenaga 1980)  
 1.15 (catfish *Ictalurus melas*, wet wt basis, Wang et al. 1996)

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

- 2.15 (soil, calculated-S, Kenaga 1980)  
 2.26 (soil, screening model calculations, Jury et al. 1987b)  
 2.00, 2.15, 2.28, 2.30 (soil, quoted values, Bottoni & Funari 1992)  
 2.46, 2.46 (soil, quoted exptl., calculated-MCI  $\chi$  and fragment contribution, Meylan et al. 1992)  
 2.30 (20–25°C, selected, Wauchope et al. 1992; Hornsby et al. 1996)  
 2.08–2.49 (Montgomery 1993; Tomlin 1994)  
 2.46 (soil, calculated-MCI  $^1\chi$ , Sabljic et al. 1995)  
 2.43 (soil, estimated-general model using molecular descriptors, Gramatica et al. 2000)  
 2.28, 2.19, 2.69 (soils: organic carbon  $OC \geq 0.1\%$ ,  $OC \geq 0.5\%$ ,  $0.1 \leq OC < 0.5\%$ , average, Delle Site 2001)

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

Volatilization:



Photolysis: under optimum exposure conditions to natural sunlight,  $t_{1/2} \sim 8$  d (Herbicide Handbook 1989).

Oxidation ;  $k_{OH} = 5.6 \times 10^{-11} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$  at 298 K in gas phase with atmospheric lifetime of 0.9 h but reduced to 0.4 h at 283 K;  $\log k_{OH}(\text{aq.}) = 1.2 \times 10^{10} \text{ M}^{-1} \text{ s}^{-1}$  in aqueous phase (Feigenbrugel et al. 2004)

Hydrolysis:  $t_{1/2} > 200$  d at 20°C and  $1 \leq \text{pH} \leq 9$  (Montgomery 1993);

$t_{1/2}(\text{calc}) > 200$  d ( $2 \leq \text{pH} \leq 10$ ) (Tomlin 1994).

Biodegradation: overall degradation rate constant  $k = 0.0154 \text{ h}^{-1}$  with  $t_{1/2} = 45.0$  h in sewage sludge and rate constant  $k = 0.0460 \text{ d}^{-1}$  with  $t_{1/2} = 15.1$  d in garden soil (Müller & Buser 1995).

Biotransformation:

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

$k_2 = 9.11 \text{ d}^{-1}$  (catfish, Ellgehausen et al. 1980)

$k_1 = 0.336 \text{ h}^{-1}$ ,  $k_2 = 0.024 \text{ h}^{-1}$  (catfish *Ictalurus melas*, Wang et al. 1996)

#### Half-Lives in the Environment:

Air:

Surface water:

Ground water: reported  $t_{1/2} = 20, 30, 42$ , and  $47\text{--}107$  d (Bottoni & Funari 1992)  
degradation time  $500\text{--}1000$  d (Tomlin 1994).

Sediment:

Soil:  $t_{1/2} = 15\text{--}38$  d in clay loam soils and  $t_{1/2} = 33\text{--}100$  d in sandy loam soils (Zimdahl & Clark 1982; quoted, Montgomery 1993);

$t_{1/2} = 42$  d from field  $t_{1/2} = 3\text{--}4$  wk by using lysimeters (Bowman 1990);

$t_{1/2}(\text{calc}) = 80, 99$  and  $142$  d for the disappearance from upper 15 cm on an Ontario clay loam soil while the decline was followed for 332, 364 and 370 d, respectively, in 1987, 1988 and 1989 (Frank et al. 1991);

$t_{1/2} \sim 6$  d in soil (Worthing & Hance 1991; quoted, Montgomery 1993);

reported  $t_{1/2} = 20, 30, 42, 47\text{--}107$  d (Bottoni & Funari 1992)

field  $t_{1/2} = 90$  d at  $20\text{--}25^\circ\text{C}$  (selected, Wauchope et al. 1992; quoted, Richards & Baker 1993; Halfon et al. 1996; Hornsby et al. 1996);

soil  $t_{1/2} = 40$  d (Pait et al. 1992);

soil  $t_{1/2} = 28\text{--}46$  d (Di Guardo et al. 1994);

$t_{1/2} \sim 30$  d (Tomlin 1994);

degradation  $t_{1/2} = 15.1$  d in garden soil (Müller & Buser 1995);

$t_{1/2} \sim 28.3$  d under conventional tillage,  $t_{1/2} \sim 25.61$  d under ridge tillage and  $t_{1/2} \sim 8.63$  d with no tillage (Otto et al. 1997).

Biota:  $t_{1/2} = 1.15$  d in catfish (Ellgehausen et al. 1980);

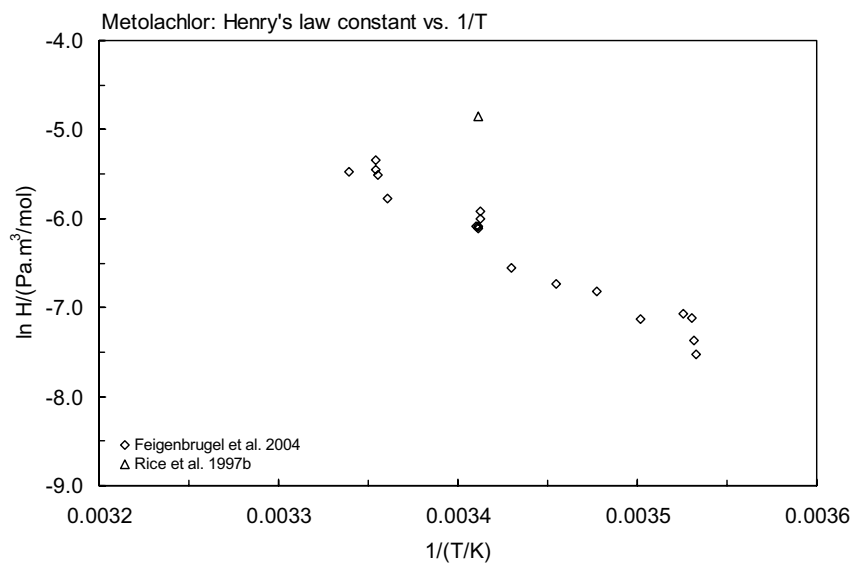
biochemical  $t_{1/2} = 42$  d from screening model calculations (Jury et al. 1987b).

**TABLE 17.1.1.49.1**

**Reported Henry's law constants of metolachlor at various temperatures**

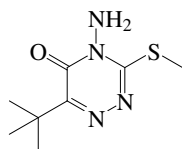
**Feigenbrugel et al. 2004**

gas stripping-GC/MS			
$t/^\circ\text{C}$	$H/(\text{Pa m}^3/\text{mol})$	$t/^\circ\text{C}$	$H/(\text{Pa m}^3/\text{mol})$
283.05	$5.39 \times 10^{-4}$	293.25	$2.262 \times 10^{-3}$
283.15	$6.34 \times 10^{-4}$	297.55	$3.099 \times 10^{-3}$
283.25	$8.126 \times 10^{-4}$	298.05	$4.053 \times 10^{-3}$
283.65	$8.465 \times 10^{-4}$	298.15	$4.757 \times 10^{-3}$
285.55	$8.01 \times 10^{-4}$	298.15	$4.312 \times 10^{-3}$
287.55	$1.088 \times 10^{-3}$	299.45	$4.170 \times 10^{-3}$
289.45	$1.193 \times 10^{-3}$		
291.55	$1.419 \times 10^{-3}$	$\ln H' = A - B/(T/K)$	
293.05	$2.702 \times 10^{-3}$	$H'/(M/\text{atm})$	
293.05	$2.471 \times 10^{-3}$	A	$-24.2298$
293.15	$2.282 \times 10^{-3}$	B	$10200$
293.15	$2.227 \times 10^{-3}$		



**FIGURE 17.1.1.49.1** Logarithm of Henry's law constant versus reciprocal temperature for metolachlor.

## 17.1.1.50 Metribuzin



Common Name: Metribuzin

Synonym: Metribuzine, Lexone, Preview, Sencor, Sencoral, Sencorer, Sencorex

Chemical Name: 4-amino-6-(t-butyl)-3-(methylthio)-1,2,4-triazin-5-(4*H*)-one

CAS Registry No: 21087-64-9

Uses: herbicide

Molecular Formula: C<sub>8</sub>H<sub>14</sub>N<sub>4</sub>OS

Molecular Weight: 214.288

Melting Point (°C):

126 (Lide 2003)

Boiling Point (°C): 132.2 Pa (Tomlin 1994)

Density (g/cm<sup>3</sup> at 20°C):

1.31 (Hartley & Kidd 1987; Montgomery 1993; Tomlin 1994)

1.28 (Herbicide Handbook 1989)

Dissociation Constant pK<sub>b</sub>:

13.0 (Wauchope et al. 1992; Hornsby et al. 1996)

1.0 (pK<sub>a</sub>, Montgomery 1993)

Enthalpy of Fusion, ΔH<sub>fus</sub> (kJ/mol):

Entropy of Fusion, ΔS<sub>fus</sub> (J/mol K):

Fugacity Ratio at 25°C (assuming ΔS<sub>fus</sub> = 56 J/mol K), F: 0.102 (mp at 126°C)

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

1220 (Kenaga & Goring 1980; Kenaga 1980b; Verschueren 1983)

1200 (20°C, Spencer 1982; Worthing & Walker 1983, 1987; Hartley & Kidd 1987)

1220 (Herbicide Handbook 1989)

1050 (20°C, Montgomery 1993; Tomlin 1994)

1220 (20–25°C, selected, Wauchope et al. 1992; Hornsby et al. 1996)

1065 (20–25°C, reported as 4.97E + 01 mol/m<sup>3</sup>, Majewski & Capel 1995)

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

< 1.3 × 10<sup>-3</sup> (20°C, Worthing 1983, 1987; Hartley & Kidd 1987; Tomlin 1994)

< 1.3 × 10<sup>-3</sup>; 2.67 × 10<sup>-2</sup> (20°C; 60°C, Herbicide Handbook 1989)

5.8 × 10<sup>-5</sup> (20°C, Montgomery 1993)

< 1.3 × 10<sup>-3</sup> (20–25°C, Wauchope et al. 1992; Hornsby et al. 1996)

5.89 × 10<sup>-4</sup> (20–25°C, Majewski & Capel 1995)

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

< 1.3 × 10<sup>-3</sup> (Spencer 1982; Worthing 1987; Hartley & Kidd 1987)

1.21 × 10<sup>-5</sup> (calculated-P/C, Montgomery 1993)

1.18 × 10<sup>-5</sup> (calculated-P/C, Majewski & Capel 1995)

Octanol/Water Partition Coefficient, log K<sub>ow</sub>:

1.60, 1.70 (quoted, Montgomery 1993)

1.58 (pH 5.6, Tomlin 1994)

1.70 (LOGPSTAR or CLOGP data, Sabljic et al. 1995)

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

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

- 2.46, 1.48, < 1.30 (algae, activated sludge, fish in 3-d testing, Korte et al. 1978)
- 1.77, 1.75 (*Chlorella*, calculated-solubility, Geyer et al. 1981)
- 1.77, 1.48, 1.04 (algae, activated sludge, *Golden orfe*, Geyer et al. 1982)
- 1.04, 0.602 (calculated-solubility, calculated- $K_{OW}$ , Kenaga 1980a)
- 1.48, 1.78, 1.0 (activated sludge, algae, *Golden ide*, Freitag et al. 1985)

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

- 1.98 (soil, Kenaga & Goring 1980)
- 1.98; 1.94 (quoted, calculated- $K_{OW}$ , Kenaga 1980b)
- 0.954–2.72 (soil, literature range, Wauchope et al. 1992)
- 1.80 (soil, estimated, Wauchope et al. 1992; Hornsby et al. 1996)
- 1.94–1.98, 2.18 (soil, Bottoni & Funari 1992)
- 1.80–2.72 (soil, Montgomery 1993)
- 1.78 (soil, Senseman et al. 1997)
- 1.71 (soil, calculated-MCI  $\chi$ , Sabljic et al. 1995)
- 1.71; 1.68, 1.33 (soil, quoted obs.; estimated-class-specific model, estimated-general model using molecular descriptors, Gramatica et al. 2000)
- 2.05, 2.06, 2.04 (soils: organic carbon  $OC \geq 0.1\%$ ,  $OC \geq 0.5\%$ ,  $0.1 \leq OC < 0.5\%$ , average, Delle Site 2001)

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

Volatilization:

Photolysis: photodecomposition in water is very rapid with  $t_{1/2} < 1$  d; on soil surface under natural sunlight conditions,  $t_{1/2} = 14$ –25 d (Tomlin 1994).

Oxidation:

Hydrolysis:  $t_{1/2} \sim 1$  wk in pond water (Hartley & Kidd 1987; Montgomery 1993).

Biodegradation: under goes microbial degradation in moist soil (Worthing 1987)

Biotransformation:

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

Half-Lives in the Environment:

Air:

Surface water: hydrolysis  $t_{1/2} \sim 1$  wk in pond water (Hartley & Kidd 1987; Montgomery 1993; Tomlin 1994); stable to dilute acids and alkalis,  $t_{1/2} = 6.7$  h at pH 1.2 and 37°C;  $t_{1/2} = 569$  h at pH 4,  $t_{1/2} = 47$  d at pH 7 and  $t_{1/2} = 191$  h at pH 9 for 70°C (Tomlin 1994).

Ground water: reported half-life or persistence  $t_{1/2} = 4$ –25, 17–301 and 56 d (Bottoni & Funari 1992).

Sediment:

Soil: undergoes microbial degradation in moist soil (Worthing 1983, 1987);

half-life varies with soil types,  $t_{1/2} \sim 90$ –115 d for Red River, Almasippi, and Stockton soils the 3 times this period for Newdale soil for normal application rates (Verschuere 1983);

$t_{1/2} \sim 1$ –2 months in soil (Hartley & Kidd 1987; Tomlin 1994);

$t_{1/2} \sim 30$ –60 d in various soil types varies greatly with climatic conditions, during the growing season (Herbicide Handbook 1989);

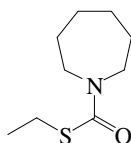
$t_{1/2} = 9$ –12 d irrespective of the number of previous treatments in the field;  $t_{1/2} = 25$ –40 d irrespective of the pretreatment history of the soil at 20°C in the laboratory (Walker & Welch 1992)

reported  $t_{1/2} = 23$ –120 d and the recommended field  $t_{1/2} = 40$  d (Wauchope et al. 1992; Hornsby et al. 1996; quoted, Senseman et al. 1997);

half-lives of in two surface soil microcosms under nitrate,  $t_{1/2} = 157$  d and non-nitrate,  $t_{1/2} = 187$  and 349 d in reducing culture conditions at 16.4°C (Pavel et al. 1999).

Biota: in mammals, following oral administration, 90% elimination within 96 h (Hartley & Kidd 1987).

## 17.1.1.51 Molinate



Common Name: Molinate

Synonym: Felan, Higalnat, Hydram, Jalan, Molmate, Ordram, Stauffer R 4572, Sakkimok, Yalan, Yulan

Chemical Name: 1*H*-azepine-1-carbothioic acid, hexahydro, *S*-ethyl ester; ethyl 1-hexa-methyleneiminocarbothioate

Uses: selective herbicide to control the germination of annual grasses and broadleaf weeds in rice crops.

CAS Registry No: 2212-67-1

Molecular Formula: C<sub>9</sub>H<sub>17</sub>NOS

Molecular Weight: 187.302

Melting Point (°C): < 25 (Montgomery 1993)

Boiling Point (°C):

202 (at 10 mmHg, Hartley & Kidd 1987; Herbicide Handbook 1989; Worthing & Hance 1991; Milne 1995)

117 (at 10 mmHg, Montgomery 1993)

Density (g/cm<sup>3</sup> at 20°C):

1.064 (Hartley & Kidd 1987)

1.0643 (Herbicide Handbook 1989; Montgomery 1993)

1.063 (Worthing & Hance 1991; Milne 1995)

Molar Volume (cm<sup>3</sup>/mol):

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

176.1 (calculated-density)

Dissociation Constant pK<sub>a</sub>:

Enthalpy of Fusion, ΔH<sub>fus</sub> (kJ/mol):

Entropy of Fusion, ΔS<sub>fus</sub> (J/mol K):

Fugacity Ratio at 25°C (assuming ΔS<sub>fus</sub> = 56 J/mol K), F: 1.0

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

880 (20°C, Weber 1972; Hartley & Kidd 1987; Worthing & Walker 1987; Worthing & Hance 1991)

800 (Martin & Worthing 1977)

800–912 (Weber et al. 1980)

912 (21°C, Spencer 1982)

800 (20°C, Herbicide Handbook 1983, 1989)

870 (Kanazawa 1989)

970 (20–25°C, selected, Wauchope et al. 1992; Hornsby et al. 1996; Armbrust 2000)

880 (20°C, Montgomery 1993; Tomlin 1994; Milne 1995)

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

0.748 (20°C, Weber 1972; Worthing & Walker 1987)

0.746 (20°C, Khan 1980)

0.185 (20°C, GC-RT correlation, Kim 1985)

0.413 (Seiber et al. 1986, 1989)

0.746 (Hartley & Kidd 1987; Montgomery 1993; Tomlin 1994)

0.746 (Herbicide Handbook 1989; Worthing & Hance 1991)

0.746 (20–25°C, selected, Wauchope et al. 1992)

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

0.097 (calculated-P/C, Seiber et al. 1986, 1989)

0.314 (20°C, calculated-P/C, Suntio et al. 1988)

0.159 (20°C, calculated-P/C as per Worthing & Walker 1987;)

0.159 (20°C, calculated-P/C, Muir 1991)

0.095	(20°C, calculated-P/C, Sagebiel et al. 1992)
0.460	(20°C, gas-stripping method, Sagebiel et al. 1992)
0.390	(20°C, headspace-GC method, Sagebiel et al. 1992)
0.162	(calculated-P/C, Montgomery 1993)
0.145	(calculated-P/C, this work)
0.132	(quoted lit., Armbrust 2000)
0.397	(20°C, selected from literature experimentally measured data, Staudinger & Roberts 2001)
$\log K_{AW} = 6.527 - 3024/(T/K)$ (van't Hoff eq. derived from literature data, Staudinger & Roberts 2001)	

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

3.21	(shake flask-GC, Kanazawa 1981)
2.88	(Worthing & Hance 1991; Tomlin 1994)
2.88	(Montgomery 1993)
3.13	(RP-HPLC-RT correlation, Saito et al. 1993)
3.26	(RP-HPLC-RT correlation, Sicbaldi & Finizio 1993)
3.21	(recommended, Sangster 1993)
2.88	(Milne 1995)
3.21	(recommended, Hansch et al. 1995)
3.25	(RP-HPLC-RT correlation, Finizio et al. 1997)

Bioconcentration Factor,  $\log BCF$ :

1.15	(calculated-S, Kenaga 1980; quoted, Pait et al. 1992)
1.41	( <i>Peudorashbora parva</i> , Kanazawa 1981)

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

2.04	(soil, calculated-S, Kenaga 1980)
1.92	(average of 2 soils, Kanazawa 1989)
1.92, 2.04	(soil, quoted values, Bottoni & Funari 1992)
1.92, 2.46	(soil, quoted exptl., calculated-MCI $\chi$ and fragments contribution, Meylan et al. 1992)
2.28	(soil, 20–25°C, selected, Wauchope et al. 1992; Hornsby et al. 1996)
1.93–1.97	(Montgomery 1993)
2.28	(selected, Lohninger 1994)
1.92	(soil, calculated-MCI $\chi$ , Sabljic et al. 1995)
2.07	(soil, quoted lit., Armbrust 2000)
1.92; 2.31, 1.86 (soil, quoted exptl.; estimated-class specific model, estimated-general model using molecular descriptors, Gramatica et al. 2000)	

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

- Volatilization:  $k = 0.0150 \text{ h}^{-1}$  (average of 2 runs, Seiber et al. 1986);  $1.1 \text{ kg ha}^{-1}$  (1st 4 day) from flooded rice fields (Seiber et al. 1986; Seiber & McChesney 1987);  
estimated  $t_{1/2} = 43 \text{ d}$  from 1 m depth of water at 20°C (Muir 1991).
- Photolysis:  $t_{1/2} = 7\text{--}10 \text{ d}$  for  $8\text{--}10 \mu\text{g mL}^{-1}$  to degrade in distilled water under  $> 290 \text{ nm}$  light (Soderquist et al. 1977; quoted, Cessna & Muir 1991);  
 $t_{1/2} = 96 \text{ h}$  for  $< 5\%$  of  $0.2 \mu\text{g mL}^{-1}$  to degrade in distilled water under sunlight (Deuel et al. 1978; quoted, Cessna & Muir 1991);  
 $t_{1/2} = 245 \text{ h}$  for  $2\text{--}54\%$  of  $10 \mu\text{g mL}^{-1}$  to degrade in distilled water under sunlight (Draper & Crosby 1984; quoted, Cessna & Muir 1991).
- Oxidation: calculated life-time of 6 h for the vapor-phase reaction with OH radicals in the troposphere (Atkinson et al. 1992; Kwok et al. 1992);  
measured rate constant for reaction with hydroxyl radical,  $k(\text{aq.}) = 0.85 \times 10^9 \text{ M}^{-1}\cdot\text{s}^{-1}$  in irradiated field water both in the laboratory and sunlit rice paddies (Mabury & Crosby 1996);  
measured hydroxy radical reaction rate constant for molinate  $k = 7.7 \times 10^{12} \text{ M}^{-1} \text{ h}^{-1}$  (Armbrust 2000).
- Hydrolysis:  $t_{1/2} > 10 \text{ d}$  in aqueous buffer at pH 5–9 in the dark (Soderquist et al. 1977; quoted, Muir 1991); stable aqueous hydrolysis rate at pH 5, 7, 9 (Armbrust 2000).

Biodegradation:  $t_{1/2} \sim 16$  d for  $0.2 \mu\text{g mL}^{-1}$  to biodegrade in flooded soils (Deuel et al. 1978; quoted, Muir 1991);  
 $t_{1/2} = 10$  wk for  $4.2 \mu\text{g mL}^{-1}$  to biodegrade in flooded soil and  $t_{1/2} < 2$  wk in water both at  $21\text{--}26^\circ\text{C}$  (Thomas & Holt 1980; quoted, Muir 1991);  
aerobic rate constant,  $k = 2.22 \times 10^{-3} \text{ h}^{-1}$  (Armbrust 2000).

Biotransformation:

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

#### Half-Lives in the Environment:

Air: calculated lifetime of 6 h for the vapor-phase reaction with OH radicals in the troposphere (Atkinson et al. 1992; Kwok et al. 1992).

Surface water:  $t_{1/2} = 84$  h from dissipation from flooded rice fields (Seiber & McChesney 1987; quoted, Seiber et al. 1989).

Ground water: reported half-lives or persistence,  $t_{1/2} = 3\text{--}14$ ,  $8\text{--}25$  and  $40\text{--}160$  d (Bottoni & Funari 1992)

Sediment:

Soil: persistence of 2 months in soil (Wauchope 1978);

$t_{1/2} \sim 3$  wk in moist loam soils at  $21\text{--}27^\circ\text{C}$  (Herbicide Handbook 1989);

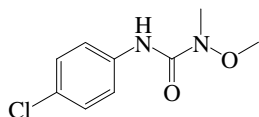
selected field  $t_{1/2} = 21$  d (Wauchope et al. 1992; quoted, Halfon et al. 1996; Hornsby et al. 1996);

soil  $t_{1/2} = 21$  d (Pait et al. 1992);

reported  $t_{1/2} = 3\text{--}14$  d,  $8\text{--}25$  d and  $40\text{--}160$  d (Bottoni & Funari 1992).

Biota:

## 17.1.1.52 Monolinuron



Common Name: Monolinuron

Synonym: Afesin, Aresin, Arresin, Hoe 02747

Chemical Name: 3-(4-chlorophenyl)-1-methoxy-1-methylurea; *N'*-(4-chlorophenyl)-*N*-methoxy-*N*-methylurea

Uses: herbicide for pre- or post-emergence control of annual broadleaf weeds and annual grasses in asparagus, berry fruit, cereals, maize, field beans, vines, leeks, onions, potatoes, herbs, lucerne, flowers, ornamental shrubs and trees, etc.

CAS Registry No: 1746-81-2

Molecular Formula: C<sub>9</sub>H<sub>11</sub>ClN<sub>2</sub>O<sub>2</sub>

Molecular Weight: 214.648

Melting Point (°C):

77 (Lide 2003)

Boiling Point (°C):

Density (g/cm<sup>3</sup> at 20°C):

Molar Volume (cm<sup>3</sup>/mol):

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

Dissociation Constant pK<sub>a</sub>:

Enthalpy of Fusion, ΔH<sub>fus</sub> (kJ/mol):

Entropy of Fusion, ΔS<sub>fus</sub> (J/mol K):

Fugacity Ratio at 25°C (assuming ΔS<sub>fus</sub> = 56 J/mol K), F: 0.309 (mp at 77°C)

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

735 (20°C, Melnikov 1971)

735 (Spencer 1973, 1982)

580 (Martin & Worthing 1977; Khan 1980)

735 (Worthing & Walker 1983, 1987, Hartley & Kidd 1987; Worthing & Hance 1991; Tomlin 1994)

735 (20–25°C, selected, Augustijn-Beckers et al. 1994; Hornsby et al. 1996)

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

0.02 (22°C, Khan 1980; Hartley & Kidd 1987)

0.0015 (20°C, Spencer 1982)

6.40 (65°C, Worthing & Hance 1991)

0.02 (20–25°C, selected, Augustijn-Beckers et al. 1994; Hornsby et al. 1996)

0.0013, 0.10 (20°C, 50°C, Tomlin 1994)

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

0.0058 (calculated-P/C, this work)

Octanol/Water Partition Coefficient, log K<sub>ow</sub>:

1.60 (Briggs 1969)

2.30 (shake flask-UV, Briggs 1981)

1.60 (selected, Dao et al. 1983)

1.99 (RP-HPLC-k' correlation, Braumann et al. 1983)

2.22 (shake flask, Mitsutake et al. 1986)

2.20 (Worthing & Hance 1991; Tomlin 1994)

2.16 (RP-HPLC-RT correlation, Sicbaldi & Finizio 1993)

2.30 (recommended, Sangster 1993)

2.30 (recommended, Hansch et al. 1995)

2.31 (Pomona-database, Müller & Kördel 1996)



2.16 (RP-HPLC-RT correlation, Finizio et al. 1997)

Bioconcentration Factor, log BCF:

- 1.23; 1.00 (calculated-S, calculated- $K_{OC}$ , Kenaga 1980)
- 1.85 (activated sludge, Freitag et al. 1982, 1984, 1985)
- 1.52, < 1.0 (algae, golden orfe, Freitag et al. 1982)
- 1.60, 1.30 (algae, golden ide, Freitag et al. 1985)

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

- 2.30 (soil, Hamaker & Thompson 1972)
- 2.11 (soil, calculated-S as per Kenaga & Goring 1980, Kenaga 1980)
- 1.60 (reported as log  $K_{OM}$ , Briggs 1981)
- 2.36, 2.08, 1.21 (estimated-S, calculated-S and mp, calculated- $K_{OW}$ , Karickhoff 1981)
- 2.40–2.70 (soil, Worthing & Hance 1991)
- 2.26–2.30, 2.40–2.70 (soil, quoted values, Bottoni & Funari 1992)
- 1.78 (soil, HPLC-screening method, mean value of different stationary and mobile phases, Kördel et al. 1993, 1995b)
- 2.30 (20–25°C, estimated, Augustijn-Beckers et al. 1994; Hornsby et al. 1996)
- 2.10 (soil, calculated-MCI  $^1\chi$ , Sabljic et al. 1995)
- 1.78; 2.33 (HPLC-screening method; calculated-PCKOC fragment method, Müller & Kördel 1996)
- 2.44, 1.50, 1.71, 1.754, 2.45 (first generation Eurosoils ES-1, ES2, ES-3, ES-4, ES-5, shake flask/batch equilibrium-HPLC/UV, Gawlik et al. 1998, 1999)
- 2.05, 1.72, 1.695, 1.825, 2.407 (second generation Eurosoils ES-1, ES2, ES-3, ES-4, ES-5, shake flask/batch equilibrium-HPLC/UV, Gawlik et al. 1999)
- 2.050, 1.721, 1.695, 1.825, 2.407 (second generation Eurosoils ES-1, ES-2, ES-3, ES-4, ES-5, shake flask-batch equilibrium-HPLC/UV and HPLC- $k'$  correlation, Gawlik et al. 2000)
- 2.10; 2.04, 2.31 (soil, quoted obs.; estimated-class-specific model, estimated-general model using molecular descriptors, Gramatica et al. 2000)
- 1.88, 1.88 (soils: organic carbon OC  $\geq 0.1\%$ , OC  $\geq 0.5\%$ , average, Delle Site 2001)

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

Photolysis:  $t_{1/2} = 23$  h for 66% of 286  $\mu\text{g/mL}$  to degrade in distilled water under > 300 nm light (Kotzias et al. 1974; quoted, Cessna & Muir 1991).

Half-Lives in the Environment:

Air:

Surface water:

Ground water: reported half-lives or persistence,  $t_{1/2} = 45$ –60 d (Bottoni & Funari 1992)

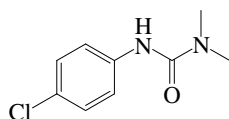
Sediment:

Soil: reported  $t_{1/2} = 45$ –60 d (Worthing & Hance 1991);

estimated field  $t_{1/2} = 60$  d (Augustijn-Beckers et al. 1994; Hornsby et al. 1996).

Biota:

## 17.1.1.53 Monuron



Common Name: Monuron

Synonym: Chlorfenidim, CMU, Karmex, Lirobetarex, Monurex, Monurox, Rosuran, Telvar, Urox

Chemical Name: *N'*-(4-chlorophenyl)-*N,N*-dimethylurea; 1,1-dimethyl-3-(*p*-chlorophenyl)urea

Uses: herbicide; also as sugar cane flowering suppressant.

CAS Registry No: 150-68-5

Molecular Formula: C<sub>9</sub>H<sub>11</sub>ClN<sub>2</sub>O

Molecular Weight: 198.648

Melting Point (°C):

170.5 (Kühne et al. 1995; Lide 2003)

Boiling Point (°C):

185–200 (decomposes, Montgomery 1993)

Density (g/cm<sup>3</sup> at 20°C):

1.27 (Spencer 1982; Hartley & Kidd 1987; Montgomery 1993)

Molar Volume (cm<sup>3</sup>/mol):

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

173.0 (modified Le Bas method, Spurlock & Biggar 1994a)

Dissociation Constant pK<sub>a</sub>:

Enthalpy of Fusion, ΔH<sub>fus</sub> (kJ/mol):

Entropy of Fusion, ΔS<sub>fus</sub> (J/mol K):

Fugacity Ratio at 25°C (assuming ΔS<sub>fus</sub> = 56 J/mol K), F: 0.0374 (mp at 170.5°C)

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

203 (Freed 1966)

230 (Günther et al. 1968; Sanborn et al. 1977; Khan 1980; Ashton & Crafts 1981)

262 (shake flask-UV, Hurle & Freed 1972)

230 (20°C, Weber 1972; Worthing & Walker 1987)

230 (Martin & Worthing 1977; Hartley & Kidd 1987)

200 (shake flask-HPLC, Ellgehausen et al. 1981)

200 (20°C, selected, Suntio et al. 1988)

275 (Spurlock 1992; Spurlock & Biggar 1994b)

230 (at pH 6.26, Montgomery 1993)

230 (20–25°C, selected, Augustijn-Beckers et al. 1994; Hornsby et al. 1996)

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

$7.60 \times 10^{-5}$ ,  $1.2 \times 10^{-5}$  (25, 27°C, Nex & Swezey 1954)

$6.67 \times 10^{-5}$  (Bailey & White 1965)

$6.72 \times 10^{-5}$  (20°C, Weber 1972; Worthing & Walker 1987)

$6.67 \times 10^{-5}$  (Ashton & Crafts 1973, 1981; Khan 1980)

$5.33 \times 10^{-5}$ \* (30.35°C, Knudsen effusion, measured range 303.5–379.1 K, Wiedemann 1972)

$\log(P/\text{mmHg}) = 13.3052 - 5988.39/(T/K)$ ; temp range 303.5–379.1 K (Antoine eq., effusion, Wiedemann 1972)

$6.70 \times 10^{-5}$  (OECD 1981)

$2.30 \times 10^{-5}$  (calculated, Jury et al. 1983)

$6.00 \times 10^{-5}$  (Hartley & Kidd 1987)

$6.67 \times 10^{-5}$  (Budavari 1989)

$2.30 \times 10^{-5}$  (selected, Taylor & Spencer 1990)

$6.00 \times 10^{-5}$  (20°C, Montgomery 1993)

$6.67 \times 10^{-5}$  (20–25°C, selected, Augustijn-Beckers et al. 1994; Hornsby et al. 1996)

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

- $5.80 \times 10^{-5}$  ( $20^\circ\text{C}$ , volatilization rate, Burkhard & Guth 1981)
- $1.88 \times 10^{-5}$  (calculated-P/C, Jury et al. 1984, 1987a; Jury & Ghodrati 1989)
- $3.00 \times 10^{-3}$  ( $20^\circ\text{C}$ , calculated-P/C, Suntio et al. 1988)
- $1.91 \times 10^{-5}$  (calculated-P/C, Taylor & Glotfelty 1988)
- $5.60 \times 10^{-5}$  ( $20^\circ\text{C}$ , calculated-P/C, Muir 1991)
- $3.00 \times 10^{-3}$  ( $20^\circ\text{C}$ , calculated-P/C, Montgomery 1993)
- $6.60 \times 10^{-5}$  (calculated-P/C, this work)

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

- 1.46 (Briggs 1969)
- 1.66 (calculated-fragment const., Rekker 1977)
- 1.80 (shake flask-UV, Erckell & Walum 1979)
- 2.08 (selected, Ellgehausen et al. 1980; Geyer et al. 1991)
- 2.12 (Rao & Davidson 1980)
- 1.98 (shake flask-UV, Briggs 1981)
- 2.08 (shake flask, Ellgehausen et al. 1980)
- 1.66 (shake flask, Ellgehausen et al. 1981)
- 1.86 (selected, Dao et al. 1983; Gerstl & Helling 1987)
- 1.91 (RP-HPLC- $k'$  correlation Braumann et al. 1983)
- 1.80 (selected, Suntio et al. 1988)
- 2.12 (shake flask-HPLC, Spurlock 1992; Spurlock & Biggar 1994b)
- 1.46, 2.12 (Montgomery 1993)
- 1.86 (RP-HPLC-RT correlation, Sicbaldi & Finizio 1993)
- 1.94 (recommended, Sangster 1993)
- 1.89; 1.88 (shake flask-UV; RP-HPLC- $k'$  correlation, Liu & Qian 1995)
- 1.94 (recommended, Hansch et al. 1995)
- 1.99 (Pomona-database, Müller & Kördel 1996)
- 1.86 (RP-HPLC-RT correlation, Finizio et al. 1997)

Bioconcentration Factor,  $\log \text{BCF}$ :

- 1.786 ( $\log \text{BF}$  bioaccumulation factor for algae, Ellgehausen et al. 1980)
- 0.32 ( $\log \text{BF}$  bioaccumulation factor for daphnids, Ellgehausen et al. 1980)
- 0.245 ( $\log \text{BF}$  bioaccumulation factor for daphnids, Ellgehausen et al. 1980)
- 1.46 (calculated-S, Kenaga 1980)
- 0.699 (calculated- $K_{oc}$ , Kenaga 1980)
- 0.0 (*Trialenodes tardus*, Belluck & Felsot 1981)
- 1.58, 1.67 (cuticle/water: tomato, pepper; Evelyne et al. 1992)

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

- 2.00 (soil, Hamaker & Thompson 1972)
- 2.34 (soil, calculated-S as per Kenaga & Goring 1980, Kenaga 1980)
- 2.26 (av. of 18 soils, Rao & Davidson 1980)
- 1.70 (soil, converted from reported  $K_{om}$ , multiplied by 1,724, Briggs 1981)
- 2.58, 1.51 (estimated-S, calculated-S and mp, Karickhoff 1981)
- 1.07, 1.73 2.58 (estimated- $K_{ow}$ , Karickhoff 1981)
- 2.03, 1.85; 2.17, 1.52 (estimated- $K_{ow}$ s; solubilities, Madhun et al. 1986)
- 1.99; 2.12 (quoted; calculated-MCI  $\chi$ , Gerstl & Helling 1987)
- 2.26 (screening model calculations, Jury et al. 1987a,b; Jury & Ghodrati 1989)
- 1.99, 2.33 (Montgomery 1993)
- 2.18 ( $20$ – $25^\circ\text{C}$ , estimated, Augustijn-Beckers et al. 1994; Hornsby et al. 1996)
- 1.99 (soil, HPLC-screening method, mean value from different stationary and mobile phases, Kördel et al. 1993, 1995a,b)
- 2.29 (calculated- $K_{ow}$ , Liu & Qian 1995)
- 1.95 (soil, calculated-MCI  $^1\chi$ , Sabljic et al. 1995)

- 1.99; 1.92 (HPLC-screening method; calculated-PCKOC fragment method, Müller & Kördel 1996)
- 2.58, 1.77, 1.85, 1.77, 2.41 (first generation Eurosoils ES-1, ES2, ES-3, ES-4, ES-5, shake flask/batch equilibrium-HPLC/UV, Gawlik et al. 1998, 1999)
- 2.14, 2.018, 1.79, 1.764, 2.243 (second generation Eurosoils ES-1, ES2, ES-3, ES-4, ES-5, shake flask/batch equilibrium-HPLC/UV, Gawlik et al. 1999)
- 2.141, 2.018, 1.793, 1.764, 2.243 (second generation Eurosoils ES-1, ES-2, ES-3, ES-4, ES-5, shake flask/batch equilibrium-HPLC/UV and HPLC- $k'$  correlation, Gawlik et al. 2000)
- 1.95; 1.96, 2.13 (soil, quoted obs.; estimated-class-specific model, estimated-general model using molecular descriptors, Gramatica et al. 2000)
- 1.80, 1.80 (soils: organic carbon OC  $\geq 0.1\%$ , OC  $\geq 0.5\%$ , average, Delle Site 2001)

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

##### Volatilization:

- Photolysis:  $t_{1/2} = 14$  d for 6% of 200  $\mu\text{g mL}^{-1}$  to degrade in distilled water under sunlight (Crosby & Tang 1969; quoted, Cessna & Muir 1991);
- $t_{1/2} = 2.25$  h for 44% of 200  $\mu\text{g mL}^{-1}$  to degrade in distilled water under 300 nm light (Tanaka et al. 1977; quoted, Cessna & Muir 1991);
- $t_{1/2} = 2.25$  s for 75% of 100  $\mu\text{g mL}^{-1}$  to degrade in 0.2% Triton X-100 aqueous solution under 300 nm light (Tanaka et al. 1981; quoted, Cessna & Muir 1991);
- $t_{1/2} = 2.25$  h for  $> 70\%$  of 200  $\mu\text{g mL}^{-1}$  to degrade in aqueous solutions of nonionic surfactants at concns. in excess of critical micelle concn. under 300 nm light (Tanaka et al. 1979; quoted, Cessna & Muir 1991);
- $t_{1/2} = 45$  h for 69% of 165  $\mu\text{g mL}^{-1}$  to degrade in distilled water under  $> 280$  nm light (Tanaka et al. 1982; quoted, Cessna & Muir 1991).

##### Oxidation:

Hydrolysis:  $t_{1/2} > 4$  months for 3974  $\mu\text{g mL}^{-1}$  to hydrolyze in phosphate buffer at pH 5–9 and 20°C (El-Dib & Aly 1976; quoted, Muir 1991).

Biodegradation: aerobic  $t_{1/2} \sim 7$  d for 0.01  $\mu\text{g mL}^{-1}$  to biodegrade in river water (Eichelberger & Lichtenberg 1971; quoted, Muir 1991);

$t_{1/2} = 166$  d for a 100 d leaching and screening test in 0–10 cm depth of soil (Jury et al. 1983, 1984, 1987a,b; Jury & Ghodrati 1989);

aerobic  $t_{1/2} \sim 10$ –15 d for 0.0005–10  $\mu\text{g mL}^{-1}$  to biodegrade in filtered sewage water at 20°C (Wang et al. 1985; quoted, Muir 1991).

##### Biotransformation:

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

$k_2 = 21.05$  d $^{-1}$  (catfish, Ellgehausen et al. 1980)

#### Half-Lives in the Environment:

##### Air:

Surface water: persistence of up to 8 wk in river water (Eichelberger & Lichtenberg 1971).

##### Ground water:

##### Sediment:

Soil:  $t_{1/2} = 5.0$  months at 15°C and 4.1 months at 30°C in soils (Freed & Haque 1973);

reported  $t_{1/2} = 166$  d from screening model calculations (Jury et al. 1987a,b; Jury & Ghodrati 1989; quoted, Montgomery 1993);

estimated field  $t_{1/2} = 170$  d (Augustijn-Beckers et al. 1994; Hornsby et al. 1996).

Biota:  $t_{1/2} = 0.45$  d in catfish (Ellgehausen et al. 1980);

biochemical  $t_{1/2} = 166$  d from screening model calculations (Jury et al. 1987a,b; Jury & Ghodrati 1989).

TABLE 17.1.1.53.1  
Reported vapor pressures of monuron at various temperatures

Wiedemann 1972			
Knudsen effusion			
T/K	P/Pa	T/K	P/Pa
303.5	$5.33 \times 10^{-5}$	358.7	0.0536
316.0	$2.44 \times 10^{-4}$	360.2	0.0561
329.8	$2.16 \times 10^{-3}$	379.1	0.399
330.6	$1.53 \times 10^{-3}$		
330.6	$2.22 \times 10^{-3}$	$\log P = A - B/(T/K)$	
338.8	$7.05 \times 10^{-3}$		P/mmHg
341.4	$9.45 \times 10^{-3}$	A	13.3952
345.7	0.0105	B	5988.39
349.5	0.0204		
357.0	0.0529	$\Delta H_{\text{subl}}/(\text{kJ mol}^{-1}) = 114.6$	

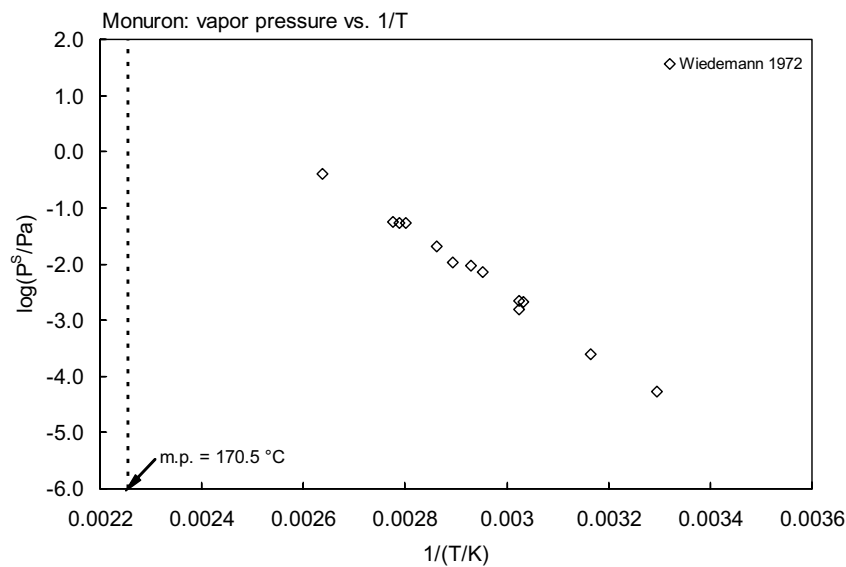
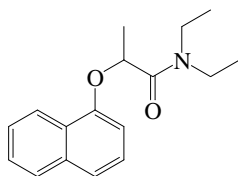


FIGURE 17.1.1.53.1 Logarithm of vapor pressure versus reciprocal temperature for monuron.

## 17.1.1.54 Napropamide



Common Name: Napropamide

Synonym: Devrinol

Chemical Name: 2-( $\alpha$ -naphthloxy)-*N,N*-diethylpropionamide

CAS Registry No: 15299-99-7

Uses: herbicide

Molecular Formula:  $C_{17}H_{21}NO_2$

Molecular Weight: 271.355

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

75 (Worthing & Walker 1987; Lide 2003)

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

Molar Volume ( $cm^3/mol$ ):

Dissociation Constant  $pK_a$ :

2.93 (Woodburn et al. 1993)

Enthalpy of Fusion,  $\Delta H_{fus}$  (kJ/mol):

Entropy of Fusion,  $\Delta S_{fus}$  (J/mol K):

Fugacity Ratio at  $25^{\circ}C$  (assuming  $\Delta S_{fus} = 56$  J/mol K), F: 0.323 (mp at  $75^{\circ}C$ )

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

69 (shake flask-LSC or GC, Gerstl & Mingelgrin 1984)

73 ( $20^{\circ}C$ , Spencer 1982; Hartley & Kidd 1987; Worthing & Walker 1987; Herbicide Handbook 1989; Montgomery 1993; Tomlin 1994)

74 ( $20$ – $25^{\circ}C$ , selected, Wauchope et al. 1992; Hornsby et al. 1996)

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

$2.67 \times 10^{-4}$  (Spencer 1982)

$5.3 \times 10^{-4}$  (Herbicide Handbook 1989)

$5.3 \times 10^{-4}$  (Hartley & Kidd 1987; Worthing & Walker 1987; Montgomery 1993; Tomlin 1994)

$2.27 \times 10^{-5}$  ( $20$ – $25^{\circ}C$ , selected, Wauchope et al. 1992; Hornsby et al. 1996)

$1.67 \times 10^{-3}$  ( $20$ – $25^{\circ}C$ , Majewski & Capel 1995)

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

0.00294 (calculated-P/C, Montgomery 1993)

0.00197 ( $20$ – $25^{\circ}C$ , Majewski & Capel 1995)

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

3.08 (shake flask-GC or LSC, Gerstl & Mingelgrin 1984)

3.36 (Montgomery 1993)

3.30 (Tomlin 1994)

3.36 (recommended, Hansch et al. 1995)

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

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

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

2.04–3.09 (various soils, Mingelgrin & Gestl 1983)

2.82, 3.56 (soil: quoted, calculated-MCI  $\chi$ , Gerstl & Helling 1987)

- 2.62 (soil, average of log  $K_{OC}$  values, Gerstl 1990)  
 3.52–4.29; 3.72 at pH 2, 3.35 at pH 6 (Dead sea sediment, Gestl & Kilger 1990)  
 2.62–3.54; 3.54 at pH 2, 3.40 at pH 6 (Kinnert F sediment, Gestl & Kilger 1990)  
 2.71–3.62; 3.62 at pH 2, 3.27 at pH 6 (Kinnert G sediment, Gestl & Kilger 1990)  
 2.40–3.31; 3.31 at pH 2, 3.20 at pH 5 (Oxford soil, Gestl & Kilger 1990)  
 2.39–3.15; 3.15 at pH 2, 2.88 at pH 6 (Malkiya soil, Gestl & Kilger 1990)  
 2.28–3.29; 3.29 at pH 2, 3.09 at pH 5 (Neve Ya'ar soil, Gestl & Kilger 1990)  
 2.85 (soil, Wauchope et al. 1992; Hornsby et al. 1996)  
 2.29–3.99 (soil/sediment, literature range, Montgomery 1993)  
 2.83 (soil, Montgomery 1993)  
 2.62 (soil, calculated-MCI  $\chi$ , Sabljic et al. 1995)  
 2.58, 2.58, 2.61 (soils: organic carbon  $OC \geq 0.1\%$ ,  $OC \geq 0.5\%$ ,  $0.1 \leq OC < 0.5\%$ , average, Delle Site 2001)  
 2.80 (sediment: organic carbon  $OC \geq 0.5\%$ , average, Delle Site 2001)

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

Volatilization: very little loss occurred by volatilization from soil surface (Herbicide Handbook 1989).

Photolysis: under condition of high sunlight intensity in the summer,  $t_{1/2} \sim 4$  d on the soil surface (Herbicide Handbook 1989);

decomposed by sunlight,  $t_{1/2} = 25.7$  min. (Tomlin 1994).

Oxidation:

Hydrolysis: stable to hydrolysis between pH 4 and 10 at 40°C (Hartley & Kidd 1987; Worthing 1987; Tomlin 1994).

Biodegradation: slowly broken down by microorganisms in soil, in pure culture, a soil fungus metabolizes rapidly with  $t_{1/2} = 2$  wk (Herbicide Handbook 1989).

Biotransformation: rapidly metabolized in plants to water-soluble metabolites (Tomlin 1994).

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

#### Half-Lives in the Environment:

Air:

Surface water:

Ground water: decomposed by sunlight,  $t_{1/2} = 25.7$  min. (Montgomery 1993; Tomlin 1994).

Sediment:

Soil:  $t_{1/2} \sim 55$  d in the plots treated for the first time whereas  $t_{1/2} = 6$ –12 d in pre-treated plots that had previously been sprayed with napropamide in the field;  $t_{1/2} = 25$ –40 d irrespective of the pre-treatment history of the soil in the laboratory at 20°C (Walker & Welch 1992)

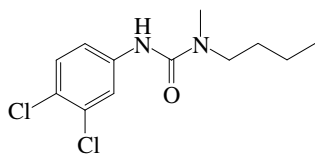
$t_{1/2} \sim 8$ –12 wk (Hartley & Kidd 1987; Tomlin 1994);

field  $t_{1/2} = 70$  d (Wauchope et al. 1992; Hornsby et al. 1996);

moist loam or sandy-loam soils at 79–90°C,  $t_{1/2} = 8$ –12 wk (Montgomery 1993).

Biota: rapidly metabolized in plants to water-soluble metabolites (Tomlin 1994).

## 17.1.1.55 Neburon



Common Name: Neburon

Synonym: Kloben, Neburea, Neburex

Chemical Name: 1-butyl-3-(3,4-dichlorophenyl)-1-methylurea; *N*-butyl-*N'*-(3,4-dichloro-phenyl)-*N*-methylurea

Uses: pre-emergence herbicide to control grasses and broadleaf weeds in peas, beans, lucerne, garlic, beets, cereals, strawberries, ornamentals and forestry.

CAS Registry No: 555-37-3

Molecular Formula:  $C_{12}H_{16}Cl_2N_2O$

Molecular Weight: 275.174

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

102–103 (Khan 1980; Spencer 1982; Worthing & Hance 1991; Tomlin 1994)

101.5–103 (Montgomery 1993)

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

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

Molar Volume ( $cm^3/mol$ ):

236.0 (modified Le Bas method at normal boiling point, Spurlock & Biggar 1994a)

Dissociation Constant  $pK_a$ :

Enthalpy of Vaporization,  $\Delta H_v$  (kJ/mol):

96.91 (Rordorf 1989)

Enthalpy of Fusion,  $\Delta H_{fus}$  (kJ/mol):

29.71 (DSC method, Plato & Glasgow 1969)

26.9 (Rordorf 1989)

Entropy of Fusion,  $\Delta S_{fus}$  (J/mol K):

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

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

4.8 ( $24^{\circ}C$ , Bailey & White 1965; Melnikov 1971)

4.8 (Martin & Worthing 1977)

4.8 ( $28^{\circ}C$ , Khan 1980)

5.0 (Hartley & Kidd 1987; Tomlin 1994)

4.8 ( $24^{\circ}C$ , Worthing & Walker 1987, Worthing & Hance 1991; Montgomery 1993)

5.2 (Spurlock 1992; Spurlock & Biggar 1994b)

5.0 ( $20$ – $25^{\circ}C$ , selected, Augustijn-Beckers et al. 1994; selected, Hornsby et al. 1996)

4.67, 9.99 (quoted, calculated-group contribution fragmentation method, Kühne et al. 1995)

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

$6.30 \times 10^{-6}$ ,  $4.10 \times 10^{-4}$ , 0.015, 0.33, 4.90 (25, 50, 70, 100,  $125^{\circ}C$ , gas saturation-GC, Rordorf 1989)

$\log(P_s/Pa) = 18.272 - 6999.1/(T/K)$ ; measured range  $50$ – $103^{\circ}C$  (solid, gas saturation-GC, Rordorf 1989)

$\log(P_L/Pa) = 13.285 - 5062.2/(T/K)$ ; measured range  $105$ – $140^{\circ}C$  (liquid, gas saturation-GC, Rordorf 1989)

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

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

4.59 (selected, Dao et al. 1983; Gerstl & Helling 1987)

4.31 (RP-HPLC- $k'$  correlation, Braumann et al. 1983)

4.22 (Spurlock 1992; Spurlock & Biggar 1994b)

3.80 (selected, Sangster 1993)

3.80 (calculated, Montgomery 1993)



- 4.10 (shake flask-UV, Liu & Qian 1995)
- 3.99 (RP-HPLC- $k'$  correlation, Liu & Qian 1995)
- 3.80 (recommended, Hansch et al. 1995)
- 3.40, 4.02, 4.13 (RP-HPLC-RT correlation, CLOGP, calculated-S, Finizio et al. 1997)

Bioconcentration Factor, log BCF:

- 2.41 (calculated-S, Kenaga 1980; quoted, Isensee 1991)
- 1.85, 2.18 (calculated-S,  $K_{OC}$ , Kenaga 1980)

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

- 3.36 (soil, Hamaker & Thompson 1972)
- 3.26, 2.72 (soil, calculated-S, Kenaga 1980)
- 3.49 (average of soils/sediments, Rao & Davidson 1980)
- 3.36, 3.23 (quoted, calculated-MCI  $\chi$ , Gerstl & Helling 1987)
- 2.95 (soil, calculated- $\chi$  and fragment contribution, Meylan et al. 1992)
- 3.49 (Montgomery 1993)
- 3.40 (20–25°C, selected, Augustijn-Beckers et al. 1994; Hornsby et al. 1996)
- 3.40 (selected, Lohninger 1994)
- 3.60 (calculated- $K_{OW}$ , Liu & Qian 1995)
- 3.140 (soil, calculated-MCI  $^1\chi$ , Sabljic et al. 1995)
- 3.40; 2.86, 2.69 (soil, quoted exptl.; estimated-class-specific model, estimated-general model using molecular descriptors, Gramatica et al. 2000)

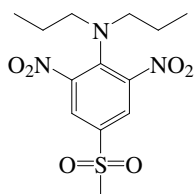
Environmental Fate Rate Constants, k, or Half-Lives,  $t_{1/2}$ :

- Hydrolysis:  $t_{1/2} > 4$  months for 5500  $\mu\text{g/mL}$  to hydrolyze in phosphate buffer at pH 5–9 and 20°C (El-dib & Aly 1976; quoted, Muir 1991).

Half-Lives in the Environment:

- Soil: residual activity in soil is limited to approximately 3–4 months (Hartley & Kidd 1987; quoted, Montgomery 1993);
- selected field  $t_{1/2} = 120$  d (Augustijn-Beckers et al. 1994; Hornsby et al. 1996).

## 17.1.1.56 Nitralin



Common Name: Nitralin

Synonym: Planavin

Chemical Name: 4-(methylsulfonyl)-2,6-dinitro-*N,N*-dipropylbenzamine

CAS Registry No: 4726-14-1

Uses: herbicide

Molecular Formula:  $C_{13}H_{19}N_3O_6S$

Molecular Weight: 345.371

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

150 (Lide 2003)

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

Density ( $g/cm^3$  at  $20^{\circ}C$ ): 1.39 (Hartley & Kidd 1987)

Molar Volume ( $cm^3/mol$ ):

Dissociation Constant  $pK_a$ :

Enthalpy of Fusion,  $\Delta H_{fus}$  ( $kJ/mol$ ):

Entropy of Fusion,  $\Delta S_{fus}$  ( $J/mol K$ ):

Fugacity Ratio at  $25^{\circ}C$  (assuming  $\Delta S_{fus} = 56 J/mol K$ ), F: 0.0594 (mp at  $150^{\circ}C$ )

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

0.60 (Melnikov 1971; Kenaga & Goring 1980; Kenaga 1980b; Isensee 1991)

0.60 (Ashton & Crafts 1981; Hartley & Kidd 1987; Worthing & Walker 1987)

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

0.240 (Ashton & Crafts 1981)

$2.0 \times 10^{-5}$  (Hartley & Kidd 1987)

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

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

6.73 (calculated-MCI  $\chi$ , Patil 1994)

2.81 (LOGPSTAR or CLOGP data, Sabljic et al. 1995)

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

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

2.90, 1.76 (calculated-solubility,  $K_{ow}$ , Kenaga 1980b)

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

2.98 (Kenaga & Goring 1980)

3.76 (calculated, Kenaga 1980a)

2.92 (soil, calculated-MCI  $\chi$ , Sabljic et al. 1995)

2.92; 3.28 (soil, quoted obs.; estimated-general model using molecular descriptors, Gramatica et al. 2000)

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

Biotransformation: Degradation by abiotic reductive transformations:

$k = 3.44 M^{-1} s^{-1}$  in  $H_2S$  with (mecapto)juglone (hydroquinone moiety, an abiotic reductant found in natural systems) solution at pH 6.65 (Wang & Arnold 2003)

Aqueous solutions with surface-bound Fe(II) species and their first-order rate constants as:

$k = 0.44 \times 10^{-3} \text{ h}^{-1}$  at pH 6.5,  $k = 0.68 \times 10^{-2} \text{ h}^{-1}$  at pH 7.0,  $k = 0.133 \text{ h}^{-1}$  at pH 7.4, and  $k = 1.96 \text{ h}^{-1}$  at pH 7.8 for aqueous ferrous ion system;

$k = 0.580 \text{ h}^{-1}$  at pH 6.5,  $k = 1.15 \text{ h}^{-1}$  at pH 6.7,  $k = 6.06 \text{ h}^{-1}$  at pH 7.0, and  $k = 20.9 \text{ h}^{-1}$  at pH 7.3 for Fe(II)/goethite system;

$k = 2.54 \times 10^{-3} \text{ h}^{-1}$  at pH 6.5,  $k = 1.83 \times 10^{-3} \text{ h}^{-1}$  at pH 7.0,  $k = 4.13 \times 10^{-3} \text{ h}^{-1}$  at pH 7.4 and  $k = 7.70 \times 10^{-3} \text{ h}^{-1}$  at pH 7.8 for Fe(II)/clay system, all with total dissolved Fe(II) = 1 mM (Wang & Arnold 2003)

#### Half-Lives in the Environment:

Air:

Surface water:

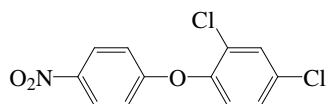
Ground water:

Sediment:

Soil:  $t_{1/2} \sim 30\text{--}54 \text{ d}$  in dry soil (Hartley & Kidd 1987)

Biota: in mammals, following oral administration, degradation and elimination occur within a few days (Hartley & Kidd 1987).

## 17.1.1.57 Nitrofen



Common Name: Nitrofen

Synonym: nitrophen Tok, Tokkron

Chemical Name: 2,4-dichloro-1-(4-nitrophenoxy)benzene

CAS Registry No: 1836-75-5

Uses: herbicide

Molecular Formula:  $C_{12}H_7Cl_2NO_3$

Molecular Weight: 284.095

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

70 (Lide 2003)

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

180–190/0.25 mmHg (Hartley & Kidd 1987)

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

Molar Volume ( $cm^3/mol$ ):

Dissociation Constant  $pK_a$ :

Enthalpy of Vaporization,  $\Delta H_v$  (kJ/mol):

93.66 (Rordorf 1989)

Enthalpy of Fusion,  $\Delta H_{fus}$  (kJ/mol):

22.7 (Rordorf 1989)

Entropy of Fusion,  $\Delta S_{fus}$  (J/mol K):

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

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

1.0 (Kenaga 1980b)

~1.0 (Spencer 1982)

0.7–1.2 ( $22^{\circ}C$ , Worthing 1987)

~1 (room temp., Hartley & Kidd 1987)

1.0 ( $20$ – $25^{\circ}C$ , selected, Augustijn-Beckers et al. 1994; Hornsby et al. 1996)

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

$1.07 \times 10^{-3}$  ( $40^{\circ}C$ , Spencer 1982)

$1.06 \times 10^{-3}$  ( $40^{\circ}C$ , Worthing 1987; Hartley & Kidd 1987)

$1.30 \times 10^{-4}$ ,  $4.50 \times 10^{-3}$ , 0.091, 1.20, 12.0 ( $25$ ,  $50$ ,  $70$ ,  $100$ ,  $125^{\circ}C$ , gas saturation-GC, Rordorf 1989)

$\log(P_s/Pa) = 15.867 - 5886.5/(T/K)$ ; measured range  $50$ – $70.2^{\circ}C$  (solid, gas saturation-GC, Rordorf 1989)

$\log(P_L/Pa) = 13.022 - 4892.8/(T/K)$ ; measured range  $72.7$ – $140^{\circ}C$  (liquid, gas saturation-GC, Rordorf 1989)

$1.33 \times 10^{-5}$  ( $20$ – $25^{\circ}C$ , selected, Augustijn-Beckers et al. 1994; Hornsby et al. 1996)

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

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

3.09 (Rao & Davidson 1980)

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

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

2.79 (fish, Kenaga 1980b)

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

3.64 (soil, calculated, Kenaga 1980b)

3.01, 3.64, 4.18, 4.05 (quoted literature values, Augustijn-Beckers et al. 1994)

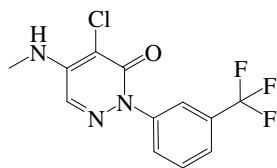
4.0 (soil, Augustijn-Beckers et al. 1994; Hornsby et al. 1996)

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

Half-Lives in the Environment:

Soil: reported field  $t_{1/2} = 3$  to 25 d and the recommended field  $t_{1/2} = 30$  d (Augustijn-Beckers et al. 1994; Hornsby et al. 1996).

## 17.1.1.58 Norflurazon



Common Name: Norflurazon

Synonym: Zorial, Solicam, Evital, Telok

Chemical Name: 4-chloro-5-(methylamino)-2[3-(trifluoromethyl)phenyl]-3-(2*H*)-pyridazinone

CAS Registry No: 27314-13-2

Uses: herbicide

Molecular Formula: C<sub>12</sub>H<sub>9</sub>ClF<sub>3</sub>N<sub>3</sub>O

Molecular Weight: 303.666

Melting Point (°C):

184 (Lide 2003)

Boiling Point (°C):

Density (g/cm<sup>3</sup> at 20°C):

Molar Volume (cm<sup>3</sup>/mol):

Dissociation Constant p*K*<sub>a</sub>:

Enthalpy of Fusion, Δ*H*<sub>fus</sub> (kJ/mol):

Entropy of Fusion, Δ*S*<sub>fus</sub> (J/mol K):

Fugacity Ratio at 25°C (assuming Δ*S*<sub>fus</sub> = 56 J/mol K), *F*: 0.0275 (mp at 184°C)

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

- 28 (Kenaga & Goring 1980; Kenaga 1980b; Gerstl & Helling 1987; Isensee 1991)
- 28 (Ashton & Crafts 1981; Worthing & Walker 1987; Herbicide Handbook 1989; Tomlin 1994)
- 40 (Spencer 1982)
- 28 (23°C, Hartley & Kidd 1987)
- 28 (20–25°C, selected, Wauchope et al. 1992; Hornsby et al. 1996; quoted, Senseman et al. 1997)

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

- 2.7 × 10<sup>-6</sup> (20°C, Ashton & Crafts 1981; Spencer 1982)
- 2.8 × 10<sup>-6</sup> (20°C, Worthing & Walker 1987; Tomlin 1994)
- 2.7 × 10<sup>-6</sup>, 3.3 × 10<sup>-5</sup>, 3.3 × 10<sup>-4</sup>, 1.6 × 10<sup>-3</sup>, 1.3 × 10<sup>-2</sup> (20, 40, 60, 80, 100°C, Herbicide Handbook 1989)
- 9.24 × 10<sup>-5</sup> (20–25°C, Majewski & Capel 1995)

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

- 3.04 × 10<sup>-5</sup> (20–25°C, Majewski & Capel 1995)

Octanol/Water Partition Coefficient, log *K*<sub>ow</sub>:

- 2.30 (22°C, shake flask-UV, Braumann & Grimme 1981)
- 2.52 (shake flask, Takahashi et al. 1993)
- 2.45 (pH 6.5, Tomlin 1994)
- 2.30 (recommended, Hansch et al. 1995)
- 2.30 (LOGPSTAR or CLOGP data, Sabljic et al. 1995)
- 2.60 (RP-HPLC-RT correlation using short ODP column, Donovan & Pescatore 2002)

Octanol/Air Partition Coefficient, log *K*<sub>OA</sub>:

Bioconcentration Factor, log BCF or log *K*<sub>B</sub>:

- 1.97 (fish, calculated-solubility, Kenaga 1980b; Isensee 1991)

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

- 3.28 (soil, Kenaga & Goring 1980)
- 2.85 (calculated-solubility, Kenaga 1980b)
- 3.28, 3.07 (soil: quoted, calculated-MCI  $\chi$ , Gerstl & Helling 1987)
- 2.85 (soil, Wauchope et al. 1992; Hornsby et al. 1996)
- 3.02, 2.64, 3.02, 2.46 2.59 (sandy loam, Mississippi loam, Mississippi sediment, Keaton sandy loam, Biggs clay, Tomlin 1994)
- 3.75 (calculated-MCI  $\chi$ , Meylan et al. 1992)
- 3.28 (soil, calculated-MCI  $\chi$ , Sabljic et al. 1995)
- 2.78 (soil, Senseman et al. 1997)

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

Volatilization: dissipated in soil by photodegradation and volatilization,  $t_{1/2} = 45\text{--}180$  d (Tomlin 1994)

Photolysis: rapidly degraded by sunlight (Worthing 1987; Tomlin 1994)

dissipated in soil by photodegradation and volatilization,  $t_{1/2} = 45\text{--}180$  d (Tomlin 1994)

Oxidation:

Hydrolysis:

Biodegradation:

Biotransformation:

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

## Half-Lives in the Environment:

Air:

Surface water:  $t_{1/2} = 3.4$  and  $1.9$  d reported in the absence and presence of 20 ppm  $H_2O_2$  (quoted, Massad et al. 2004)

Ground water:

Sediment:

Soil: the average  $t_{1/2} = 45\text{--}130$  d residues in soil from the Delta and Southeast depending on clay and organic content (Herbicide Handbook 1989)

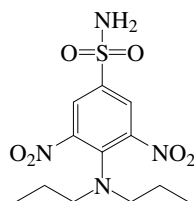
field  $t_{1/2} \sim 30$  d (estimated, Wauchope et al. 1992; Hornsby et al. 1996)

dissipated in soil by photodegradation and volatilization,  $t_{1/2} = 45\text{--}180$  d (Tomlin 1994)

soil  $t_{1/2} = 90$  d (Senseman et al. 1997)

Biota:

## 17.1.1.59 Oryzalin



Common Name: Oryzalin

Synonym: Dirimal, EL 119, Rycelan, Ryzelon, Ryzelan, Surflan

Chemical Name: 4-(dipropylamino)-3,5-dinitrobenzene-sulfonamide; 3,5-dinitro-*N*<sup>d</sup>, *N*<sup>d</sup>-dipropylsulfanilamide

Uses: herbicide for pre-emergence control of many annual grasses and broadleaf weeds in cotton, fruit trees, vines, nut trees, soybeans, groundnuts, oilseed rape, sunflowers, lucerne, peas, sweet potatoes, mint, ornamentals and also used in noncrop areas.

CAS Registry No: 19044-88-3

Molecular Formula: C<sub>12</sub>H<sub>18</sub>N<sub>4</sub>O<sub>6</sub>S

Molecular Weight: 346.359

Melting Point (°C):

141 (Lide 2003)

Boiling Point (°C): 265 (dec. Tomlin 1994)

Density (g/cm<sup>3</sup> at 20°C):

Molar Volume (cm<sup>3</sup>/mol):

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

Dissociation Constant pK<sub>a</sub>:

9.40 (Worthing & Hance 1991; Tomlin 1994)

8.60 (Wauchope et al. 1992; Hornsby et al. 1996)

Enthalpy of Fusion, ΔH<sub>fus</sub> (kJ/mol):

Entropy of Fusion, ΔS<sub>fus</sub> (J/mol K):

Fugacity Ratio at 25°C (assuming ΔS<sub>fus</sub> = 56 J/mol K), F: 0.0728 (mp at 141°C)

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

2.4 (Martin & Worthing 1977; Spencer 1982; Ashton & Crafts 1981)

2.6 (Weber et al. 1980)

2.5 (Hartley & Kidd 1987; Budavari 1989; Milne 1995)

2.4 (Worthing & Walker 1987, Worthing & Hance 1991)

2.6 (Herbicide Handbook 1989; Tomlin 1994)

2.5 (20–25°C, selected, Wauchope et al. 1992; Hornsby et al. 1996)

3.5 (calculated-group contribution fragmentation method, Kühne et al. 1995)

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

< 1.33 × 10<sup>-5</sup> (30°C, Ashton & Crafts 1981)

< 1.30 × 10<sup>-5</sup> (30°C, Hartley & Kidd 1987)

< 1.33 × 10<sup>-6</sup> (Herbicide Handbook 1989; Tomlin 1994)

< 1.33 × 10<sup>-5</sup> (30°C, Budavari 1989)

< 1.30 × 10<sup>-6</sup> (Worthing & Hance 1991)

< 1.30 × 10<sup>-6</sup> (20–25°C, selected, Wauchope et al. 1992; Hornsby et al. 1996)

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

0.000188 (calculated-P/C, this work)

Octanol/Water Partition Coefficient, log K<sub>ow</sub>:

4.13 (selected, Dao et al. 1983)

3.73 (Worthing & Hance 1991)



- 3.72 (pH 7, Tomlin 1994)
- 3.73 (Milne 1995)
- 3.73 (selected, Hansch et al. 1995)
- 2.79 (MedChem master file or ClogP program, Sabljic et al. 1995)

Bioconcentration Factor, log BCF:

- 2.58 (calculated-S, Kenaga 1980)

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

- 3.43 (soil, calculated-S, Kenaga 1980)
- 2.78 (soil, 20–25°C, selected, Wauchope et al. 1992; Hornsby et al. 1996)
- 2.78 (estimated-chemical structure, Lohninger 1994)
- 2.85–3.04 (Tomlin 1994)
- 3.40 (quoted or calculated-QSAR MCI  $^1\chi$ , Sabljic et al. 1995)
- 3.40; 3.18 (soil, quoted obs.; estimated-general model using molecular descriptors, Gramatica et al. 2000)

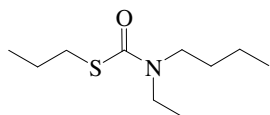
Environmental Fate Rate Constants, k, or Half-Lives,  $t_{1/2}$ :

Biodegradation: in soil, microbial degradation occurs rapidly,  $t_{1/2}$  = 2.1 months for aerobic and  $t_{1/2}$  = 10 d for anaerobic metabolism (Tomlin 1994).

Half-Lives in the Environment:

Soil: selected field  $t_{1/2}$  = 20 d (Wauchope et al. 1992; Hornsby et al. 1996);  
 $t_{1/2}$  = 2.1 months for aerobic degradation and  $t_{1/2}$  = 10 d for anaerobic degradation (Tomlin 1994).

## 17.1.1.60 Pebulate



Common Name: Pebulate

Synonym: PEBC, R-2061, Stauffer 2061, Tillam, Timmam-6-E

Chemical Name: *S*-propyl butylethyl(thiocarbamate); *S*-propyl butylethylcarbamothioate

Uses: selective pre-emergence herbicide to control annual grasses and broadleaf weeds in tomatoes, sugar beet, and tobacco.

CAS Registry No: 1114-71-2

Molecular Formula: C<sub>10</sub>H<sub>21</sub>NOS

Molecular Weight: 203.345

Melting Point (°C): liquid

Boiling Point (°C):

142 (at 20 mmHg, Hartley & Kidd 1987; Budavari 1989; Montgomery 1993; Milne 1995)

142 (at 21 mmHg, Herbicide Handbook 1989)

Density (g/cm<sup>3</sup> at 20°C):

0.956 (Hartley & Kidd 1987; Worthing & Hance 1991; Tomlin 1994; Milne 1995)

0.9555 (Herbicide Handbook 1989; Montgomery 1993)

Molar Volume (cm<sup>3</sup>/mol):

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

Dissociation Constant pK<sub>a</sub>:

Enthalpy of Fusion, ΔH<sub>fus</sub> (kJ/mol):

Entropy of Fusion, ΔS<sub>fus</sub> (J/mol K):

Fugacity Ratio at 25°C (assuming ΔS<sub>fus</sub> = 56 J/mol K), F: 1.0

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

92 (21°C, Woodford & Evans 1963)

92 (21°C, Spencer 1973, 1982)

60 (Herbicide Handbook 1978, 1989; quoted, Kenaga 1980; Kenaga & Goring 1980)

60 (Ashton & Crafts 1973, 1981)

60 (20°C, Khan 1980; Hartley & Kidd 1987; Tomlin 1994; Montgomery 1993; Milne 1995)

60 (20°C, Worthing & Walker 1987, Worthing & Hance 1991)

100 (20–25°C, selected, Wauchope et al. 1992; Hornsby et al. 1996)

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

4.67 (Ashton & Crafts 1973, 1981; Herbicide Handbook 1989)

3.60 (20°C, Hartley & Graham-Bryce 1980)

9.06 (30°C, Khan 1980)

0.216 (20°C, GC-RT correlation, Kim 1985)

9.00 (30°C, Hartley & Kidd 1987; Tomlin 1994)

3.50 (20°C, selected, Suntio et al. 1988)

4.70 (Worthing & Hance 1991; Tomlin 1994)

1.186 (20–25°C, selected, Wauchope et al. 1992; Hornsby et al. 1996)

9.064 (20°C, Montgomery 1993)

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

11.67 (20°C, calculated-P/C, Suntio et al. 1988)

11.65 (20°C, calculated-P/C, Montgomery 1993)

Octanol/Water Partition Coefficient, log K<sub>OW</sub>:

3.78 (selected, Magee 1991)

3.84 (Worthing & Hance 1991; Montgomery 1993; Milne 1995)

- 3.83 (Tomlin 1994)
- 3.84 (selected, Hansch et al. 1995)
- 4.19, 3.74, 3.27 (RP-HPLC, CLOGP, calculated-S, Finizio et al. 1997)

Bioconcentration Factor, log BCF:

- 1.79 (calculated-S, Kenaga 1980)
- 1.54 (calculated- $K_{OC}$ , Kenaga 1980)

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

- 2.80 (soil, Hamaker & Thompson 1972)
- 2.66 (soil, calculated-S as per Kenaga & Goring 1980, Kenaga 1980)
- 2.80 (reported as log  $K_{OM}$ , Magee 1991)
- 2.65 (estimated as log  $K_{OM}$ , Magee 1991)
- 2.63 (soil, 20–25°C, selected, Wauchope et al. 1992; Hornsby et al. 1996)
- 2.80 (Montgomery 1993)
- 2.63 (selected, Lohninger 1994)
- 2.80 (quoted or calculated-QSAR MCI  $\chi$ , Sabljic et al. 1995)
- 2.48, 2.10 (soil, estimated-class-specific model, estimated-general model using molecular descriptors, Gramatica et al. 2000)

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

Biodegradation: in soil, microbial degradation  $t_{1/2} = 2\text{--}3$  wk (Tomlin 1994).

Half-Lives in the Environment:

Air:

Surface water:  $t_{1/2} = 11$  d, at pH 4 and pH 10,  $t_{1/2} = 12$  d at pH 7 (40°C, Tomlin 1994).

Ground water:

Sediment:

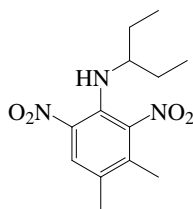
Soil:  $t_{1/2} \sim 2$  wk in moist loam soil at 21–27°C (Herbicide Handbook 1989; Montgomery 1993);

selected field  $t_{1/2} = 14$  d (Wauchope et al. 1992; Hornsby et al. 1996);

$t_{1/2} = 2\text{--}3$  wk (Tomlin 1994);.

Biota:

## 17.1.1.61 Pendimethalin



Common Name: Pendimethalin

Synonym: penoxalin

Chemical Name: *N*-(1-ethylpropyl-3,4-dimethyl-2,6-dinitrobenzenamine

CAS Registry No: 40487-42-1

Uses: herbicide

Molecular Formula: C<sub>13</sub>H<sub>19</sub>N<sub>3</sub>O<sub>4</sub>

Molecular Weight: 281.308

Melting Point (°C):

56 (Lide 2003)

Boiling Point (°C):

330 (Ashton & Crafts 1981; Herbicide Handbook 1989)

decomposes on heating (Hartley & Kidd 1987; Tomlin 1994)

Density (g/cm<sup>3</sup> at 25°C):

1.19 (Ashton & Crafts 1981; Montgomery 19993; Tomlin 1994)

1.12 (Hartley & Kidd 1987)

1.17 (Herbicide Handbook 1989)

Molar Volume (cm<sup>3</sup>/mol):

Dissociation Constant pK<sub>a</sub>:

Enthalpy of Fusion, ΔH<sub>fus</sub> (kJ/mol):

Entropy of Fusion, ΔS<sub>fus</sub> (J/mol K):

Fugacity Ratio at 25°C (assuming ΔS<sub>fus</sub> = 56 J/mol K), F: 0.496 (mp at 56°C)

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

0.50 (23°C, Ashton & Crafts 1981)

0.30 (20°C, Hartley & Kidd 1987; Worthing & Walker 1987; Montgomery 1993; Tomlin 1994)

0.275 (Herbicide Handbook 1989)

0.275 (20–25°C, selected, Wauchope et al. 1992; Hornsby et al. 1996)

0.61 (20–25°C, Majewski & Capel 1995)

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

0.004 (Ashton & Crafts 1981; Herbicide Handbook 1989)

0.004 (Hartley & Kidd 1987; Worthing & Walker 1987; Tomlin 1994)

1.25 × 10<sup>-3</sup> (20–25°C, selected, Wauchope et al. 1992; Hornsby et al. 1996)

0.004 (Montgomery 1993)

8.16 × 10<sup>-3</sup> (20–25°C, Majewski & Capel 1995)

0.00123; 0.00776 (liquid P<sub>L</sub>, GC-RT correlation; quoted lit., Donovan 1996)

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

0.0867 (Montgomery 1993)

3.75 (20–25, calculated-P/C, Majewski & Capel 1995)

Octanol/Water Partition Coefficient, log K<sub>ow</sub>:

5.18 (Montgomery 1993)

5.18 (Tomlin 1994)

5.24 (RP-HPLC-RT correlation using short ODP column, Donovan & Pescatore 2002)

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

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

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

2.95	(soil, Wauchope et al. 1992; Hornsby et al. 1996)
4.20	(soil, Bottoni & Funari 1992)
4.14, 4.47	(loam, pH 7, pH 6.5, quoted, Montgomery 1993)
3.81	(sand, pH 7.6, Montgomery 1993)
4.07, 4.14	(sandy loam pH 6.4, silty loam, pH 7.0, Montgomery 1993)
1.48–2.93	(soil, Montgomery 1993)
3.70	(soil, Senseman et al. 1997)
3.14	(soil, estimated-general model using molecular descriptors, Gramatica et al. 2000)

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

Volatilization:

Photolysis: slowly decomposed by light (Hartley & Kidd 1987; Tomlin 1994).

Oxidation:

Hydrolysis:  $t_{1/2} < 21$  d (Montgomery 1993).

Biodegradation: observed  $t_{1/2} = 33$  d, 45 d, 52 d and 67 d in flooded and nonflooded conditions in nonsterile and sterile soils, respectively, in the study of degradation of pendimethalin under the influence of soil moisture and microbial activity in a sandy loam soil, in both nonsterile nonflooded and flooded soil, degradation followed first-order kinetics. (Kulshrestha & Singh 1992; quoted, Montgomery 1993).

Biotransformation: Degradation by abiotic reductive transformations:

$k = 1.25 \text{ M}^{-1} \text{ s}^{-1}$  in  $\text{H}_2\text{S}$  with (mecapto)juglone (hydroquinone moiety, an abiotic reductant found in natural systems) solution at pH 6.65 (Wang & Arnold 2003)

Aqueous solutions with surface-bound Fe(II) species and their first-order rate constants as:

$k = 0.50 \times 10^{-3} \text{ h}^{-1}$  at pH 6.5,  $k = 0.27 \times 10^{-2} \text{ h}^{-1}$  at pH 7.0,  $k = 0.093 \text{ h}^{-1}$  at pH 7.4, and  $k = 0.81 \text{ h}^{-1}$  at pH 7.8 for aqueous ferrous ion system;

$k = 0.216 \text{ h}^{-1}$  at pH 6.5,  $k = 0.274 \text{ h}^{-1}$  at pH 6.7,  $k = 0.918 \text{ h}^{-1}$  at pH 7.0, and  $k = 2.10 \text{ h}^{-1}$  at pH 7.3 for Fe(II)/goethite system;

$k = 3.81 \times 10^{-3} \text{ h}^{-1}$  at pH 6.5,  $k = 2.66 \times 10^{-3} \text{ h}^{-1}$  at pH 7.0,  $k = 1.13 \times 10^{-2} \text{ h}^{-1}$  at pH 7.4 and  $k = 1.74 \times 10^{-2} \text{ h}^{-1}$  at pH 7.8 for Fe(II)/clay system, all with total dissolved Fe(II) = 1 mM (Wang & Arnold 2003)

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

Half-Lives in the Environment:

Air:

Surface water:  $t_{1/2} < 21$  d in water (Tomlin 1994).

Ground water: reported  $t_{1/2} = 30$ –90 d (Bottoni & Funari 1992)

Sediment:

Soil:  $t_{1/2} = 98$  and 409 d at 30 and 10°C in a sandy loam soil with 75% moisture (Walker & Bond 1977)

$t_{1/2} = 4$  d on Bosket silt loam,  $t_{1/2} = 6$  d on Sharkey clay for the first 3 to 5 days when sprayed onto soil surface, rate of loss much slower for the remainder of the 7- or 12-d sampling period with  $t_{1/2} = 18$  d on Bosket silt loam,  $t_{1/2} = 27$  d on Sharkey clay (Savage & Jordon 1980)

$t_{1/2} = 58$ –63 d in IARI sandy loam soil under Indian tropical climate (Kulshrestha & Yaduraju 1987)

$t_{1/2} = 30$ –90 d or persistence (Bottoni & Funari 1992)

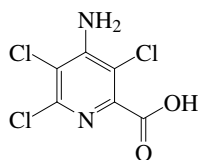
$t_{1/2} = 66.9$  d in sterile,  $t_{1/2} = 52.2$  d in nonsterile non-flooded sandy loam soil;  $t_{1/2} = 44.9$  d in sterile and 33.4 d in nonsterile flooded sandy loam soil in the study of degradation under the influence of soil moisture and microbial activity (Kulshrestha & Singh 1992; quoted, Montgomery 1993)

reported field  $t_{1/2} = 8$ –480 d, recommended  $t_{1/2} = 90$  d (Wauchope et al 1992; Hornsby et al. 1996);

soil  $t_{1/2} = 90$  d (Senseman et al. 1997).

Biota:  $t_{1/2} = 3$ –4 months (quoted, Hartley & Kidd 1987; Tomlin 1994)

## 17.1.1.62 Picloram



Common Name: Picloram

Synonym: Amdon, ATCP, Borolin, Grazon, K-Pin, Tordon

Chemical Name: 4-amino-3,5,6-trichloropicolinic acid; 4-amino-3,5,6-trichloro-2-pyridinecarboxylic acid

Uses: systemic herbicide to control most broadleaf weeds on grassland and noncropland.

CAS Registry No: 1918-02-1

Molecular Formula:  $C_6H_3Cl_3N_2O_2$

Molecular Weight: 241.459

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

218.5 (Lide 2003)

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

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

Molar Volume ( $cm^3/mol$ ):

204.2 (calculated-Le Bas method at normal boiling point, Suntio et al. 1988)

Dissociation Constant  $pK_a$ :

3.43, 3.42, 3.39, 3.36 (10, 20, 30,  $40^{\circ}C$ , Cheung & Biggar 1974)

1.90 (Weber et al. 1980; Willis & McDowell 1982)

3.60 (Windholz 1983; quoted, Howard 1991; Yao & Haag 1991; Haag & Yao 1992; Montgomery 1993)

2.3 ( $22^{\circ}C$ , Worthing & Hance 1991; Montgomery 1993; Tomlin 1994)

1.94 (Hornsby et al. 1996)

Enthalpy of Fusion,  $\Delta H_{fus}$  (kJ/mol):

Entropy of Fusion,  $\Delta S_{fus}$  (J/mol K):

Fugacity Ratio at  $25^{\circ}C$  (assuming  $\Delta S_{fus} = 56$  J/mol K), F: 0.0126 (mp at  $218.5^{\circ}C$ )

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

430 (Bailey & White 1965; Freed 1966; Khan 1980; Weber et al. 1980; Ashton & Crafts 1981; Spencer 1982)

546\* ( $20^{\circ}C$ , shake flask-IR, measured range  $10-40^{\circ}C$ , pH 2.8, distilled water, Cheung & Biggar 1974)

73.65\* ( $20^{\circ}C$ , shake flask-IR, measured range  $10-40^{\circ}C$  at pH 0.2, Cheung & Biggar 1974)

62.7\* ( $20^{\circ}C$ , shake flask-IR, measured range  $10-40^{\circ}C$  at pH 1.1, Cheung & Biggar 1974)

137\* ( $20^{\circ}C$ , shake flask-IR, measured range  $10-40^{\circ}C$  at pH 2.0, Cheung & Biggar 1974)

19560\* ( $20^{\circ}C$ , shake flask-IR, measured range  $10-40^{\circ}C$  at pH 4.2, Cheung & Biggar 1974)

74593\* ( $20^{\circ}C$ , shake flask-IR, measured range  $10-40^{\circ}C$  at pH 4.7, Cheung & Biggar 1974)

430 (Martin & Worthing 1977, Worthing & Hance 1991; quoted, Kenaga 1980; Kenaga & Goring 1980; Isensee 1991; Howard 1991)

430 (Hartley & Graham-Bryce 1980; Taylor & Glotfelty 1988)

430 (Hartley & Kidd 1987; Herbicide Handbook 1989; Tomlin 1994; Milne 1995)

400-430 (Montgomery 1993)

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

$7.30 \times 10^{-7}$  ( $20^{\circ}C$ , Hartley & Graham-Bryce 1980)

$8.20 \times 10^{-5}$  ( $35^{\circ}C$ , Khan 1980; Ashton & Crafts 1981; Hartley & Kidd 1987; Herbicide Handbook 1989)

$8.26 \times 10^{-5}$  ( $20-25^{\circ}C$ , Weber et al. 1980; Willis & McDowell 1982)

$9.70 \times 10^{-9}$  (Dobbs & Cull 1982; quoted, Howard 1991)

$7.30 \times 10^{-6}$  ( $20^{\circ}C$ , quoted from Hartley & Graham-Bryce 1980, Dobbs et al. 1984)

$6.00 \times 10^{-5}$  ( $20^{\circ}C$ , selected, Suntio et al. 1988)

$1.40 \times 10^{-4}$  ( $45^{\circ}C$ , Herbicide Handbook 1989)

- $4.50 \times 10^{-8}$  (quoted, Nash 1989)
- $7.40 \times 10^{-7}$  (20°C, selected, Taylor & Spencer 1990)
- $8.20 \times 10^{-5}$  (35°C, Worthing & Hance 1991; Montgomery 1993; Tomlin 1994)

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

- $3.40 \times 10^{-5}$  (20°C, calculated-P/C, Suntio et al. 1988; quoted, Mabury & Crosby 1996)
- $4.20 \times 10^{-7}$  (calculated-P/C, Taylor & Glotfelty 1988)
- $2.50 \times 10^{-5}$  (calculated-P/C, Nash 1989)
- $4.10 \times 10^{-6}$  (calculated-P/C, Howard 1991)
- $3.40 \times 10^{-5}$  (20–35°C, calculated-P/C, Montgomery 1993)
- $3.17 \times 10^{-5}$  (calculated-P/C, this work)

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

- 0.30 (Kenaga 1975)
- 0.63 (selected, Dao et al. 1983)
- 0.30 (Hansch & Leo 1985; Hansch et al. 1995;)
- −3.47 (selected, Gerstl & Helling 1987)
- 1.166 (calculated as per Broto et al. 1984, Karcher & Devillers 1990)
- 0.26, 0.30 (quoted, Sangster 1993)
- 1.87 (LOGPSTAR or CLOGP data, Sabljic et al. 1995)

Bioconcentration Factor,  $\log BCF$ :

- −1.70 (fish in static water, quoted from Dow Chemical data, Kenaga & Goring 1980)
- 1.30 (calculated-S, Kenaga 1980; quoted, Isensee 1991)
- −0.222 (calculated- $K_{oc}$ , Kenaga 1980)
- 0.0 (estimated- $K_{ow}$ , Lyman et al. 1982; quoted, Howard 1991)
- 1.49 (fish in flowing water, Garten & Trabalka 1983; quoted, Howard 1991)

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

- 1.23 (soil, Hamaker & Thompson 1972)
- 1.10 (average in soil, Hamaker & Thompson 1972)
- 1.10 (average in soil, Reinhold et al. 1979)
- 1.23 (Kenaga & Goring 1980; quoted, Bahnick & Doucette 1988)
- 2.20 (soil, calculated-S as per Kenaga & Goring 1980, Kenaga 1980)
- 1.41 (av. of 26 soils, Rao & Davidson 1980)
- 1.40 (soil, Rao & Davidson 1982)
- 1.31, 1.05, 1.34, 1.0, 1.26, 1.10, 1.05 (Catlin soil, Commerce soil, Fargo soil, Holdredge soil, Norfolk soil, Kawkawlin soil, Walla-Walla soil, McCall & Agin 1985; quoted, Brusseau & Rao 1989)
- 2.11 (calculated-MCI  $\chi$ , Gerstl & Helling 1987)
- 1.68 (screening model calculations, Jury et al. 1987b)
- 1.47 (calculated-MCI  $\chi$ , Bahnick & Doucette 1988)
- 1.88 (Nash 1989)
- 1.23 (reported as  $\log K_{OM}$ , Magee 1991)
- 1.20 (organic carbon, Wauchope et al. 1991)
- 1.11, 1.41, 1.68 (soil, quoted values, Bottoni & Funari 1992)
- 1.41 (Montgomery 1993)
- 1.30 (soil, calculated-QSAR MCI  $^1\chi$ , Sabljic et al. 1995)
- 1.55, 1.39, 2.38 (soils: organic carbon  $OC \geq 0.1\%$ ,  $OC \geq 0.5\%$ ,  $0.1 \leq OC < 0.5\%$ , and pH 2.0–10.5, average, Delle Site 2001)
- 3.07, 2.96, 3.30 (soils: organic carbon  $OC \geq 0.1\%$ ,  $OC \geq 0.5\%$ ,  $0.1 \leq OC < 0.5\%$ , and pH  $\leq 2.0$  undissociated, average, Delle Site 2001)
- 1.80, 1.76 (soils: organic carbon  $OC \geq 0.1\%$ ,  $OC \geq 0.5\%$ , pH 4.2–5.9, average, Delle Site 2001)
- 1.12, 2.02, 1.93 (soils: organic carbon  $OC \geq 0.1\%$ ,  $OC \geq 0.5\%$ ,  $0.1 \leq OC < 0.5\%$ , pH  $\geq 6.0$ , dissociated, average, Delle Site 2001)

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

## Volatilization:

Photolysis:  $t_{1/2} = 200$  h for 40% of 4,840  $\mu\text{g/mL}$  to degrade in dilute NaOH solution under sunlight (Hall et al 1968; quoted, Cessna & Muir 1991);

$t_{1/2} = 2.3$  d to 9.58 d direct photolysis by sunlight under various conditions, at depths of 2.54 cm–3.65 m at various times of the year; one result at 3.65 m during Sept.–Oct. gave  $t_{1/2} = 41.3$  d; distilled water and canal water gave essentially the same results in one set of experiments (Hedlund & Youngson 1972; quoted, Cessna & Muir 1991; Howard 1991);

$t_{1/2} = 72$  h for 99% of 548  $\mu\text{g mL}^{-1}$  to degrade in Na salt solution under 300–380 nm light (Mosier & Guenzi 1973; quoted, Cessna & Muir 1991);

$t_{1/2} = 0.5$  h for 38% of 265  $\mu\text{g mL}^{-1}$  to degrade in distilled water under 254 nm light (Glass 1975; quoted, Cessna & Muir 1991);

$t_{1/2} = 2.2$  d for  $< 2.4$   $\mu\text{g mL}^{-1}$  L to degrade in distilled water under sunlight (Skurlatov et al. 1983; quoted, Cessna & Muir 1991);

$t_{1/2} = 16$  h in surface water estimated from direct midday sunlight photolysis in mid-summer at 40°N (Zepp 1991).

## Oxidation:

photooxidation:  $t_{1/2} = 12.21$  d in air, based on estimated rate constant for the reaction with photochemically produced hydroxyl radical in the atmosphere (GEMS 1986; quoted, Howard 1991)

$k = 5.9 \times 10^9 \text{ M}^{-1} \text{ s}^{-1}$  for the reaction (Fenton with reference to acetophenone) with hydroxyl radical in aqueous solutions at pH 2.1–3.7 and at  $24 \pm 1^\circ\text{C}$  (Buxton et al. 1988; quoted, Haag & Yao 1992)

$k(\text{aq.}) = (50\text{--}150) \text{ M}^{-1} \text{ s}^{-1}$  for direct reaction with ozone in water at pH 1.5–4.9 and  $21 \pm 1^\circ\text{C}$ , with  $t_{1/2} = 4.0$  min at pH 7 (Yao & Haag 1991).

$k(\text{aq.}) = (3.4 \pm 0.3) \times 10^9 \text{ M}^{-1} \text{ s}^{-1}$  for the reaction (Fenton with reference to acetophenone) with hydroxyl radicals in aqueous solutions at pH 2.1–3.7 and at  $24 \pm 1^\circ\text{C}$  (Haag & Yao 1992)

$k(\text{aq.}) = 1.3 \times 10^9 \text{ M}^{-1} \text{ s}^{-1}$  for reaction with hydroxyl radical, in irradiated field water both in the laboratory and sunlit rice paddies (Mabury & Crosby 1996).

## Hydrolysis:

Biodegradation:  $t_{1/2} = 128\text{--}144$  h in mixture of 5 g soil and 1–4 mL water,  $t_{1/2} = 90\text{--}1000$  h in mixture of 1 mL water with 0.25–10 g soil, (Hance 1969; quoted, Howard 1991);

$t_{1/2} > 15$  months for 0.07, 0.72 and 10  $\mu\text{g mL}^{-1}$  to biodegrade in groundwater (Weidner 1974; quoted, Muir 1991);

$k = 0.0073 \text{ d}^{-1}$  by soil incubation die-away test studies (Rao & Davidson 1980; quoted, Scow 1982);

biochemical  $t_{1/2} = 100$  d from screening model calculations (Jury et al. 1987b);

$t_{1/2} = 30\text{--}300$  d, degraded slowly by soil microorganisms (Tomlin 1994).

## Biotransformation:

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

## Half-Lives in the Environment:

Air:  $t_{1/2} = 12.21$  d, based on estimated rate constant for the vapor-phase reaction with photochemically produced hydroxyl radicals in the atmosphere (GEMS 1986; quoted, Howard 1991).

Surface water:  $t_{1/2} = 2.6$  d decomposed by UV irradiation (Tomlin 1994);

measured rate constant  $k = (50 - 150) \text{ M}^{-1} \text{ s}^{-1}$  for direct reaction with ozone in water at pH 1.5–4.9 and  $21^\circ\text{C}$ , with  $t_{1/2} = 4.0$  min at pH 7 (Yao & Haag 1991).

Ground water:  $t_{1/2} > 15$  months for 0.07, 0.72 and 10  $\mu\text{g/mL}$  to biodegrade in ground water (Weidner 1974; quoted, Muir 1991);

measured rate constant  $k \leq 0.005 \text{ M}^{-1} \text{ s}^{-1}$  for direct reaction with ozone in water at pH 2 and  $21^\circ\text{C}$ , with  $t_{1/2} \geq 80$  d at pH 7 (Yao & Haag 1991)

reported  $t_{1/2} = 30\text{--}330, 138, 180$  and  $206$  d (Bottoni & Funari 1992).

## Sediment:

Soil: estimated persistence of 18 months (Kearney et al. 1969; Edwards 1973; quoted, Morrill et al. 1982; Jury et al. 1987b);

persistent in soils with  $t_{1/2} > 5$  yr (Alexander 1973; quoted, Howard 1991);

estimated first-order  $t_{1/2} = 95$  d in soil from biodegradation rate constant  $k = 0.0073 \text{ d}^{-1}$  by soil incubation die-away test studies (Rao & Davidson 1980; quoted, Scow 1982);



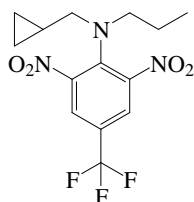
persistent in soil with  $t_{1/2} > 100$  d (Willis & McDowell 1982);  
 $t_{1/2} = 100$  d from screening model calculations (Jury et al. 1987b);  
 selected  $t_{1/2} = 90$  d (Wauchope et al. 1991; quoted, Dowd et al. 1993);  
 reported  $t_{1/2} = 30$ –330 d, 18 d, 180 d and 206 d (Bottoni & Funari 1992);  
 $t_{1/2} = 3$ –330 d (Tomlin 1994).

Biota: biochemical  $t_{1/2} = 100$  d from screening model calculations (Jury et al. 1987b);  
 average  $t_{1/2} = 60$  d in the forest (USDA 1989; quoted, Neary et al. 1993).

**TABLE 17.1.1.62.1**
**Reported aqueous solubilities of picloram at various temperatures**
**Cheung & Biggar 1974**

shake flask-IR spec.						
$t/^{\circ}\text{C}$	$\text{S/g}\cdot\text{m}^{-3}$	$\text{S/g}\cdot\text{m}^{-3}$	$\text{S/g}\cdot\text{m}^{-3}$	$\text{S/g}\cdot\text{m}^{-3}$	$\text{S/g}\cdot\text{m}^{-3}$	$\text{S/g}\cdot\text{m}^{-3}$
	pH 0.20	pH 1.10	pH 2.0	pH 2.8	pH 4.2	pH 4.7
10	43.95	39.12	89.11	475	22240	84446
20	73.65	62.78	136.92	545.74	19560	74953
30	119.5	108.9	205.3	683.4	21395	82248
40	214.9	199	316.3	704.5	21371	78240
$\Delta H_{\text{sol}}/(\text{kJ mol}^{-1})$	38.49	38.91	31.38	12.97	0	0

## 17.1.1.63 Profluralin



Common Name: Profluralin

Synonym: CGA 10832, Pregard, Tolban

Chemical Name: *N*-(cyclopropylmethyl)-2,6-dinitro-*N*-propyl-4-(trifluoromethyl)benzenamine; *N*-(cyclopropylmethyl)-2,6-dinitro-*N*-propyl-4-(trifluoromethyl) benzenamine

Uses: herbicide for pre-planting by soil incorporation to control annual and perennial broadleaf and grass weeds in cotton, soybeans, brassicas, capsicums, tomatoes and other crops.

CAS Registry No: 26399-36-0

Molecular Formula:  $C_{14}H_{16}F_3N_3O_4$

Molecular Weight: 347.290

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

34 (Lide 2003)

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

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

1.45 ( $25^{\circ}C$ , Ashton & Crafts 1981)

1.38 (Hartley & Kidd 1987; Worthing & Hance 1991)

Molar Volume ( $cm^3/mol$ ):

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

Dissociation Constant  $pK_a$ :

Enthalpy of Fusion,  $\Delta H_{fus}$  (kJ/mol):

Entropy of Fusion,  $\Delta S_{fus}$  (J/mol K):

Fugacity Ratio at  $25^{\circ}C$  (assuming  $\Delta S_{fus} = 56$  J/mol K), F: 0.816 (mp at  $34^{\circ}C$ )

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

0.10 ( $20^{\circ}C$ , Weber 1972)

0.10 (Spencer 1973, 1982; Wauchope 1978; Kenaga 1980)

0.10 ( $27^{\circ}C$ , Ashton & Crafts 1973, 1981)

0.10 (shake flask-HPLC, Ellgehausen et al. 1981)

0.10 ( $20^{\circ}C$ , Hartley & Kidd 1987; Milne 1995)

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

0.10 ( $20$ – $25^{\circ}C$ , selected, Augustijn-Beckers et al. 1994; Hornsby et al. 1996)

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

0.0092 ( $20^{\circ}C$ , Weber 1972; Worthing & Walker 1987)

0.0092 ( $20^{\circ}C$ , Ashton & Crafts 1973, 1981)

0.0084 ( $20^{\circ}C$ , Hartley & Kidd 1987)

0.0084 ( $20^{\circ}C$ , Worthing & Hance 1991)

0.0084 ( $20$ – $25^{\circ}C$ , selected, Augustijn-Beckers et al. 1994; Hornsby et al. 1996)

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

39.07 ( $20^{\circ}C$ , calculated-P/C, Suntio et al. 1988)

31.91 ( $20^{\circ}C$ , calculated-P/C, Muir 1991)

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

5.16 (selected, Dao et al. 1983)

6.34 (shake flask-HPLC/UV, Ellgehausen et al. 1981)

6.34 (recommended, Sangster 1993)

- 4.46 (calculated-fragment const., Pinsuwan et al. 1995)  
 6.34 (recommended, Hansch et al. 1995)  
 5.08 (LOGPSTAR or CLOGP data, Sabljic et al. 1995)

Bioconcentration Factor, log BCF:

- 3.35 (calculated-S, Kenaga 1980; quoted, Isensee 1991)  
 2.83 (calculated- $K_{OC}$ , Kenaga 1980)

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

- 3.93 (soil, exptl., Kenaga 1980)  
 4.19 (soil, calculated-S as per Kenaga & Goring 1980, Kenaga 1980)  
 3.83 (estimated as log  $K_{OM}$ , Magee 1991)  
 3.93 (soil, quoted exptl., Meylan et al. 1992)  
 4.26 (soil, calculated-MCI  $\chi$  and fragment contribution, Meylan et al. 1992)  
 4.00 (20–25°C, estimated, Augustijn-Beckers et al. 1994; Hornsby et al. 1996)  
 4.16 (selected, Lohninger 1994)  
 4.01 (soil, calculated-QSAR MCI  $^1\chi$ , Sabljic et al. 1995)  
 3.87 (soil, estimated-general model using molecular descriptors, Gramatica et al. 2000)

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

Volatilization: estimated  $t_{1/2} \sim 1.2$  d from 1 m depth of water at 20°C (Muir 1991).

Photolysis:

Oxidation:

Hydrolysis:

Biodegradation:  $t_{1/2} = 12$  d for 0.5  $\mu\text{g mL}^{-1}$  to biodegrade in flooded soils at 20–42°C (Savage 1978; quoted, Muir 1991);

Degradation  $t_{1/2} < 1$  month in three soils, Goldsborol loamy sand, Cecil loamy sand Drummer clay loam treated with 1 ppm profluralin) for 4 month under aerobic conditions, no degradation in sterile controls. (shake flask-TLC, Camper et al. 1980)

$t_{1/2} < 1$  month for 1  $\mu\text{g/mL}$  to biodegrade in flooded soils at 25°C (derived from results of Camper et al. 1980, Muir 1991);

biodegradation  $t_{1/2} < 20$  d in water and sediment with flooded soils and terrestrial-aquatic model ecosystems (Muir 1991).

Biotransformation:

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

Half-Lives in the Environment:

Air:

Surface water: biodegradation  $t_{1/2} < 20$  d in water and sediment with flooded soils and terrestrial-aquatic model ecosystems (Muir 1991).

Ground water:

Sediment: biodegradation  $t_{1/2} < 20$  d in water and sediment with flooded soils and terrestrial-aquatic model ecosystems (Muir 1991).

Soil:  $t_{1/2} = 12$  d for 0.5  $\mu\text{g mL}^{-1}$  to biodegrade in flooded soils at 20–42°C (Savage 1978, Muir 1991) persistence of 12 months in soil (Wauchope 1978);

aerobic and anaerobic degradation  $t_{1/2} < 1$  month in 3 flooded soils at 25°C (Camper et al. 1980);

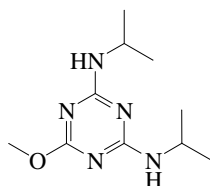
field studies,  $t_{1/2} = 10.9$  wk - 1978 first study;  $t_{1/2} = 10.1$  wk -1978 second study;  $t_{1/2} = 11.5$  wk -1979, in a Crowley silt loam at Stuttgart, Arkansas (Brewer et al. 1982)

laboratory studies:  $t_{1/2} = 19.9$  wk at 4°C,  $t_{1/2} = 6.7$  wk at 25°C for soil of field capacity moisture (27% w/w for Crowley silt loam),  $t_{1/2} = 20.4$  wk at 4°C,  $t_{1/2} = 4.8$  wk at 25°C for flooded soils, Crowley silt loam; and  $t_{1/2} = 25.8$  wk at 4°C,  $t_{1/2} = 8.6$  wk at 25°C for soil of field capacity moisture (34% w/w for Sharkey silty clay),  $t_{1/2} = 21.3$  wk at 4°C and  $t_{1/2} = 6.2$  wk at 25°C for flooded soils, Sharkey silty clay (Brewer et al. 1982);

selected field  $t_{1/2} = 110$  d (Augustijn-Beckers et al. 1994; Hornsby et al. 1996).

Biota:

## 17.1.1.64 Prometon



Common Name: Prometon

Synonym: G 31435, Gesafram, Gesagram, Methoxypropazine, Ontracac 800, Ontrack, Pramitol, Prometone

Chemical Name: 6-methoxy-*N,N'*-bis(methylethyl)-1,3,5-triazine-2,4-diamine; 2,4-bis(isopropylamino)-6-methoxy-1,3,5-triazine

Uses: nonselective pre-emergence and post-emergence herbicide to control most annual and broadleaf weeds, grasses, and brush weeds on noncropland.

CAS Registry No: 1610-18-0

Molecular Formula: C<sub>10</sub>H<sub>19</sub>N<sub>5</sub>O

Molecular Weight: 225.291

Melting Point (°C):

91.5 (Lide 2003)

Boiling Point (°C):

Density (g/cm<sup>3</sup> at 20°C):

1.088 (Hartley & Kidd 1987; Worthing & Hance 1991; Montgomery 1993)

Molar Volume (cm<sup>3</sup>/mol):

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

Dissociation Constant:

4.28 (pK<sub>a</sub>, Weber 1970; quoted, Bintein & Devillers 1994)

4.30 (pK<sub>a</sub>, 21°C, Worthing & Hance 1991; Montgomery 1993)

9.73 (pK<sub>b</sub>, Wauchope et al. 1992; Hornsby et al. 1996)

9.7 (21°C, pK<sub>b</sub>, Tomlin 1994)

Enthalpy of Vaporization, ΔH<sub>v</sub> (kJ/mol):

90.77 (Rordorf 1989)

Enthalpy of Fusion, ΔH<sub>fus</sub> (kJ/mol):

22.175 (DSC method, Plato & Glasgow 1969)

21.6 (Rordorf 1989)

Entropy of Fusion, ΔS<sub>fus</sub> (J/mol K):

Fugacity Ratio at 25°C (assuming ΔS<sub>fus</sub> = 56 J/mol K), F: 0.223 (mp at 91.5°C)

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

750 (20°C, Bailey & White 1965; Ashton & Crafts 1981; Herbicide Handbook 1989)

1000, 678, 669 (26°C, pH 3.0, 7.0, 10.0, shake flask-UV, Ward & Weber 1968)

750 (Martin & Worthing 1977; Herbicide Handbook 1978)

677 (Weber et al. 1980)

620 (20°C, Spencer 1982)

750 (20°C, Verschueren 1983)

750 (20°C, Hartley & Kidd 1987; Montgomery 1993)

620 (20°C, Worthing & Walker 1987, 1991; Tomlin 1994)

720 (20–25°C, selected, Wauchope et al. 1992; Hornsby et al. 1996)

Vapor Pressure (Pa at 25°C or as indicated and reported temperature dependence equations.):

3.07 × 10<sup>-4</sup> (20°C, extrapolated-Antoine eq. from gas saturation-GC measurements, measured range 50–130°C, Friedrich & Stambach 1964) (See figure at the end of this section.)

log (P/mmHg) = 11.911 – 4933/(T/K), temp range 50–130°C (gas saturation-GC, data presented in Antoine eq., Friedrich & Stambach 1964)

0.00030 (20°C, Khan 1980)  
 0.00031 (20°C, Ashton & Crafts 1981; Worthing & Hance 1991)  
 0.00083 (Jury et al. 1984; selected, Spencer et al. 1988; Spencer & Cliath 1990; Taylor & Spencer 1990)  
 0.00031 (20°C, Hartley & Kidd 1987)  
 0.00031, 0.00105 (20°C, 30°C, Herbicide Handbook 1989)  
 $1.0 \times 10^{-3}$ ,  $3.30 \times 10^{-2}$ , 0.65, 8.60, 82 (25, 50, 70, 100, 125°C, gas saturation-GC, Rordorf 1989)  
 $\log (P_g/P_a) = 16.525 - 5817.4/(T/K)$ ; measured range 32.1–89.3°C (gas saturation-GC, Rordorf 1989)  
 $\log (P_L/P_a) = 13.617 - 4741.7/(T/K)$ ; measured range 92.3–140°C (gas saturation-GC, Rordorf 1989)  
 0.00103 (20–25°C, selected, Wauchope et al. 1992; Hornsby et al. 1996)  
 0.00031 (20°C, Montgomery 1993)  
 0.000306 (20°C, Tomlin 1994)

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

$2.50 \times 10^{-4}$  (calculated-P/C, Jury et al. 1984; Spencer et al. 1988; Spencer & Cliath 1990)  
 $9.02 \times 10^{-5}$  (20°C, calculated-P/C, Montgomery 1993)  
 $9.01 \times 10^{-5}$  (calculated-P/C, this work)

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

1.94 (selected, Dao et al. 1983)  
 1.94 (Gerstl & Helling 1987)  
 2.99 (RP-HPLC-RT correlation, Finizio et al. 1991; quoted, Sangster 1993)  
 2.85 (selected, Magee 1991)  
 2.55 (shake flask-UV, Liu & Qian 1995)  
 2.69, 2.99 (Montgomery 1993)  
 2.99 (recommended, Hansch et al. 1995)  
 2.82 (RP-HPLC-RT correlation, Finizio et al. 1997)

Bioconcentration Factor,  $\log \text{BCF}$ :

1.18 (calculated-S, Kenaga 1980; quoted, Isensee 1991)  
 1.28 (calculated- $K_{oc}$ , Kenaga 1980)

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

2.54 (soil, Hamaker & Thompson 1972; Kenaga 1980; Kenaga & Goring 1980)  
 2.04 (soil, calculated-S as per Kenaga & Goring 1980, Kenaga 1980)  
 2.61 (Jury et al. 1984; quoted, Spencer & Cliath 1990)  
 2.40 (calculated-MCI  $\chi$ , Gerstl & Helling)  
 2.48 (Spencer et al. 1988)  
 2.35 (estimated as  $\log K_{om}$ , Magee 1991)  
 2.20 (soil, calculated-MCI  $\chi$  and fragment contribution, Meylan et al. 1992)  
 2.18 (soil, 20–25°C, selected, Wauchope et al. 1992; Hornsby et al. 1996)  
 1.92–2.24 (Montgomery 1993)  
 2.77 (selected, Lohninger 1994)  
 2.39 (calculated- $K_{ow}$ , Liu & Qian 1995)  
 2.50 (soil, calculated-MCI  $\chi$ , Sabljic et al. 1995)  
 2.60; 2.70, 2.68 (soil, quoted obs.; estimated-class-specific model, estimated-general model using molecular descriptors, Gramatica et al. 2000)  
 2.47, 2.50 (soils: organic carbon  $\text{OC} \geq 0.1\%$ ,  $\text{OC} \geq 0.5\%$ , pH 4.3–7.1, average, Delle Site 2001)  
 2.81, 2.65, 2.53 (soils with organic carbon  $\text{OC} \geq 0.5\%$  at: pH 4.3–4.9, pH 5.0–5.9, pH- 6.0, average, Delle Site 2001)

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

Volatilization: estimated  $t_{1/2} \sim 100$  d (Spencer & Cliath 1990).

Photolysis:  $t_{1/2} = 2.25$  h for 1% of  $100 \mu\text{g mL}^{-1}$  to degrade in distilled water under 300 nm light (Tanaka et al. 1981; quoted, Cessna & Muir 1991).

Oxidation:

Hydrolysis:

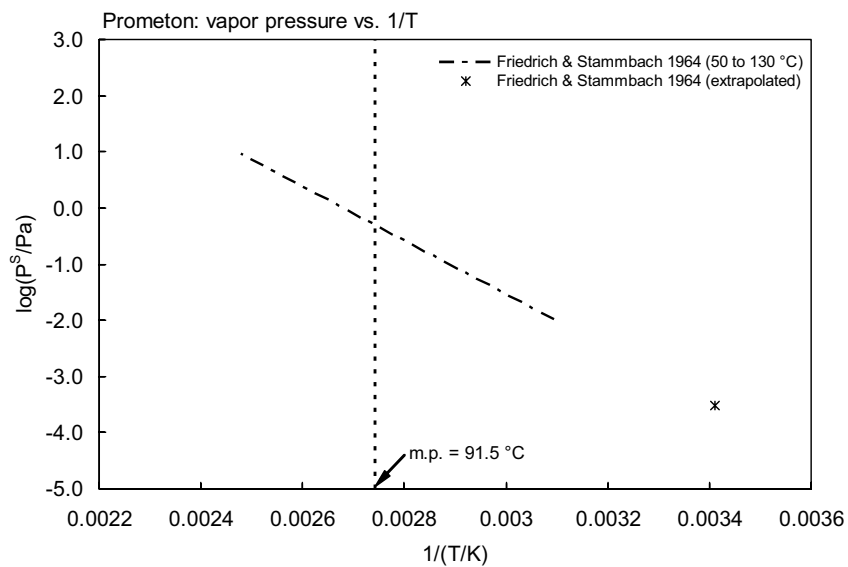
Biodegradation:

Biotransformation:

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

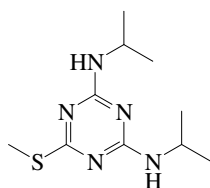
Half-Lives in the Environment:

Soil: selected field  $t_{1/2} = 500$  d (Wauchope et al. 1992; Hornsby et al. 1996).



**FIGURE 17.1.1.64.1** Logarithm of vapor pressure versus reciprocal temperature for prometon.

## 17.1.1.65 Prometryn



Common Name: Prometryn

Synonym: Caparol, Cotton-Pro, Gesagard, G-34161, Mercasin, Mercazin, Polisin, Primatol, Prometrex, Prometrin, Selectin, Sesagard, Uvon

Chemical Name: *N,N'*-bis(1-methylethyl)-6-(methylthio)-1,3,5-triazine-2,4-diamine; 2,4-bis(isopropylamino)-6-(methylthio)-1,3,5-triazine

Uses: selective herbicide to control many annual grass and broadleaf weeds in celery, cotton and peas.

CAS Registry No: 7287-19-6

Molecular Formula: C<sub>10</sub>H<sub>19</sub>N<sub>5</sub>S

Molecular Weight: 241.357

Melting Point (°C):

119 (Lide 2003)

Boiling Point (°C):

Density (g/cm<sup>3</sup> at 20°C):

1.157 (Hartley & Kidd 1987; Worthing & Hance 1991; Montgomery 1993; Milne 1995)

Molar Volume (cm<sup>3</sup>/mol):

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

Dissociation Constant:

4.05 (pK<sub>a</sub>, Weber 1970; Pacakova et al. 1988; Somasundaram et al. 1991; Bintein & Devillers 1994)

4.10 (pK<sub>a</sub>, 21°C, Weber et al. 1980; Willis & McDowell 1982; Worthing & Hance 1991)

9.95 (pK<sub>b</sub>, Wauchope et al. 1992; Hornsby et al. 1996)

4.05 (pK<sub>a</sub>, 21°C, Montgomery 1993)

Enthalpy of Vaporization, ΔH<sub>v</sub> (kJ/mol):

96.43 (Rordorf 1989)

Enthalpy of Fusion, ΔH<sub>fus</sub> (kJ/mol):

26.36 (DSC method, Plato & Glasgow 1969)

25.4 (Rordorf 1989)

Entropy of Fusion, ΔS<sub>fus</sub> (J/mol K):

Fugacity Ratio at 25°C (assuming ΔS<sub>fus</sub> = 56 J/mol K), F: 0.120 (mp at 119°C)

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

48 (20°C, Woodford & Evans 1963)

48 (20°C, Bailey & White 1965; Ashton & Crafts 1973, 1981; Khan 1980)

206, 40.3, 41.8 (26°C, shake flask-UV at pH 3.0, 7.0, 10.0, Ward & Weber 1968)

48 (Martin & Worthing 1977; Herbicide Handbook 1978)

40 (Weber et al. 1980)

48 (20°C, Hartley & Kidd 1987; Herbicide Handbook 1989; Montgomery 1993; Milne 1995)

33 (20°C, Worthing & Walker 1987, Worthing & Hance 1991)

33 (20–25°C, selected, Wauchope et al. 1992; Hornsby et al. 1996)

33 (Tomlin 1994; selected, Lohninger 1994)

241 (calculated-group contribution method, Kühne et al. 1995)

Vapor Pressure (Pa at 25°C or as indicated and reported temperature dependence equations.):

1.33 × 10<sup>-4</sup> (20°C, extrapolated-Antoine eq. from gas saturation-GC measurements, measured range 50–130°C, Friedrich & Stambach 1964) (See figure at the end of this section.)

log (P/mmHg) = 11.911 – 4933/(T/K), temp range 50–130°C (gas saturation-GC, data presented in Antoine eq., Friedrich & Stambach 1964)

0.00028 (from Friedrich & Stambach 1964; Jury et al. 1983; 1984; Spencer & Cliath 1990)  
 0.00013 (20°C, Ashton & Crafts 1973, 1981)  
 0.00013 (20–25°C, Weber et al. 1980)  
 0.00028 (quoted, Jury et al. 1984; Spencer & Cliath 1990)  
 0.00013 (20°C, Hartley & Kidd 1987; Worthing & Hance 1991; Montgomery 1993)  
 0.00010 (20°C, selected, Suntio et al. 1988)  
 0.00013, 0.00053 (20, 30°C, Herbicide Handbook 1989)  
 $1.60 \times 10^{-4}$ ,  $6.70 \times 10^{-3}$ , 0.16, 2.50, 28.0 (25, 50, 70, 100, 125°C, gas saturation-GC, Rordorf 1989)  
 $\log (P_g/P_a) = 17.063 - 6215.6/(T/K)$ ; measured range 32.4–117°C (gas saturation-GC, Rordorf 1989)  
 $\log (P_L/P_a) = 14.013 - 5037.2/(T/K)$ ; measured range 129–140°C (gas saturation-GC, Rordorf 1989)  
 0.00017 (20–25°C, selected, Wauchope et al. 1992; Hornsby et al. 1996)  
 0.000169 (Tomlin 1994)

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

0.00139 (calculated-P/C, Jury et al. 1984; quoted, Spencer & Cliath 1990)  
 0.00139 (calculated-P/C, Jury et al. 1987a,b; Jury & Ghodrati 1989)  
 0.00050 (20°C, calculated-P/C, Suntio et al. 1988; quoted, Majewski & Capel 1995)  
 0.00050 (20°C, calculated-P/C, Montgomery 1993)

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

2.99 (selected, Dao et al. 1983)  
 1.91 (RP-HPLC- $k'$  correlation, Braumann et al. 1983)  
 3.46 (selected, Yoshioka et al. 1986)  
 3.51 (shake flask, Mitsutake et al. 1986)  
 2.99 (Gerstl & Helling 1987)  
 3.34 (RP-HPLC-RT correlation, Finizio et al. 1991)  
 3.43 (selected, Magee 1991)  
 3.34 (Worthing & Hance 1991; Milne 1995)  
 3.34, 3.46 (Montgomery 1993)  
 3.51 (recommended, Sangster 1993)  
 2.93 (RP-HPLC- $k'$  correlation, Liu & Qian 1995)  
 3.51 (recommended, Hansch et al. 1995)  
 3.35 (Pomona-database, Müller & Kördel 1996)  
 3.25 (RP-HPLC-RT correlation, Finizio et al. 1997)  
 2.99 (RP-HPLC-RT correlation using short ODP column, Donovan & Pescatore 2002)

Bioconcentration Factor,  $\log \text{BCF}$ :

1.85, 1.67 (calculated-S,  $K_{oc}$ , Kenaga 1980)

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

2.91 (soil, Hamaker & Thompson 1972; Kenaga 1980; Kenaga & Goring 1980)  
 2.72 (soil, calculated-S as per Kenaga & Goring 1980, Kenaga 1980)  
 2.79 (Rao & Davidson 1980)  
 3.17 (calculated-MCI  $\chi$ , Gerstl & Helling)  
 2.78 (screening model calculations, Jury et al. 1987a,b; Jury & Ghodrati 1989)  
 2.75 (estimated as  $\log K_{om}$ , Magee 1991)  
 2.72–2.91, 2.79, 2.83 (soil, quoted values, Bottoni & Funari 1992)  
 2.60 (soil, 20–25°C, selected, Wauchope et al. 1992; Hornsby et al. 1996)  
 2.38 (soil, HPLC-screening method, mean value from different stationary and mobile phases, Kördel et al. 1993, 1995b)  
 2.28–2.79 (Montgomery 1993)  
 3.15 (estimated-chemical structure, Lohninger 1994)  
 2.60 (soil, Tomlin 1994)  
 2.63 (calculated- $K_{ow}$ , Liu & Qian 1995)  
 2.85 (soil, calculated-QSAR MCI  $^1\chi$ , Sabljic et al. 1995)



2.38; 2.84 (HPLC-screening method; calculated-PCKOC fragment method, Müller & Kördel 1996)  
 3.54, 1.595, 1.968, 1.77, 2.67 (first generation Eurosoils ES-1, ES-2, ES-3, ES-4, ES-5, shake flask/batch equilibrium-HPLC/UV, Gawlik et al. 1998)  
 3.24, 2.16, 2.86, 2.59, 2.53 (calculated- $K_{OW}$ ; HPLC-screening method with different LC-columns, Szabo et al. 1999)  
 2.544, 2.635, 2.484, 1.816, 2.933 (second generation Eurosoils ES-1, ES-2, ES-3, ES-4, ES-5, shake flask/batch equilibrium-HPLC/UV and HPLC- $k'$  correlation, Gawlik et al. 2000)  
 2.85, 2.89 (soil, estimated-class-specific model, estimated-general model using molecular descriptors, Gramatica et al. 2000)

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

Volatilization:  $t_{1/2} = 60$  d (Jury et al. 1984).

Photolysis:

Oxidation:

Hydrolysis:  $t_{1/2} = 22$  d in 0.1 N hydrochloric acid solution,  $t_{1/2} = 500$  yr at pH 7 in distilled water and  $t_{1/2} = 30$  yr in 0.01 sodium hydroxide solution all at 25°C (Montgomery 1993).

Biodegradation:  $t_{1/2} = 60$  d (Wauchope 1978);

$t_{1/2} = 60$  d for a 100 d leaching and screening test in 0–10 cm depth of soil (Jury et al. 1987a,b; Jury & Ghodrati 1989);  
 soil microbial degradation  $t_{1/2} = 70$  d (Tomlin 1994).

Biotransformation:

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

#### Half-Lives in the Environment:

Air:

Surface water: completely decomposed when exposed to UV light for 3 h (Montgomery 1993).

Ground water: reported half-lives or persistence,  $t_{1/2} = 40$ –70, 60 and 94 d (Bottoni & Funari 1992)

Sediment:

Soil: estimated persistence of 3 months (Kearney et al. 1969; Edwards 1973; quoted, Morrill et al. 1982; Jury et al. 1987a,b; Jury & Ghodrati 1989);

$t_{1/2} \sim 6$  months to biodegrade in flooded soils (Plimmer et al. 1970; quoted, Muir 1991);

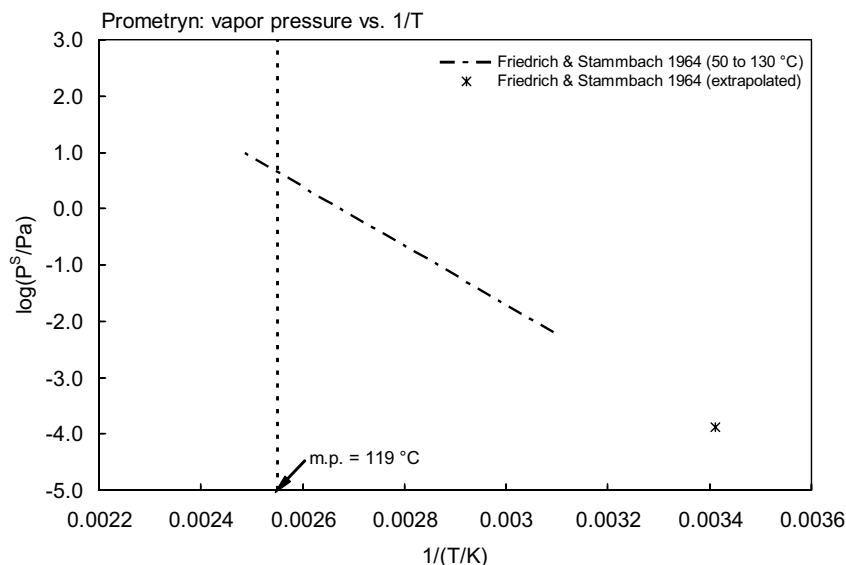
persistence of 2 months in soil (Wauchope 1978);

reported  $t_{1/2} = 40$ –70 d, 60 d and 94 d (Bottoni & Funari 1992);

selected field  $t_{1/2} = 60$  d (Wauchope et al. 1992; Hornsby et al. 1996);

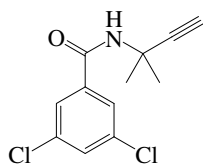
$t_{1/2} = 70$  d for microbial degradation in soil (Tomlin 1994).

Biota: biochemical  $t_{1/2} = 60$  d from screening model calculations (Jury et al. 1987a,b; Jury & Ghodrati 1989).



**FIGURE 17.1.1.65.1** Logarithm of vapor pressure versus reciprocal temperature for prometryn.

## 17.1.1.66 Pronamide



Common Name: Pronamide

Synonym: Kerb, Promamide, Propyzamide, RH-315

Chemical Name: 3,5-dichloro-N-(1,1-dimethylpropynyl)benzamide

Uses: herbicide.

CAS Registry No: 23950-58-5

Molecular Formula:  $C_{12}H_{11}Cl_2NO$

Molecular Weight: 256.127

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

155 (Lide 2003)

Boiling Point ( $^{\circ}C$ ): 321

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

Molar Volume ( $cm^3/mol$ ):

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

Dissociation Constant  $pK_a$ :

Enthalpy of Fusion,  $\Delta H_{fus}$  (kJ/mol):

Entropy of Fusion,  $\Delta S_{fus}$  (J/mol K):

Fugacity Ratio at  $25^{\circ}C$  (assuming  $\Delta S_{fus} = 56$  J/mol K), F: 0.0530 (mp at  $155^{\circ}C$ )

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

15 (Martin & Worthing 1977; Herbicide Handbook 1978, 1983; Worthing & Walker 1987)  
 15 ( $15^{\circ}C$ , Khan 1980)  
 15 (Ashton & Crafts 1981)  
 15 ( $24^{\circ}C$ , Herbicide Handbook 1989)  
 15 ( $20$ – $25^{\circ}C$ , selected, Wauchope et al. 1992; Hornsby et al. 1996)  
 15 (Tomlin 1994; Milne 1995)

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

0.0113 (Khan 1980)  
 0.0113 (Ashton & Crafts 1981; Herbicide Handbook 1989)  
 0.0536 (Dixon & Rissman 1985; quoted, Howard 1991)  
 0.227 (Worthing & Walker 1987)  
 0.0113 ( $20$ – $25^{\circ}C$ , selected, Wauchope et al. 1992; Hornsby et al. 1996)  
 0.000058 (Tomlin 1994)

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

0.912 (Dixon & Rissman 1985)  
 0.193 (calculated-P/C as per Worthing & Walker 1987, Majewski & Capel 1995)  
 0.188 (calculated-P/C, this work)

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

3.26 (estimated, Lyman et al. 1982; quoted, Howard 1991)  
 3.36 (selected, Magee 1991)  
 3.26 (selected, Dao et al. 1983)  
 2.95 (estimated-QSAR and SPARC, Kollig et al. 1993)  
 3.09–3.28 (Tomlin 1994; Milne 1995)  
 3.87 (LOGPSTAR or CLOGP data, Sabljic et al. 1995)

## Bioconcentration Factor, log BCF:

2.13	(calculated-S, Kenaga 1980)
1.00	(calculated- $K_{OC}$ , Kenaga 1980)
2.25	(estimated- $K_{OW}$ , Lyman et al. 1982; quoted, Howard 1991)
2.13	(estimated-S, Lyman et al. 1982; quoted, Howard 1991)

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

2.30	(soil, Leistra et al. 1974; Carlson et al.)
2.30	(measured for single soil, Kenaga 1980)
3.00	(soil, calculated-S as per Kenaga & Goring 1980, Kenaga 1980)
2.99	(soil, estimated-S, Lyman et al. 1982; quoted, Howard 1991)
2.30; 2.42	(reported as log $K_{OM}$ , estimated as log $K_{OM}$ , Magee 1991)
2.30; 3.20	(soil, quoted; calculated-MCI $\chi$ and fragment contribution, Meylan et al. 1992)
2.90	(soil, 20–25°C, selected, Wauchope et al. 1992; Hornsby et al. 1996)
2.63	(estimated-QSAR and SPARC, Kollig 1993)
2.54	(selected, Lohninger 1994)
2.31	(soil, calculated-QSAR MCI $^1\chi$ , Sabljic et al. 1995)

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

Volatilization: based on a Henry's law constant of 0.9118 Pa·m<sup>3</sup>/mol,  $t_{1/2}$  ~ 6.6 d from a river 1-m deep flowing 1 m/s with a wind velocity of 3 m/s (estimated, Lyman et al. 1982; quoted, Howard 1991).

Photolysis: degraded photolytically on soil thin films,  $t_{1/2}$  = 13–57 d in artificial sunlight (Tomlin 1994).

Oxidation: photooxidation  $t_{1/2}$  = 4.2 h in air, based on an estimated rate constant for the vapor-phase reaction with photochemically produced hydroxyl radicals in the atmosphere (Atkinson 1985; quoted, Howard 1991).

Hydrolysis: neutral hydrolysis rate constant  $k < 1.5 \times 10^{-5} \text{ h}^{-1}$  with a calculated  $t_{1/2} > 700 \text{ d}$  in neutral solution and with faster hydrolysis rates in acidic and basic solutions to be expected (Ellington et al. 1987, 1988; quoted, Howard 1991).

Biodegradation: depending on soil and climatic conditions, the degradation  $t_{1/2}$  = 10 to 112 d, but a  $t_{1/2}$  = 40 d may be more common under field conditions (Walker 1976, 1978; Zandvoort et al. 1979; quoted, Howard 1991).

Biotransformation: second-order rate constant  $k = 5 \times 10^{-14} \text{ L/organisms} \cdot \text{h}$  with an estimated  $t_{1/2}$  ~ 580 d for microbial degradation in natural water (Steen & Collette 1989; quoted, Howard 1991).

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

## Half-Lives in the Environment:

Air:  $t_{1/2}$  = 4.2 h, based on an estimated rate constant for the vapor-phase reaction with photochemically produced hydroxyl radicals in the atmosphere (Atkinson 1985; quoted, Howard 1991).

Surface water:

Ground water:

Sediment:

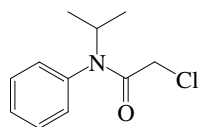
Soil: depending on soil and climatic conditions, the degradation  $t_{1/2}$  = 10 to 112 d, but a  $t_{1/2}$  = 40 d may be more common under field conditions (Walker 1976, 1978; Zandvoort et al. 1979; quoted, Howard 1991);

selected field  $t_{1/2}$  = 60 d (Wauchope et al. 1992; Hornsby et al. 1996);

degraded photolytically on soil thin films,  $t_{1/2}$  = 13–57 d in artificial sunlight (Tomlin 1994).

Biota:

## 17.1.1.67 Propachlor



Common Name: Propachlor

Synonym: Albrass, Bexton, CIPA, CP 31393, Niticid, Propachlore, Prolex, Ramrod, Satecid

Chemical Name: 2-chloro-*N*-(1-methylethyl)-*N*-phenylacetamide; 2-chloro-*N*-isopropyl-acetanilide

Uses: selective pre-emergence herbicide to control most annual grasses and some broadleaf weeds in brassicas, corn, cotton, flax, leeks, maize, milo, onions, peas, roses, ornamental trees and shrubs, soybeans, and sugar cane.

CAS Registry No: 1918-16-7

Molecular Formula:  $C_{11}H_{14}ClNO$

Molecular Weight: 211.688

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

77 (Herbicide Handbook 1989; Worthing & Hance 1991; Tomlin 1994; Milne 1995; Lide 2003)

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

110 (at 0.03 mmHg, Ashton & Crafts 1981; Hartley & Kidd 1987; Herbicide Handbook 1989; Worthing & Hance 1991; Montgomery 1993; Milne 1995)

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

1.13 ( $25^{\circ}C$ , Ashton & Crafts 1981)

1.242 ( $25^{\circ}C$ , Hartley & Kidd 1987; Worthing & Hance 1991; Montgomery 1993; Tomlin 1994; Milne 1995)

1.134 ( $25^{\circ}C$ , Herbicide Handbook 1989)

Molar Volume ( $cm^3/mol$ ):

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

Dissociation Constant  $pK_a$ :

Enthalpy of Fusion,  $\Delta H_{fus}$  ( $kJ/mol$ ):

27.614 (DSC method, Plato 1972)

Entropy of Fusion,  $\Delta S_{fus}$  ( $J/mol K$ ):

Fugacity Ratio at  $25^{\circ}C$  (assuming  $\Delta S_{fus} = 56 J/mol K$ ),  $F$ : 0.309 (mp at  $77^{\circ}C$ )

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

700 (Melnikov 1971; Khan 1980)

614 ( $20^{\circ}C$ , Weber 1972)

693 (Spencer 1973, 1982)

580 ( $20^{\circ}C$ , Ashton & Crafts 1973)

580 (Martin & Worthing 1977; Herbicide Handbook 1978)

839 (generator column-HPLC-RI, Swann et al. 1983)

2300 (HPLC-RT correlation, Swann et al. 1983)

613 (Hartley & Kidd 1987; Worthing & Walker 1987, Herbicide Handbook 1989 Worthing & Hance 1991; Tomlin 1994; Milne 1995)

613 ( $20$ – $25^{\circ}C$ , selected, Wauchope et al. 1992; Hornsby et al. 1996)

613–700 (Montgomery 1993)

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

0.032 ( $20$ – $25^{\circ}C$ , Weber et al. 1980)

0.0307 ( $24^{\circ}C$ , Beestman & Demming 1974)

0.0307 (Ashton & Crafts 1981; Herbicide Handbook 1989)

0.03 (Hartley & Kidd 1987)

0.03 ( $20^{\circ}C$ , selected, Suntio et al. 1988)

0.0306 (Worthing & Hance 1991; Tomlin 1994)

0.0307 (20–25°C, selected, Wauchope et al. 1992; Hornsby et al. 1996)  
 0.03 (Montgomery 1993)

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

0.011 (20°C, calculated-P/C, Suntio et al. 1988)  
 0.011 (20°C, calculated-P/C, Muir 1991)  
 0.011 (calculated-P/C, Montgomery 1993)

Octanol/Water Partition Coefficient, log K<sub>OW</sub>:

2.75 (Leo et al. 1971)  
 1.61 (Rao & Davidson 1980)  
 2.80 (selected, Gerstl & Helling 1987)  
 2.18 (shake flask, Log P Database, Hansch & Leo 1987)  
 2.18 (selected, Magee 1991)  
 1.61 (Montgomery 1993)  
 2.18 (recommended, Sangster 1993)  
 1.62–2.30 (Tomlin 1994)  
 2.18 (recommended, Hansch et al. 1995)  
 2.36 (RP-HPLC-RT correlation, Finizio et al. 1997)  
 2.88 ± 0.17, 2.86 ± 0.12 (isocratic RP-HPLC-k' correlation, gradient RP-HPLC-k' correlation, Paschke et al. 2004)

Bioconcentration Factor, log BCF:

1.23 (calculated-S, Kenaga 1980)  
 1.15 (calculated-K<sub>OC</sub>, Kenaga 1980)

Sorption Partition Coefficient, log K<sub>OC</sub>:

2.42 (soil, Beestman & Demming 1976; Kenaga 1980; Kenaga & Goring 1980)  
 2.11 (soil, calculated-S as per Kenaga & Goring 1980, Kenaga 1980)  
 2.43 (calculated-MCI  $\chi$ , Gerstl & Helling 1987)  
 2.62 (screening model calculations, Jury et al. 1987b)  
 2.31 (estimated as log K<sub>OM</sub>, Magee 1991)  
 2.45 (soil, calculated-MCI  $\chi$  and fragment contribution, Meylan et al. 1992)  
 1.90 (soil, 20–25°C, selected, Wauchope et al. 1992; Hornsby et al. 1996)  
 2.07–2.11 (Montgomery 1993)  
 2.62 (estimated-chemical structure, Lohninger 1994)  
 2.42 (quoted or calculated-QSAR MCI  $\chi$ , Sabljic et al. 1995)  
 2.18 (soil, estimated-general model using molecular descriptors, Gramatica et al. 2000)

Environmental Fate Rate Constants, k, or Half-Lives, t<sub>1/2</sub>:

Volatilization: estimated t<sub>1/2</sub> = 671 d from 1 m depth of water at 20°C (Muir 1991).

Photolysis: t<sub>1/2</sub> = 2.25 h in distilled water (Tanaka et al. 1981; quoted, Cessna & Muir 1991);

1 ppb contaminated water in the presence of TiO<sub>2</sub> and H<sub>2</sub>O<sub>2</sub> completely photodegraded after 3 h by solar irradiation (Muszkat et al. 1992).

Oxidation:

Hydrolysis:

Biodegradation: t<sub>1/2</sub>  $\mu$ 10–14 d for 0.001–1.0  $\mu$ g/mL to biodegrade in sewage effluent lake water (Novick & Alexander 1985; quoted, Muir 1991);

biochemical t<sub>1/2</sub> = 7 d from screening model calculations (Jury et al. 1987b).

Biotransformation: second-order microbial rate constant k = 1.1 × 10<sup>-9</sup> L·organisms<sup>-1</sup> h<sup>-1</sup> (Steen & Collette 1989).

Bioconcentration, Uptake (k<sub>1</sub>) and Elimination (k<sub>2</sub>) Rate Constants:

Half-Lives in the Environment:

Air:

Surface water: t<sub>1/2</sub> ~ 10–14 d for 0.001–1.0  $\mu$ g/mL to biodegrade in sewage effluent lake water (Novick & Alexander 1985; quoted, Muir 1991).

Ground water:

Sediment:

Soil: persistence of 2 months (Wauchope 1978);

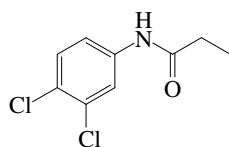
$t_{1/2} = 7$  d from screening model calculations Jury et al. 1987b);

persists in soil for 28–42 d (Worthing & Hance 1991);

selected field  $t_{1/2} = 6.3$  d (Wauchope et al. 1992; Hornsby et al. 1996).

Biota: biochemical  $t_{1/2} = 7$  d from screening model calculations (Jury et al. 1987b).

## 17.1.1.68 Propanil



Common Name: Propanils

Synonym: Bay 30130, Chem rice, Crystal Propanil-4, DCPA, Dipram, DPA, DPA, Erban, Erbanil, Farmco propanil, FW-734, Grascide, Herbax technical, Prop-Job, Propanex, Propanid, Riselect, Rogue, Rosanil, S 10165, Stam F-34, Stampede, Stam Supernox, Strel, Supernox, Surcopur, Surpur, STAM, Synpran N, Vertac, Wham EZ

Chemical Name: *N*-(3,4-dichlorophenyl)propionamide; *N*-(3,4-dichlorophenyl)propanamide

Uses: selective emergence and post-emergence herbicide to control many grasses and broadleaf weeds in potatoes, rice and wheat.

CAS Registry No: 709-98-8

Molecular Formula:  $C_9H_9Cl_2NO$

Molecular Weight: 218.079

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

92 (Lide 2003)

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

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

1.25 ( $25^{\circ}C$ , Ashton & Crafts 1981; Hartley & Kidd 1987; Herbicide Handbook 1989; Montgomery 1993; Milne 1995)

1.41 ( $22^{\circ}C$ , Tomlin 1994)

Molar Volume ( $cm^3/mol$ ):

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

Dissociation Constant  $pK_a$ :

Enthalpy of Vaporization,  $\Delta H_v$  (kJ/mol):

95.1 (Rordorf 1989)

Enthalpy of Fusion,  $\Delta H_{fus}$  (kJ/mol):

20.08 (DSC method, Plato & Glasgow 1969)

15.3 (Rordorf 1989)

Entropy of Fusion,  $\Delta S_{fus}$  (J/mol K):

Fugacity Ratio at  $25^{\circ}C$  (assuming  $\Delta S_{fus} = 56$  J/mol K), F: 0.220 (mp at  $92^{\circ}C$ )

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

225 (Woodford & Evans 1963; Khan 1980)

500 (Bailey & White 1965; Ashton & Crafts 1973; Herbicide Handbook 1989)

268 (Freed 1966)

225 (Martin & Worthing 1977; Worthing & Walker 1987; Herbicide Handbook 1983)

268–500 (Weber et al. 1980)

130 ( $20^{\circ}C$ , Spencer 1982)

225 (Hartley & Kidd 1987; Milne 1995)

130 ( $20^{\circ}C$ , Worthing & Hance 1991)

200 ( $20$ – $25^{\circ}C$ , selected, Wauchope et al. 1992; Hornsby et al. 1996)

130, 225 ( $20^{\circ}C$ ,  $25^{\circ}C$ , Montgomery 1993)

130 (Tomlin 1994)

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

0.012 ( $60^{\circ}C$ , Khan 1980)

0.012 ( $60^{\circ}C$ , Verschueren 1983)

0.012 ( $60^{\circ}C$ , Hartley & Kidd 1987)

0.005 ( $20^{\circ}C$ , selected, Suntio et al. 1988)

$2.50 \times 10^{-4}$ ,  $7.20 \times 10^{-3}$ , 0.130, 1.50, 13.0 (25, 50, 70, 100,  $125^{\circ}C$ , gas saturation-GC, Rordorf 1989)

$\log (P_s/P_a) = 15.201 - 5604.1/(T/K)$ ; measured range 36.4–92.6°C (gas saturation-GC, Rordorf 1989)  
 $\log (P_L/P_a) = 13.192 - 4863.1/(T/K)$ ; measured range 95.1–160°C (gas saturation-GC, Rordorf 1989)  
 $2.60 \times 10^{-5}$  (20°C, Worthing & Hance 1991)  
 0.00533 (20–25°C, selected, Wauchope et al. 1992; Hornsby et al. 1996)  
 $2.67 \times 10^{-5}$  (20°C, Montgomery 1993)

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

0.0036 (20°C, calculated-P/C, Suntio et al. 1988)  
 0.0036 (20°C, calculated-P/C, Montgomery 1993)  
 0.00545 (calculated-P/C, this work)

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

2.02 (Rao & Davidson 1980)  
 2.80 ( $20 \pm 2^\circ\text{C}$ , shake flask-UV, Briggs 1981)  
 3.12 (selected, Dao et al. 1983)  
 3.07 (shake flask, Log P Database, Hansch & Leo 1987)  
 2.99 (selected, Gerstl & Helling 1987)  
 2.29 (Worthing & Hance 1991; Milne 1995)  
 2.34 (quoted from Kenaga 1980, Bottoni & Funari 1992)  
 2.73 (RP-HPLC-RT correlation, Sicbaldi & Finizio 1993)  
 2.03, 2.29 (Montgomery 1993)  
 3.07 (recommended, Sangster 1993)  
 2.80 (RP-HPLC-RT correlation, Saito et al. 1993)  
 3.30 (Tomlin 1999)  
 3.07 (selected, Hansch et al. 1995)  
 2.73 (RP-HPLC-RT correlation, Finizio et al. 1997)  
 3.21 (RP-HPLC-RT correlation using short ODP column, Donovan & Pescatore 2002)

Bioconcentration Factor,  $\log \text{BCF}$ :

1.46 (calculated-S, Kenaga 1980)  
 1.34 (calculated, Pait et al. 1992)

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

2.34 (calculated-S, Kenaga 1980)  
 2.23 (calculated-MCI  $\chi$ , Gerstl & Helling 1987)  
 2.33 (selected, Trevisan et al. 1991)  
 2.19 (Montgomery 1993)  
 2.17 (soil, 20–25°C, selected, Wauchope et al. 1992; Hornsby et al. 1996)  
 2.38–2.90 (Tomlin 1994)

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

Volatilization:

Photolysis:  $t_{1/2} = 34$  d for 82% of 200  $\mu\text{g/mL}$  to degrade in distilled water under sunlight (Moilanen & Crosby 1972; quoted, Cessna & Grover 1991);

$t_{1/2} = 2.25$  h for 37–51% of 100  $\mu\text{g mL}^{-1}$  to degrade in distilled water under  $> 300$  nm light (Tanaka et al. 1981; quoted, Cessna & Grover 1991);

$t_{1/2} = 245$  h for 14–81% of 15  $\mu\text{g mL}^{-1}$  to degrade in distilled water under sunlight (Draper & Crosby 1984; quoted, Cessna & Grover 1991);

photolysis  $t_{1/2} = 12$ –13 h in water (Tomlin 1994).

Oxidation: measured rate constant for reaction with hydroxyl radical,  $k(\text{aq.}) = 1.60 \times 10^9 \text{ M}^{-1} \text{ s}^{-1}$  in irradiated field water both in the laboratory and sunlit rice paddies (Mabury & Crosby 1996).

Hydrolysis:  $t_{1/2} > 4$  months for 4360  $\mu\text{g mL}^{-1}$  to hydrolyze in phosphate buffers pH 5–9 at 20°C (El-dib & Aly 1976; quoted, Muir 1991);

hydrolysis  $t_{1/2} \gg 1$  yr at pH 4, 7, 9 at 22°C (Tomlin 1994).



Biodegradation:  $t_{1/2} = 1-2$  d for  $30 \mu\text{g mL}^{-1}$  to biodegrade in flooded soil at  $30^\circ\text{C}$  (Kuwatsuka 1972; quoted, Muir 1991);

$t_{1/2} \sim 10$  d for  $40 \mu\text{g mL}^{-1}$  to biodegrade in pond sediment (Stepp et al. 1985; quoted, Muir 1991).

Biotransformation: second-order microbial degradation rate constant  $k = 5 \times 10^{-10} \text{ L} \cdot \text{organisms}^{-1} \text{ h}^{-1}$  (Steen & Collette 1989).

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

#### Half-Lives in the Environment:

Air:

Surface water: hydrolysis  $t_{1/2} \gg 1$  yr (pH 4, 7, 9) at  $22^\circ\text{C}$  and photolysis  $t_{1/2} = 12-13$  h in aqueous solution (Tomlin 1994).

Groundwater: reported  $t_{1/2} < 5$  d (Bottoni & Funari 1992)

Sediment:  $t_{1/2} \sim 10$  d for  $40 \mu\text{g mL}^{-1}$  to biodegrade in pond sediment (Stepp et al. 1985; quoted, Muir 1991).

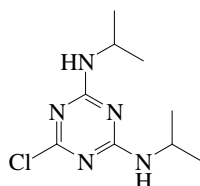
Soil:  $t_{1/2} = 1-2$  d for  $30 \mu\text{g mL}^{-1}$  to biodegrade in flooded soil at  $30^\circ\text{C}$  (Kuwatsuka 1972; quoted, Muir 1991);  
selected field  $t_{1/2} = 1.0$  d (Wauchope et al. 1992; Hornsby et al. 1996; quoted, Halfon et al. 1996);

soil  $t_{1/2} = 15$  d (Pait et al. 1992);

$t_{1/2} < 5$  d (Bottoni & Funari 1992).

Biota:

## 17.1.1.69 Propazine



Common Name: Propazine

Synonym: G-30028, Geigy 30028, Gesamil, Maax, Milogard, Plantulin, Primatol P, Propasin, Prozinex

Chemical Name: 6-chloro-*N,N'*-bis(1-methylethyl)-1,3,5-triazine-2,4-diamine; 2-chloro-4,6-bis(isopropylamino)-1,3,5-triazine

Uses: selective pre-emergence herbicide to control annual grasses and broadleaf weeds in milo and sweet sorghum.

CAS Registry No: 139-40-2

Molecular Formula: C<sub>9</sub>H<sub>16</sub>ClN<sub>5</sub>

Molecular Weight: 229.710

Melting Point (°C):

213 (Lide 2003)

Boiling Point (°C):

Density (g/cm<sup>3</sup> at 20°C):

1.162 (Hartley & Kidd 1987; Worthing & Hance 1991; Montgomery 1993; Tomlin 1994; Milne 1995)

Molar Volume (cm<sup>3</sup>/mol):

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

Dissociation Constant:

1.85 (pK<sub>a</sub>, Weber 1970; quoted, Bintein & Devillers 1994)

1.80 (pK<sub>a</sub>, Weber et al. 1980; Willis & McDowell 1982)

1.85 (pK<sub>a</sub>, Herbicide Handbook 1989)

1.70 (pK<sub>a</sub>, 21°C, Worthing & Hance 1991)

12.15 (pK<sub>b</sub>, Wauchope et al. 1992)

1.85 (pK<sub>a</sub>, 22°C, Montgomery 1993)

12.3 (pK<sub>b</sub>, 21°C, Tomlin 1994)

Enthalpy of Fusion, ΔH<sub>fus</sub> (kJ/mol):

41.84 (DSC method, Plato 1972)

Entropy of Fusion, ΔS<sub>fus</sub> (J/mol K):

Fugacity Ratio at 25°C (assuming ΔS<sub>fus</sub> = 56 J/mol K), F: 0.0143 (mp at 213°C)

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

10 (Gysin 1962)

8.6 (20–22°C, Bailey & White 1965; Spencer 1973; Quellette & King 1977)

4.82, 4.60, 5.05 (26°C, shake flask-UV at pH 3.0, 7.0, 10.0, Ward & Weber 1968)

8.60 (Martin & Worthing 1977)

4.8–8.6 (Weber et al. 1980)

5.0 (20°C, Spencer 1982)

8.60 (20°C, Hartley & Kidd 1987; Herbicide Handbook 1989)

5.0 (20°C, Worthing & Walker 1987, Worthing & Hance 1991; Tomlin 1994; Milne 1995)

8.60 (20–25°C, selected, Wauchope et al. 1992; Hornsby et al. 1996)

8.50 (20°C, Montgomery 1993)

Vapor Pressure (Pa at 25°C or as indicated and reported temperature dependence equations):

3.87 × 10<sup>-6</sup> (20°C, extrapolated-Antoine eq. from gas saturation-GC measurements, measured range 50–130°C, Friedrich & Stambach 1964) (See figure at the end of this section.)

log (P/mmHg) = 11.911 – 4933/(T/K), temp range 50–130°C (gas saturation-GC, data presented in graph and Antoine eq., Friedrich & Stambach 1964)

3.90 × 10<sup>-6</sup> (20°C, Quellette & King 1977)

- $4.00 \times 10^{-6}$  (20–25°C, Weber et al. 1980)
- $3.90 \times 10^{-6}$  (20°C, Ashton & Crafts 1981; Herbicide Handbook 1989)
- $4.00 \times 10^{-6}$  (20°C, Hartley & Kidd 1987)
- $2.10 \times 10^{-5}$  (30°C, Herbicide Handbook 1989)
- $3.90 \times 10^{-6}$  (20°C, Worthing & Hance 1991; Montgomery 1993)
- $1.75 \times 10^{-5}$  (20–25°C, selected, Wauchope et al. 1992; Hornsby et al. 1996)

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

- $1.00 \times 10^{-4}$  (20°C, selected, Suntio et al. 1988; quoted, Majewski & Capel 1995)
- $1.00 \times 10^{-3}$  (20°C, calculated-P/C, Montgomery 1993)
- $1.04 \times 10^{-3}$  (calculated-P/C, this work)

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

- 2.89 (Kenaga & Goring 1980; Yoshioka et al. 1986)
- 2.94 (shake flask-GC or UV, Brown & Flagg 1981)
- 2.59 (RP-HPLC- $k'$  correlation, Braumann et al. 1983)
- 2.93 (shake flask, Biagi et al. 1991)
- 2.91 (RP-HPLC-RT correlation, Finizio et al. 1991)
- 2.91, 2.94 (Montgomery 1993)
- 2.77 (RP-HPLC-RT correlation, Sicbaldi & Finizio 1993)
- 2.93 (recommended, Sangster 1993; Hansch et al. 1995)
- 2.89 (shake flask-UV, Liu & Qian 1995)
- 3.13 (Pomona-database, Müller & Kördel 1996)
- 2.77 (RP-HPLC-RT correlation, Finizio et al. 1997)

Bioconcentration Factor, log BCF:

- 2.26 (calculated-S, Kenaga 1980)
- 0.903 (calculated- $K_{oc}$ , Kenaga 1980)

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

- 2.20 (soil, Hamaker & Thompson 1972; Brown 1978; Kenaga 1980; Kenaga & Goring 1980; Sabljic 1987)
- 3.11 (soil, calculated-S per Kenaga & Goring 1980; Kenaga 1980)
- 2.56 (Georgia's Hickory Hill pond sediment, Brown & Flagg 1981)
- 2.78 (calculated-MCI  $\chi$ , Gerstl & Helling 1987)
- 2.34 (estimated as log  $K_{OM}$ , Magee 1991)
- 2.18 (soil, quoted, Bottoni & Funari 1992)
- 2.19 (soil, 20–25°C, selected, Wauchope et al. 1992; Hornsby et al. 1996)
- 1.94 (soil, HPLC-screening method, mean value from different stationary and mobile phases, Kördel et al. 1993, 1995b)
- 1.69–2.56 (Montgomery 1993)
- 2.44 (selected, Lohninger 1994)
- 1.90, 2.0 (Tomlin 1994)
- 2.57 (calculated- $K_{ow}$ , Liu & Qian 1995)
- 2.40 (soil, calculated-MCI  $\chi$ , Sabljic et al. 1995)
- 1.94; 2.55 (HPLC-screening method; calculated-PCKOC fragment method, Müller & Kördel 1996)
- 2.59, 1.93, 2.08, 1.95, 2.70 (first generation Eurosoils ES-1, ES-2, ES-3, ES-4, ES-5, shake flask/batch equilibrium-HPLC/UV, Gawlik et al. 1998, 1999)
- 2.18, 2.148, 2.10, 1.98, 2.58 (second generation Eurosoils ES-1, ES-2, ES-3, ES-4, ES-5, shake flask/batch equilibrium-HPLC/UV, Gawlik et al. 1999)
- 2.818, 2.148, 2.100, 1.977, 2.579 (second generation Eurosoils ES-1, ES-2, ES-3, ES-4, ES-5, shake flask/batch equilibrium-HPLC/UV and HPLC- $k'$  correlation, Gawlik et al. 2000)
- 2.40; 2.43, 2.84 (soil, quoted obs.; estimated-class-specific model, estimated-general model using molecular descriptors, Gramatica et al. 2000)
- 2.15, 2.17 (soils: organic carbon OC  $\geq$  0.1%, OC  $\geq$  0.5%, pH 3.2–7.4, average, Delle Site 2001)

2.29, 2.21, 2.03 (soil with organic carbon  $OC \geq 0.5\%$  at: pH 4.3–5.0, pH 5.1–5.0, pH  $\geq 6.0$ , average, Delle Site 2001)

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

Volatilization:

Photolysis: 1 ppb contaminated water in presence of  $TiO_2$  and  $H_2O_2$  completely photodegraded after 3.5 h by solar irradiation (Muszkat et al. 1992).

Oxidation:

Hydrolysis: calculated rate constant  $k = 9.70 \times 10^{-6} \text{ s}^{-1}$  with  $t_{1/2} = 83 \text{ d}$  at  $20^\circ\text{C}$  in a buffer at pH 5 (Burkhard & Guth 1981).

Biodegradation:

Biotransformation:

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

Half-Lives in the Environment:

Air:

Surface water:

Ground water: reported half-lives or persistence,  $t_{1/2} = 80\text{--}100 \text{ d}$  (Bottoni & Funari 1992)

Sediment:

Soil: persistence of 18 months (Edwards 1973; quoted, Morrill et al. 1982);

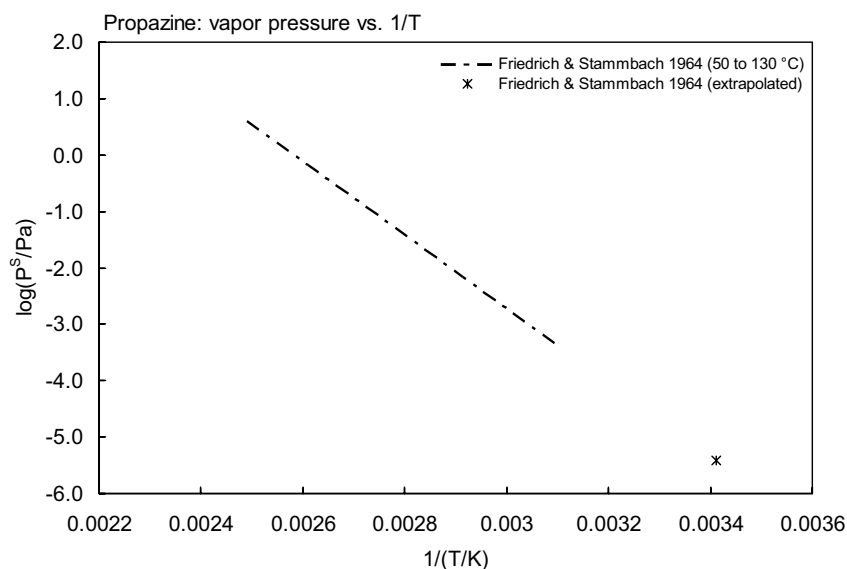
persistence of 12 months in soil (Wauchope 1978);

$t_{1/2} = 62 \text{ d}$  and  $127 \text{ d}$  in a Hatzenbühl soil at pH 4.8 and Neuhoefen soil at pH 6.5 respectively at  $22^\circ\text{C}$  under laboratory conditions (Burkhard & Guth 1981; quoted, Montgomery 1993);

reported  $t_{1/2} = 80\text{--}100 \text{ d}$  (Bottoni & Funari 1992);

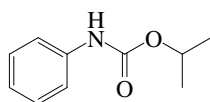
selected field  $t_{1/2} = 135 \text{ d}$  (Wauchope et al. 1992; Hornsby et al. 1996).

Biota:



**FIGURE 17.1.1.69.1** Logarithm of vapor pressure versus reciprocal temperature for propazine.

## 17.1.1.70 Protham



Common Name: Protham

Synonym: Agermin, Ban-Hoe, Beet-Kleen, Birgin, Chem-Hoe, Collavin, IFC, IFK, INPC, IPC

Chemical Name: carbanilate acid isopropyl ester; isopropyl carbanilate; isopropyl-N-phenyl carbamate; 1-methylethyl phenylcarbamate

Uses: pre-emergence and post-emergence herbicide to control annual grass weeds in peas, beans, sugar beet, lettuce, lucerne, clover, flax, sunflowers and lentils.

CAS Registry No: 122-42-9

Molecular Formula:  $C_{10}H_{13}NO_2$

Molecular Weight: 179.2 16

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

90 (Lide 2003)

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

> 150 (sublimes but decomposes, Montgomery 1993)

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

1.09 (Spencer 1982; Tomlin 1994; Hartley & Kidd 1987; Milne 1995)

1.09 ( $30^{\circ}C$ , Ashton & Crafts 1981; Herbicide Handbook 1989; Montgomery 1993)

Molar Volume ( $cm^3/mol$ ):

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

Dissociation Constant  $pK_a$ :

Enthalpy of Fusion,  $\Delta H_{fus}$  (kJ/mol):

Entropy of Fusion,  $\Delta S_{fus}$  (J/mol K):

Fugacity Ratio at  $25^{\circ}C$  (assuming  $\Delta S_{fus} = 56$  J/mol K), F: 0.230 (mp at  $90^{\circ}C$ )

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

100 (Freed 1953)

250 (Nex & Swezey 1954; Ashton & Crafts 1981)

22.5–32 (Bailey & White 1965)

250 ( $20^{\circ}C$ , Spencer 1973, 1982)

250 (Martin & Worthing 1977; Herbicide Handbook 1978, 1983, 1989; Hartley & Kidd 1987)

250–254 (Weber et al. 1980)

127 (selected, Gerstl & Helling 1987)

32–250 ( $20$ – $25^{\circ}C$ , Worthing & Hance 1991; Montgomery 1993)

250 ( $20$ – $25^{\circ}C$ , selected, Wauchope et al. 1992; Hornsby et al. 1996)

250 ( $20^{\circ}C$ , Tomlin 1994; Milne 1995)

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

sublimes (rm. temp., Herbicide Handbook 1989)

sublimes (rm. temp., Montgomery 1993; Tomlin 1994)

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

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

2.60 ( $20 \pm 2^{\circ}C$ , shake flask-UV, Briggs 1981)

2.16 (selected, Dao et al. 1983; Gerstl & Helling 1987)

2.27 (shake flask, Mitsutake et al. 1986)

2.60 (recommended, Sangster 1993)

## Bioconcentration Factor, log BCF:

1.43	(calculated-S, Kenaga 1980)
0.301	(calculated- $K_{OC}$ , Kenaga 1980)

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

1.71	(Hamaker & Thompson 1972; Kenaga 1980; Kenaga & Goring 1980)
2.32	(soil, calculated-S as per Kenaga & Goring 1980, Kenaga 1980)
1.71	(20 $\pm$ 2°C, reported as log $K_{OM}$ , Briggs 1981)
1.93	(calculated-MCI $\chi$ , Gerstl & Helling 1987)
2.30	(soil, 20–25°C, estimated, Wauchope et al. 1992; Hornsby et al. 1996)
1.71	(Montgomery 1993)
2.30	(estimated-chemical structure, Lohninger 1994)

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

## Volatilization:

Photolysis: direct  $t_{1/2}$  = 254 d in clear water body near the surface for a mid-summer day at latitude 40° (Wolfe et al. 1978)

direct  $t_{1/2}$  = 254 d in distilled water assuming for a mid-summer day at latitude 40°;  $t_{1/2}$  = 2.25 h for 1% of 100  $\mu\text{g/mL}$  to degrade in distilled water under 300 nm light (Tanaka et al. 1981; quoted, Cessna & Muir 1991).

## Oxidation:

Hydrolysis:  $t_{1/2}$  > 4 months for 3550  $\mu\text{g/mL}$  to hydrolyze in phosphate buffer at pH 5–9 and 20°C (El-Dib & Aly 1976; quoted, Muir 1991)

$k(\text{alkaline}) = 7.6 \times 10^{-6} \text{ M}^{-1} \text{ s}^{-1}$  at 27°C,  $k = 5.6 \times 10^{-5} \text{ M}^{-1} \text{ s}^{-1}$  at 50°C,  $k = 2.6 \times 10^{-4} \text{ M}^{-1} \text{ s}^{-1}$  at 70°C; with  $t_{1/2} > 1 \times 10^4$  d at pH 5, 7 and 9 (Wolfe et al. 1978)

Biodegradation:  $t_{1/2}$  = 190 d by 1 mg/L fungus *Asperillus fumigaurs*,  $t_{1/2}$  = 3.2 d by bacteria (Wolfe et al. 1978)

$k = 1.5 \times 10^{-4} \text{ L (mg M)}^{-1} \text{ h}^{-1}$  with  $t_{1/2}$  = 190 d for 2–25  $\mu\text{g/mL}$  fungus *Aspergillus fumigatus*;  $k = 9 \times 10^{-2} \text{ L (mg M)}^{-1} \text{ h}^{-1}$  with  $t_{1/2}$  = 3.2 d for bacteria *Pseudomonas striata* to biodegrade in stream water at pH 7 and 28°C (Muir 1991)

$t_{1/2} \sim 30\text{--}40$  d for 1–0.0004  $\mu\text{g/mL}$  to biodegrade in filtered sewage water at 20–22°C and  $t_{1/2} \sim 20$  to 50 d at 29°C in filtered lake water (Wang et al. 1984; quoted, Muir 1991)

$t_{1/2}(\text{aerobic}) > 4$  months for 6–7  $\mu\text{g/mL}$  to biodegrade in river water at 25°C (Stepp et al. 1985; quoted, Muir 1991)

## Biotransformation:

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

## Half-Lives in the Environment:

## Air:

Surface water: hydrolysis  $t_{1/2} > 1 \times 10^4$  d based on neutral and alkaline hydrolysis assuming pseudo-first order kinetics; direct photolysis  $t_{1/2}$  = 254 d assuming a mid-summer day at altitude 40°, and biolysis  $t_{1/2}$  = 190 d for 1 mg/L of fungus and  $t_{1/2}$  = 3.2 d for bacteria at 28°C (Wolfe et al. 1978);

$t_{1/2} \sim 30\text{--}40$  d for 1–0.0004  $\mu\text{g/mL}$  to biodegrade in filtered sewage water at 20–22°C and  $t_{1/2} \sim 20$  to 50 d at 29°C in filtered lake water (Wang et al. 1984; quoted, Muir 1991);

aerobic  $t_{1/2} > 4$  months for 6–7  $\mu\text{g/mL}$  to biodegrade in river water at 25°C (Stepp et al. 1985; quoted, Muir 1991).

## Ground water:

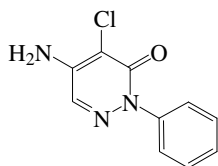
## Sediment:

Soil:  $t_{1/2} \sim 15$  d in soil and  $t_{1/2}$  = 5 d at 16 and 29°C (Hartley & Kidd 1987; Herbicide Handbook 1989; quoted, Montgomery 1993; Tomlin 1994);

selected field  $t_{1/2}$  = 10 d (Wauchope et al. 1992; Hornsby et al. 1996).

## Biota:

## 17.1.1.71 Pyrazon



Common Name: Pyrazon

Synonym: chloridazon, chloridazone, Blurex, Burex, Dazon, Phenosane, Piramin, Pyramin

Chemical Name: 5-amino-4-chloro-2-phenylpyridazin-3(2H)-one

Uses: as pre- and post-emergence herbicide to control of annual broadleaf weeds in sugar-beet, fodder beet and beet root; and also used in combination with other herbicides, etc.

CAS Registry No: 1698-60-8

Molecular Formula:  $C_{10}H_8ClN_3O$

Molecular Weight: 221.643

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

205 (Lide 2003)

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

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

1.54 (Tomlin 1994)

Molar Volume ( $cm^3/mol$ ):

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

143.9 (calculated-density)

Dissociation Constant  $pK_a$ :

Enthalpy of Fusion,  $\Delta H_{fus}$  ( $kJ/mol$ ):

26.59 (DSC method, Plato & Glasgow 1969)

Entropy of Fusion,  $\Delta S_{fus}$  ( $J/mol K$ ):

Fugacity Ratio at  $25^{\circ}C$  (assuming  $\Delta S_{fus} = 56 J/mol K$ ), F: 0.0171 (mp at  $205^{\circ}C$ )

0.013 ( $20^{\circ}C$ , Suntio et al. 1988)

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

400 ( $20^{\circ}C$ , Ashton & Crafts 1973, 1981)

300 ( $20^{\circ}C$ , Khan 1980)

400 ( $20^{\circ}C$ , Spencer 1982)

400 ( $20^{\circ}C$ , Worthing & Walker 1987; Hartley & Kidd 1987; Milne 1995)

360 ( $20^{\circ}C$ , selected, Suntio et al. 1988)

400 ( $20$ – $25^{\circ}C$ , selected, Wauchope et al. 1992; Hornsby et al. 1996)

340 ( $20^{\circ}C$ , Tomlin 1994)

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

9.86 ( $40^{\circ}C$ , Ashton & Craft 1973; Spencer 1982)

< 0.00001 ( $20^{\circ}C$ , Worthing & Walker 1987; Hartley & Kidd 1987; Tomlin 1994)

7.0 ( $20^{\circ}C$ , estimated, Suntio et al. 1988)

6.67 ( $20$ – $25^{\circ}C$ , selected, Wauchope et al. 1992; Hornsby et al. 1996)

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

4.31 ( $20^{\circ}C$ , calculated-P/C, Suntio et al. 1988)

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

1.14 ( $22^{\circ}C$ , shake flask-AS, Braumann & Grimme 1981; quoted, Sangster 1993)

1.50 (selected, Gerstl & Helling 1987)

1.12 (RP-HPLC-RT correlation, Sicbaldi & Finizio 1993)

1.19 (pH 7, Tomlin 1994)

- 2.20 (Milne 1995)
- 1.14 (recommended, Hansch et al. 1995)
- 1.12 (RP-HPLC-RT correlation, Finizio et al. 1997)

Bioconcentration Factor, log BCF:

- 1.32 (calculated-S per Kenaga 1980, this work)

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

- 2.12, 2.18 (selected, calculated-MCI  $\chi$ , Gerstl & Helling 1987)
- 2.74 (soil, calculated-MCI and fragments contribution method, Meylan et al. 1992)
- 2.08 (soil, Wauchope et al. 1992; Hornsby et al. 1996)
- 1.95–2.53 (soil, Tomlin 1994)

Environmental Fate Rate Constants, or Half-Lives:

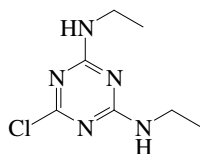
Photolysis:  $t_{1/2} = 150$  h at pH 7 in simulated sunlight and  $t_{1/2} = 47.7$  h by 80000 lux, xenon lamp (Tomlin 1994).

Half-Lives in the Environment:

Soil: field  $t_{1/2} = 21$  d (Wauchope et al. 1992; Hornsby et al. 1996)



## 17.1.1.72 Simazine



Common Name: Simazine

Synonym: A 2079, Aktinit S, Amizine, Aquazine, Batazina, Bitemol, Cekusan, CAT, CET, DCT, Framed, G 27692, Gesapun, Gesaran, Gesatop, Herbazin, Herbex, Herboxy, Premazine, Primatol, Primcep, Princep, Printop, Radocon, Radokor, Simadex, Simanex, Sim-Trol, Tafazine, Weedex, Zeapur

Chemical Name: 6-chloro-*N,N'*-diethyl-1,3,5-triazine-2,4-diamine; 2-chloro-4,6-bis(ethyl-amino)-1,3,5-triazine

Uses: selective pre-emergence systemic herbicide to control many broadleaf weeds and annual grasses in deep-rooted fruit and vegetable crops.

CAS Registry No: 122-34-9

Molecular Formula:  $C_7H_{12}ClN_5$

Molecular Weight: 201.657

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

226 (Lide 2003)

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

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

1.302 (Hartley & Kidd 1987; Milne 1995)

1.203 (Montgomery 1993)

Molar Volume ( $cm^3/mol$ ):

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

Dissociation Constant:

1.65 ( $pK_a$ , Weber 1970; quoted, Bintein & Devillers 1994)

1.60 ( $pK_a$ , Weber et al. 1980; Willis & McDowell 1982)

1.70 ( $pK_a$ ,  $21^{\circ}C$ , Worthing & Hance 1991; Montgomery 1993)

2.00 ( $pK_a$ , Yao & Haag 1991; Haag & Yao 1992)

12.35 ( $pK_b$ , Wauchope et al. 1992; Hornsby et al. 1996)

12.3 ( $pK_b$ , Tomlin 1994)

Enthalpy of Fusion,  $\Delta H_{fus}$  (kJ/mol):

43.932 (DSC method, Plato 1972)

Entropy of Fusion,  $\Delta S_{fus}$  (J/mol K):

Fugacity Ratio at  $25^{\circ}C$  (assuming  $\Delta S_{fus} = 56$  J/mol K), F: 0.0107 (mp at  $226^{\circ}C$ )

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

5.0 (Bailey & White 1965 Freed 1976; Wauchope 1978)

5.8, 5.0, 5.0 ( $26^{\circ}C$ , shake flask-UV at pH 3.0, 7.0, 10.0, Ward & Weber 1968)

15.1 ( $26^{\circ}C$ , Getzen & Ward 1971)

5.0 ( $20^{\circ}C$ , Weber 1972; Spencer 1973; Khan 1980)

5.0 ( $20^{\circ}C$ , Martin & Worthing 1977; Worthing & Walker 1987; Worthing & Hance 1991; Milne 1995)

3.5 (Herbicide Handbook 1978, 1989)

3.5 ( $20^{\circ}C$ , Ashton & Crafts 1981; Hartley & Kidd 1987)

5.0, 3.50, 7.4 ( $20^{\circ}C$ , quoted, exptl., calculated-Parachor & mp, Briggs 1981)

6.2 ( $20$ – $25^{\circ}C$ , selected, Wauchope et al. 1992; Hornsby et al. 1996)

3.5–5.0 ( $20^{\circ}C$ ), Montgomery 1993)

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

$8.13 \times 10^{-7}$  ( $20^{\circ}C$ , extrapolated-Antoine eq. from gas saturation-GC measurements, measured range  $50$ – $130^{\circ}C$ , Friedrich & Stambach 1964) (See figure at the end of this section.)

$\log (P/mmHg) = 11.911 - 4933/(T/K)$ , temp range  $50$ – $130^{\circ}C$  (gas saturation-GC, data presented in graph and Antoine eq., Friedrich & Stambach 1964)

- 8.10 × 10<sup>-7</sup> (20°C, Weber 1972; Khan 1980; Ashton & Crafts 1981; Herbicide Handbook 1989)
- 2.00 × 10<sup>-6</sup> (gas saturation, Spencer & Cliath 1974)
- 8.00 × 10<sup>-7</sup> (20–25°C, Weber et al. 1980; Willis & McDowell 1982)
- 8.10 × 10<sup>-7</sup> (20°C, Hartley & Kidd 1987; Worthing & Walker 1987; Worthing & Hance 1991; Montgomery 1993)
- 8.50 × 10<sup>-6</sup> (20°C, selected, Suntio et al. 1988)
- 4.80 × 10<sup>-6</sup> (30°C, Herbicide Handbook 1989)
- 2.95 × 10<sup>-6</sup> (20–25°C, selected, Wauchope et al. 1992; Hornsby et al. 1996)
- 2.94 × 10<sup>-6</sup> (OECD 104, Tomlin 1994)

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

- 8.40 × 10<sup>-5</sup> (calculated-P/C, Jury et al. 1983, 1984, 1987a; Jury & Ghodrati 1989)
- 3.40 × 10<sup>-4</sup> (20°C, calculated-P/C, Suntio et al. 1988)
- 8.40 × 10<sup>-5</sup> (calculated-P/C, Taylor & Glotfelty 1988)
- 3.30 × 10<sup>-5</sup> (20°C, calculated-P/C, Muir 1991)
- 3.40 × 10<sup>-4</sup> (20°C, calculated-P/C, Montgomery 1993)

Octanol/Water Partition Coefficient, log K<sub>OW</sub>:

- 2.19 (Kenaga & Goring 1980)
- 1.94 (Rao & Davidson 1980)
- 1.51 (shake flask-UV, Lord et al. 1980)
- 1.51 (20 ± 2°C, shake flask-UV, Briggs 1981)
- 2.16 (shake flask, Brown & Flagg 1981)
- 1.96, 2.06 (RP-HPLC-k' correlation, McDuffie et al. 1981)
- 2.27 (selected, Dao et al. 1983; Gerstl & Helling 1987)
- 2.14 (shake flask, Mitsutake et al. 1986)
- 1.50 (Nicholls 1988)
- 2.18 (shake flask, Biagi et al. 1991)
- 2.26, 2.20 (RP-HPLC-RT correlation, calculated, Finizio et al. 1991)
- 1.96 (Worthing & Hance 1991; Milne 1995)
- 2.00 (shake flask, pH 7, Baker et al. 1992)
- 1.94–2.26 (Montgomery 1993)
- 2.07 (RP-HPLC-RT correlation, Sicbaldi & Finizio 1993)
- 2.18 (recommended, Sangster 1993)
- 2.10 (Tomlin 1994)
- 2.18 (shake flask-UV, Liu & Qian 1995)
- 2.18 (recommended, Hansch et al. 1995)
- 2.51 (Pomona-database, Müller & Kördel 1996)
- 2.07 (RP-HPLC-RT correlation, Finizio et al. 1997)
- 1.83 (RP-HPLC-RT correlation, Nakamura et al. 2001)
- 1.49 (RP-HPLC-RT correlation using short ODP column, Donovan & Pescatore 2002)

Bioconcentration Factor, log BCF:

- 2.48 (calculated-S, Kenaga 1980)
- 0.778 (calculated-K<sub>OC</sub>, Kenaga 1980)
- 2.16 (earthworms, Lord et al. 1980)
- 0.699 (calculated-K<sub>OW</sub>, Briggs 1981)

Sorption Partition Coefficient, log K<sub>OC</sub>:

- 2.13 (soil, Hamaker & Thompson 1972; Brown 1978; Kenaga 1980; Kenaga & Goring 1980)
- 3.34 (soil, calculated-S as per Kenaga & Goring 1980, Kenaga 1980)
- 2.15 (av. soils/sediments, Rao & Davidson 1980)
- 1.68 (20 ± 2°C, K<sub>OM</sub> multiplied by 1.724, Briggs 1981)
- 2.33 (Georgia's Hickory Hill pond sediment, Brown & Flagg 1981)
- 3.66, 2.53, 1.77 (estimated-S, calculated-S and mp, estimated-K<sub>OW</sub>, Karickhoff 1981)
- 2.14 (soil average, Jury et al. 1983)

- 2.20, 2.15 (selected, calculated-MCI  $\chi$ , Gerstl & Helling 1987)  
 2.15 (screening model calculations, Jury et al. 1987a,b; Jury & Ghodrati 1989)  
 1.60–2.20 (Carsel 1989)  
 1.92 (estimated as  $\log K_{OM}$ , Magee 1991)  
 2.13–3.34, 2.15, 2.45, 2.70 (soil, quoted values, Bottoni & Funari 1992)  
 2.11 (soil, 20–25°C, selected, Wauchope et al. 1991, Hornsby et al. 1996)  
 3.02 (average of 12 soils, calculated-linearize Freundlich Isotherm, Sukop & Cogger 1992)  
 2.14 (Montgomery 1993)  
 1.78 (soil, HPLC-screening method, mean value from different stationary and mobile phases, Kördel et al. 1993, 1995b)  
 2.37 (selected, Lohninger 1994)  
 2.01–2.58 (Tomlin 1994)  
 2.18 (calculated- $K_{OW}$ , Liu & Qian 1995)  
 2.10 (soil, calculated-MCI  $\chi$ , Sabljic et al. 1995)  
 1.79; 2.17 (HPLC-screening method; calculated-PCKOC fragment method, Müller & Kördel 1996)  
 3.07, 1.65, 1.68, 1.61, 2.48 (soil, first generation Eurosoils ES-1, ES-2, ES-3, ES-4, ES-5, shake flask/batch equilibrium-HPLC/UV, Gawlik et al. 1998, 1999)  
 2.625, 1.90, 1.69, 1.66, 2.382 (soil, second generation Eurosoils ES-1, ES-2, ES-3, ES-4, ES-5, shake flask/batch equilibrium-HPLC/UV, Gawlik et al. 1999)  
 2.625, 1.901, 1.689, 1.656, 2.382 (soil, second generation Eurosoils ES-1, ES-2, ES-3, ES-4, ES-5, shake flask/batch equilibrium-HPLC/UV and HPLC- $k'$  correlation, Gawlik et al. 2000)  
 2.10; 2.10, 2.47 (soil, quoted obs.; estimated-class-specific model, estimated-general model using molecular descriptors, Gramatica et al. 2000)  
 2.29, 2.29, 2.29 (soils: organic carbon  $OC \geq 0.1\%$ ,  $OC \geq 0.5\%$ ,  $0.1 \leq OC < 0.5\%$ , pH 3.2–8.0, average, Delle Site 2001)  
 2.50, 2.34, 2.10 (soils with organic carbon  $OC \geq 0.5\%$  at: pH 3.2–5.0, pH 5.1–5.9, pH  $\geq 6.0$ , average, Delle Site 2001)

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

Volatilization:  $t_{1/2} = 276$  d (Jury et al. 1983; quoted, Grover 1991); measured rate constant  $k = 600$  d<sup>-1</sup> and estimated rate constant  $k = 1000$  d<sup>-1</sup> (Glottfelty et al. 1989).

Photolysis:

Oxidation:

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

$k(aq.) = (4.8 \pm 0.2)$  M<sup>-1</sup> s<sup>-1</sup> for direct reaction with ozone in water at pH 4.3 and  $23^\circ\text{C}$ , with  $t_{1/2} = 1.9$  h at pH 7 (Yao & Haag 1991).

$k(aq.) = (2.8 \pm 0.2) \times 10^9$  M<sup>-1</sup> s<sup>-1</sup> for the reaction (photo-Fenton with reference to acetophenone) with hydroxyl radical in aqueous solutions at pH 3.5 and  $24 \pm 1^\circ\text{C}$  (Haag & Yao 1992).

Hydrolysis: calculated rate constant  $k = 8.32 \times 10^{-6}$  s<sup>-1</sup> with  $t_{1/2} = 96$  d at  $20^\circ\text{C}$  in a buffer at pH 5 (Burkhard & Guth 1981).

Biodegradation: rate constant  $k = 0.014$  d<sup>-1</sup> by soil incubation die-away studies (Rao & Davidson 1980; quoted, Scow 1982);

$t_{1/2} = 8$ –27 d for  $3 \mu\text{g mL}^{-1}$  to biodegrade in pond sediment/water and  $t_{1/2} > 32$  d in pond water both at  $25^\circ\text{C}$  (Tucker & Boyd 1981; quoted, Muir 1991);

$t_{1/2} = 75$  d for a 100 d leaching and screening test in 0–10 cm depth of soil (Rao & Davidson 1980; quoted, Jury et al. 1983, 1984, 1987a,b; Jury & Ghodrati 1989; Grover 1991);  
 microbial degradation  $t_{1/2} = 70$ –11 d in soil (Tomlin 1994).

Biotransformation:

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

#### Half-Lives in the Environment:

Air:

Surface water:  $t_{1/2} > 32$  d for  $3 \mu\text{g mL}^{-1}$  to biodegrade in pond water at  $25^\circ\text{C}$  (Tucker & Boyd 1981; quoted, Muir 1991);

$t_{1/2} = 1$ –4 wk in estuarine systems (Jones et al. 1982; quoted, Meakins et al. 1994);

$t_{1/2} \sim 30$  d in ponds (Herbicide Handbook 1989);  
 measured rate constant  $k = (4.8 \pm 0.2) \text{ M}^{-1} \text{ s}^{-1}$  for direct reaction with ozone in water at pH 4.3 and  $23^\circ\text{C}$ ,  
 with  $t_{1/2} = 1.9$  h at pH 7 (Yao & Haag 1991).  
 Ground water: reported half-lives or persistence,  $t_{1/2} = 15\text{--}75$ ,  $46\text{--}174$  and  $56$  d (Bottoni & Funari 1992)  
 Sediment:  $t_{1/2} = 8\text{--}27$  d for  $3 \mu\text{g mL}^{-1}$  to biodegrade in pond sediment/water at  $25^\circ\text{C}$  (Tucker & Boyd 1981;  
 quoted, Muir 1991).  
 Soil: estimated persistence of 12 months (Kearney et al. 1969; Edwards 1973; quoted, Morrill et al. 1982; Jury  
 et al. 1987a);  
 persistence of 12 months (Wauchope 1978);  
 estimated first-order  $t_{1/2} = 49.5$  d from biodegradation rate constant  $k = 0.014 \text{ d}^{-1}$  by soil incubation die-away  
 studies (Rao & Davidson 1980; quoted, Scow 1982);  
 $t_{1/2} = 45$  d in Hatzenbühl soil at pH 4.8 and  $t_{1/2} = 100$  d in Neuhausen soil at pH 6.5 both at  $22^\circ\text{C}$ , respectively,  
 under lab. conditions (Burkhard & Guth 1981; quoted, Montgomery 1993);  
 $t_{1/2} = 1\text{--}6$  months (Jones et al. 1982; quoted, Meakins et al. 1994);  
 $t_{1/2} = 75$  d from screening model calculations (Jury et al. 1987a,b; Jury & Ghodrati 1989);  
 moderately persistent in soils with  $t_{1/2} = 20\text{--}100$  d (Willis & McDowell 1982);  
 degradation rate constant  $k = (1.51 \pm 0.086) \times 10^{-2} \text{ d}^{-1}$  with  $t_{1/2} = 45.9$  d in control soil and  $k = (1.76 \pm 0.177)$   
 $\times 10^{-2} \text{ d}^{-1}$  with  $t_{1/2} = 39.4$  d in pretreated soil in the field;  $k = (0.943 \pm 0.047) \times 10^{-2} \text{ d}^{-1}$  with  $t_{1/2} = 73.5$  d  
 in control soil and  $k = (0.864 \pm 0.048) \times 10^{-2} \text{ d}^{-1}$  with  $t_{1/2} = 80.2$  d in pretreated soil once only in the  
 laboratory (Walker & Welch 1991);  
 reported  $t_{1/2} = 15\text{--}75$  d,  $46\text{--}174$  d and  $56$  d;  $29$  d at  $5^\circ\text{C}$  and  $t_{1/2} = 209$  d at  $30^\circ\text{C}$  (Bottoni & Funari 1992);  
 selected field  $t_{1/2} = 60$  d (Wauchope et al. 1991, 1992; quoted, Dowd et al. 1993; Richards & Baker 1993;  
 quoted, Halfon et al. 1996; Hornsby et al. 1996);  
 soil  $t_{1/2} = 75$  d (Pait et al. 1992);  
 degradation by microorganism in biometer systems:  $t_{1/2} = 58$  d in silty sand standard laboratory conditions,  
 $t_{1/2} = 87$  d for corrected standard conditions and  $t_{1/2} = 91$  d in simulated outdoor conditions;  $t_{1/2} = 51$  d in  
 silty loam standard laboratory conditions,  $t_{1/2} = 77$  d corrected standard conditions,  $t_{1/2} = 63$  d in simulated  
 outdoor conditions at constant soil moisture and  $20^\circ\text{C}$ . Degradation by microorganism in outdoor exper-  
 iments in small lysimeter systems:  $t_{1/2} = 32$  d outdoor fallow,  $t_{1/2} = 35$  d outdoor barley in silty sand, and  
 $t_{1/2} = 49$  d outdoor fallow,  $t_{1/2} = 53$  d outdoor barley in silty loam (Rüdel et al. 1993)  
 $t_{1/2} = 49\text{--}50$  d in  $0\text{--}40$  cm soil cores taken from: cultivated field; from meadow  $t_{1/2} = 32\text{--}39$  d and from gravel  
 track  $t_{1/2} = 62\text{--}51$  d (Hassink et al. 1994);  
 degradation  $t_{1/2} = 70\text{--}110$  d (Tomlin 1994).  
 Biota: biochemical  $t_{1/2} = 75$  d from screening model calculations (Jury et al. 1987a,b; Jury & Ghodrati 1989).

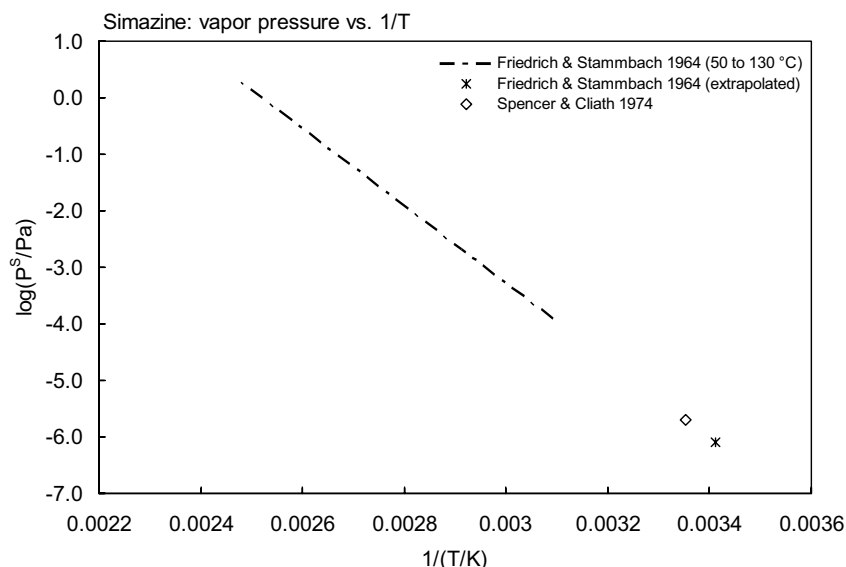
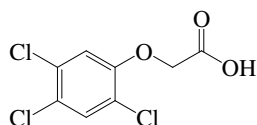


FIGURE 17.1.1.72.1 Logarithm of vapor pressure versus reciprocal temperature for simazine.

## 17.1.1.73 2,4,5-T



Common Name: 2,4,5-T

Synonym: Amine 2,4,5-T for rice, BCF-bushkiller, Brush rhap, Brush-Khap, Brushtox, Dacamine, Ded-Weed, Dinoxol, Envert-T, Estercide T-2 & T-245, Esterone 245, Fence rider, Forron, Fortex, Fruitone A, Gesatop, Inverton 245, Line rider, Phortox, Reddon, Reddox, Spontox, Super D Weedone, Tippon, Tormona, Transamine, Tributon, Trinoxol, Trioxone, Veon, Weddar, Weedone

Chemical Name: 2,4,5-trichlorophenoxyacetic acid

Uses: herbicide to control undesirable brush and woody plants; also used as plant hormone, defoliant.

CAS Registry No: 93-76-5

Molecular Formula:  $C_8H_5Cl_3O_3$

Molecular Weight: 255.483

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

153 (Lide 2003)

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

> 200 (dec., Howard 1991)

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

1.80 (Ashton & Crafts 1981; Hartley & Kidd 1987; Montgomery 1993)

1.80 ( $25^{\circ}C$ , Que Hee et al. 1981)

1.80 (Spencer 1982; Budavari 1989; Milne 1995)

Molar Volume ( $cm^3/mol$ ):

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

Dissociation Constant  $pK_a$ :

2.88 (potentiometric titration, Nelson & Faust 1969)

2.85 (Cessna & Grover 1978; Somasundaram et al. 1991; Augustijn-Beckers et al. 1994)

2.70 (Haag & Yao 1992)

2.80–2.88 (Montgomery 1993)

Enthalpy of Vaporization,  $\Delta H_v$  ( $kJ/mol$ ):

107.8 (Rordorf 1989)

Enthalpy of Fusion,  $\Delta H_{fus}$  ( $kJ/mol$ ):

34.936 (DSC method, Plato & Glasgow 1969)

34.2 (Rordorf 1989)

Entropy of Fusion,  $\Delta S_{fus}$  ( $J/mol K$ ):

Fugacity Ratio at  $25^{\circ}C$  (assuming  $\Delta S_{fus} = 56 J/mol K$ ), F: 0.0555 (mp at  $153^{\circ}C$ )

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

268 (shake flask-UV, Leopold et al. 1960)

238 ( $20^{\circ}C$ , Loos 1975)

238 (Martin & Worthing 1977)

238–280 (Weber et al. 1980)

238 ( $30^{\circ}C$ , Ashton & Crafts 1981; Budavari 1989)

278 (Spencer 1982; Verschueren 1983)

278 ( $20^{\circ}C$ , Hartley & Kidd 1987)

280 (selected, Gerstl & Helling 1987)

150 (Worthing & Walker 1987, Worthing & Hance 1991)

220 ( $20^{\circ}C$ , Montgomery 1993)

278 ( $20$ – $25^{\circ}C$ , selected, Augustijn-Beckers et al. 1994)

238 ( $20^{\circ}C$ , Milne 1995)

Vapor Pressure (Pa at 25°C or as indicated and reported temperature dependence equations):

- 0.0063 (effusion method, Hamaker & Kerlinger 1971)
- $< 1.0 \times 10^{-6}$  (20°C, Hartley & Kidd 1983)
- 0.005 (20°C, selected, Suntio et al. 1988; Riederer 1990)
- $< 1.0 \times 10^{-5}$  (20°C, Hartley & Kidd 1983; 1987)
- $2.30 \times 10^{-6}$ ,  $1.90 \times 10^{-4}$ ,  $8.50 \times 10^{-3}$ , 0.230, 4.0 (25, 50, 70, 100, 125°C, gas saturation-GC, Rordorf 1989)
- $\log (P_s/\text{Pa}) = 19.238 - 7418.9/(T/K)$ ; measured range 80.4–145°C (solid, gas saturation-GC, Rordorf 1989)
- $\log (P_L/\text{Pa}) = 15.058 - 5632.4/(T/K)$ ; measured range 80.4–145°C (liquid, gas saturation-GC, Rordorf 1989)
- $7.00 \times 10^{-7}$  (Worthing & Hance 1991)
- 0.0040 (20°C, Montgomery 1993)
- 0.0 (20–25°C at pH 7, selected, Augustijn-Beckers et al. 1994)

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

- $8.79 \times 10^{-4}$  (Hine & Mookerjee 1975)
- 0.0058 (20°C, calculated-P/C, Suntio et al. 1988)
- 0.0049 (20°C, calculated-P/C, Montgomery 1993)

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

- 3.13 (electrometric titration, Freese et al. 1979)
- 0.60 (pH dependent quoted from Dow Chemical data, Kenaga & Goring 1980)
- 0.85 (Rao & Davidson 1980)
- 2.99 (RP-HPLC- $k'$  correlation, Braumann et al. 1983)
- 3.13 (Hansch & Leo 1985)
- 3.40 (OECD 81 method, Kerler & Schönherr 1988)
- 3.36 (selected, Travis & Arms 1988)
- 3.31 (shake flask-HPLC/UV, Jafvert et al. 1990)
- 0.60–3.40 (Montgomery 1993)
- 3.13 (countercurrent LC, Ilchmann et al. 1993)
- 3.13 (selected, Sangster 1993)
- 3.13 (recommended, Hansch et al. 1995)
- 3.31 (LOGPSTAR or CLOGP data, Sabljic et al. 1995)

Bioconcentration Factor,  $\log BCF$ :

- 4.55 (milk biotransfer factor  $\log B_m$ , correlated- $K_{OW}$ , Bjerke et al. 1972)
- 1.18 (measured, Isensee 1976)
- 4.82 (beef biotransfer factor  $\log B_b$ , correlated- $K_{OW}$ , Kenaga 1980)
- 1.63 (fish under flowing water conditions, Kenaga & Goring 1980)
- 1.45 (calculated-S, Kenaga 1980)
- 0.301 (calculated- $K_{OC}$ , Kenaga 1980)
- 1.36–1.40 (fish under static ecosystem tests, Kenaga & Goring 1980; Garten & Tralbalka 1983)
- 1.41 (mosquito fish 32 d under unspecified conditions, Ang et al. 1989)

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

- 1.72 (soil, Hamaker & Thompson 1972; Kenaga 1980; Kenaga & Goring 1980; Sabljic 1987)
- 2.34 (soil, calculated-S as per Kenaga & Goring 1980, Kenaga 1980)
- 1.93, 2.27, 2.31, 2.31, 2.45, 2.31 (sand soil, whole soil, fine soil, coarse clay soil, medium silt soil, coarse silt soil, Nkedi-Kizza et al. 1983)
- 2.38 (calculated-MCI  $\chi$ , Gerstl & Helling 1987)
- 1.90 (soil, screening model calculations, Jury 1987b)
- 1.72 (soil, Sabljic 1987)
- 1.77; 2.63; 1.94 (Alfisol soil, Podzol soil; sediment, von Oepen et al. 1991)
- 1.72, 2.27 (Montgomery 1993)
- 1.90 (20–25°C at pH 7, selected, Augustijn-Beckers et al. 1994)

- 1.72 (estimated-chemical structure, Lohninger 1994)  
 1.99 (soil, calculated-QSAR MCI  $^1\chi$ , Sabljic et al. 1995)  
 1.99 (1.63–2.35) (soils: organic carbon OC  $\geq$  0.5%, average, Delle Site 2001)

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

##### Volatilization:

Photolysis:  $t_{1/2} = 48$  h for 17–80% of 1  $\mu\text{g/mL}$  to degrade in buffered aqueous solution at pH 7.8 under sunlight (Crosby & Wong 1973; quoted, Cessna & Muir 1991);

$t_{1/2} = 15$  d for  $< 2.6$   $\mu\text{g/mL}$  to degrade in distilled water under sunlight (Skurlatov et al. 1983; quoted, Cessna & Muir 1991);

$t_{1/2} = 8.7$  d for  $< 2.6$   $\mu\text{g/mL}$  to degrade in aqueous fulvic acid solution (17 mg/L) and  $t_{1/2} = 3.5$  d for  $< 2.6$   $\mu\text{g/mL}$  to degrade in aqueous fulvic acid solution (55 mg/L) under sunlight (Skurlatov et al. 1983; quoted, Cessna & Muir 1991).

##### Oxidation:

photooxidation  $t_{1/2} = 12.2$ –122 h in air, based on an estimated rate constant for the reaction with hydroxyl radical in the atmosphere (Atkinson 1987; quoted, Howard et al. 1991)

$k(\text{aq.}) = (8.9 \pm 1.3) \text{ M}^{-1} \text{ s}^{-1}$  for direct reaction with ozone in water at pH 1.7–5.0 and 26°C, with  $t_{1/2} = 1.0$  h at pH 7 (Yao & Haag 1991)

$k_{\text{OH}}(\text{calc}) = 4.0 \times 10^9 \text{ M}^{-1} \text{ s}^{-1}$  for reaction with hydroxy radical in aqueous solutions (Haag & Yao 1992).

Hydrolysis: will not hydrolyze to any reasonable extent; however, it may undergo other abiotic transformation processes (Kollig 1993).

##### Biodegradation:

$t_{1/2}(\text{aerobic}) = 27$  d for 50  $\mu\text{g/mL}$  in sediment-water microcosm by long lag phase degradation (Alexander 1974; quoted, Muir 1991)

$t_{1/2}(\text{aq. aerobic}) = 240$ –480 h, based on unacclimated soil grab sample data (Smith 1978, 1979; quoted, Howard et al. 1991)

$k = 0.001 \text{ d}^{-1}$  by river die-away test in aquatic systems (Lee & Ryan 1979; quoted, Scow 1982)

$k = 0.035 \text{ d}^{-1}$  by soil incubation die-away studies (Rao & Davidson 1980; quoted, Scow 1982)

$k = 0.01$ –0.03  $\text{d}^{-1}$  at 9–21°C by river die-away test in slurry sediment of aquatic systems (Lee & Ryan 1979; quoted, Scow 1982)

$t_{1/2} = 33$  d from screening model calculations (Jury et al. 1987b)

$t_{1/2}(\text{aq. anaerobic}) = 672$ –4320 h, based on anaerobic digester sludge data (Battersby & Wilson 1989; quoted, Howard et al. 1991).

##### Biotransformation:

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

#### Half-Lives in the Environment:

Air:  $t_{1/2} = 12.2$ –122 h, based on an estimated rate constant for the vapor-phase reaction with hydroxyl radical in the atmosphere (Atkinson 1987; quoted, Howard et al. 1991).

Surface water: estimated first-order  $t_{1/2} = 693$  d from biodegradation rate constant  $k = 0.001 \text{ d}^{-1}$  by river die-away test in aquatic systems (Lee & Ryan 1979; quoted, Scow 1982);

$t_{1/2} = 240$ –480 h, based on estimated unacclimated aqueous aerobic biodegradation half-life (Howard et al. 1991);

extremely resistant degradation in natural water with  $t_{1/2} = 580$  d for static sediment-sea water to  $t_{1/2} = 1400$  d for static estuarine river water (Muir 1991);

measured rate constant  $k = (8.9 \pm 1.3) \text{ M}^{-1} \text{ s}^{-1}$  for direct reaction with ozone in water at pH 1.7–5.0 and  $21 \pm 1^\circ\text{C}$ , with  $t_{1/2} = 3.9$  h at pH 7 (Yao & Haag 1991).

Ground water:  $t_{1/2} = 480$ –4320 h, based on estimated unacclimated aqueous aerobic and anaerobic biodegradation half-life (Howard et al. 1991).

Sediment: estimated first-order  $t_{1/2} = 23$ –69.3 d from biodegradation rate constant  $k = 0.01$ –0.03  $\text{d}^{-1}$  at 9–21°C by river die-away test in slurry sediment of aquatic systems (Lee & Ryan 1979; quoted, Scow 1982);

$t_{1/2} = 27$  d for sediment-water microcosm under aerobic conditions (quoted, Muir 1991).

Soil: degradation  $t_{1/2} = 24$  d and 14 d in Quachita Highlands' forest and grassland soil, respectively,  $t_{1/2} = 21$  d in Gross Timbers Forest soil, average  $t_{1/2} = 17$  d in 3 soils (Altom & Stritzke 1973);

$t_{1/2} = 240\text{--}480$  h, based on unacclimated soil grab sample data (Smith 1978, 1979; quoted, Howard et al. 1991); estimated first-order  $t_{1/2} = 19.8$  d from rate constant  $k = 0.035\text{ d}^{-1}$  by soil incubation die-away studies (Rao & Davidson 1980; quoted, Scow 1982);

$t_{1/2} = 33$  d from screening model calculations (Jury et al. 1987b);

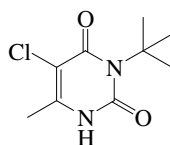
aerobic degradation  $t_{1/2} > 25$  d at  $29^{\circ}\text{C}$ , to  $t_{1/2} = 58$  d at  $21^{\circ}\text{C}$  in soil suspension from pre-incubated soil (Muir 1991);

selected field  $t_{1/2} = 30$  d (Augustijn-Beckers et al. 1994).

Biota: biochemical  $t_{1/2} = 33$  d from screening model calculations (Jury et al. 1987b).



## 17.1.1.74 Terbacil



Common Name: Terbacil

Synonym: Sinbar, Turbacil

Chemical Name: 3-*tert*-butyl-5-chloro-6-methyluracil

CAS Registry No: 5902-51-2

Uses: control of most annual grasses and broadleaf weeds, and some perennial weeds in established apples, asparagus, blueberries, citrus, lucerne, mint, peaches, pecans, strawberries, and sugar cane, etc.

Molecular Formula: C<sub>9</sub>H<sub>13</sub>ClN<sub>2</sub>O<sub>2</sub>

Molecular Weight: 216.664

Melting Point (°C):

176 (Lide 2003)

Boiling Point (°C):

sublime(below mp, Hartley & Kidd 1987; Tomlin 1994)

Density (g/cm<sup>3</sup> at 20°C):

1.34 (25°C, Hartley & Kidd 1987; Montgomery 1993; Tomlin 1994)

Molar Volume (cm<sup>3</sup>/mol):

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

Dissociation Constant pK<sub>a</sub>:

9.0 (Wauchope et al. 1992)

Enthalpy of Fusion, ΔH<sub>fus</sub> (kJ/mol):

Entropy of Fusion, ΔS<sub>fus</sub> (J/mol K):

Fugacity Ratio at 25°C (assuming ΔS<sub>fus</sub> = 56 J/mol K), F: 0.0330 (mp at 176°C)

0.027 (20°C, Suntio et al. 1988)

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

710 (Ashton & Crafts 1973; 1981; Spencer 1982)

710 (Martin & Worthing 1977; Hartley & Kidd 1987; Montgomery 1993; Tomlin 1994)

600 (20°C, selected, Suntio et al. 1988)

710 (20–25°C, selected, Wauchope et al. 1992; Hornsby et al. 1996)

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

6.40 × 10<sup>-5</sup> (29.5°C, Ashton & Crafts 1973; 1981)

6.00 × 10<sup>-5</sup> (30°C, Hartley & Kidd 1987)

5.00 × 10<sup>-5</sup> (20°C, selected, Suntio et al. 1988)

6.00 × 10<sup>-5</sup> (20°C, Montgomery 1993)

6.25 × 10<sup>-5</sup> (29.5°C, Tomlin 1994)

1.91 × 10<sup>-3</sup> (20–25°C, supercooled liquid value, quoted, Majewski & Capel 1995)

4.13 × 10<sup>-5</sup> (20–25°C, selected, Wauchope et al. 1992; Hornsby et al. 1996)

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

1.80 × 10<sup>-5</sup> (20°C, calculated-P/C, Suntio et al. 1988)

1.82 × 10<sup>-5</sup> (20–25°C, calculated, Montgomery 1993)

1.53 × 10<sup>-5</sup> (calculated-P/C, this work)

Octanol/Water Partition Coefficient, log K<sub>ow</sub>:

1.89 (Karickhoff et al. 1979)

1.89 (Rao & Davidson 1980)

- 1.89, 1.90 (quoted, Montgomery 1993)
- 1.89 (recommended, Sangster 1993)
- 1.91 (Tomlin 1994)
- 1.89 (recommended, Hansch et al. 1995)

Bioconcentration Factor, log BCF:

- 1.18 (calculated-S, Kenaga 1980)
- 1.74 (Montgomery 1993)

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

- 1.71, 2.08 (soil: exptl., calculated, Kenaga 1980; Kenaga & Goring 1980)
- 1.62, 1.98 (soil, quoted, Madhun et al. 1986)
- 1.89, 1.76; 1.82, 1.04 (estimated- $K_{OW}$ ; solubilities, Madhun et al. 1986)
- 1.62 (soil, screening model calculations, Jury et al. 1987b)
- 1.74 (soil, Wauchope et al. 1992; Hornsby et al. 1996)
- 1.32–2.20 (soil, quoted, Montgomery 1993)
- 1.66 (soil, calculated-QSAR MCI  $^1\chi$ , Sabljic et al. 1995)
- 1.58 (1.38–1.78) (soils: organic carbon OC  $\geq 0.5\%$ , average, Delle Site 2001)

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

Biodegradation:  $t_{1/2} = 50$  d (Jury et al. 1987b).

Half-Lives in the Environment:

Air:

Surface water:

Ground water:

Sediment:

Soil: moderately persistent in soil with  $t_{1/2} = 20$ –100 d (Willis & McDowell 1982);

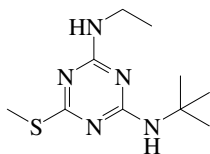
$t_{1/2} \sim 5$ –7 months (Hartley & Kidd 1987);

$t_{1/2} = 50$  d from screening model calculations (Jury et al. 1987b);

field  $t_{1/2} = 50$ –175 d and the selected  $t_{1/2} = 120$  d (Wauchope et al. 1992; Hornsby et al. 1996).

Biota: biochemical  $t_{1/2} = 50$  d (Jury et al. 1987b).

## 17.1.1.75 Terbutryn



Common Name: Terbutryn

Synonym: Clarosan, GS 14260, Igran, Prebane, Shortstop, Terbutrex, Terbutrin, Terbutryn

Chemical Name: *N*-(1,1-dimethylethyl)-*N'*-ethyl-6-(methylthio)-1,3,5-triazine-2,4-diamine; 2-(*tert*-butylamino)-4-(ethylamino)-6-(methylthio)-*s*-triazine

Uses: selective herbicide to control annual broadleaf and grass weeds in wheat.

CAS Registry No: 886-50-0

Molecular Formula: C<sub>10</sub>H<sub>19</sub>N<sub>5</sub>S

Molecular Weight: 241.357

Melting Point (°C):

104 (Herbicide Handbook 1989, Lide 2003)

Boiling Point (°C):

154–160 (at 0.06 mmHg, Hartley & Kidd 1987; Worthing & Hance 1991; Montgomery 1993; Milne 1995)

Density (g/cm<sup>3</sup> at 20°C):

1.115 (Hartley & Kidd 1987; Worthing & Hance 1991; Montgomery 1993; Milne 1995)

Molar Volume (cm<sup>3</sup>/mol):

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

Dissociation Constant:

4.30 (pK<sub>a</sub>, Worthing & Hance 1991)

9.70 (pK<sub>b</sub>, Wauchope et al. 1992; Hornsby et al. 1996)

4.07 (pK<sub>a</sub>, Montgomery 1993)

Enthalpy of Vaporization, ΔH<sub>v</sub> (kJ/mol):

101.4 (Rordorf 1989)

Enthalpy of Fusion, ΔH<sub>fus</sub> (kJ/mol):

22.4 (Rordorf 1989)

Entropy of Fusion, ΔS<sub>fus</sub> (J/mol K):

59 (Rordorf 1989)

Fugacity Ratio at 25°C (assuming ΔS<sub>fus</sub> = 56 J/mol K), F: 0.168 (mp at 104°C)

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

25 (20°C, Weber 1972; Ashton & Crafts 1973, 1981)

58 (20°C, Quellette & King 1977)

25 (Martin & Worthing 1977; Worthing & Walker 1987, Worthing & Hance 1991; Herbicide Handbook 1978)

25 (shake flask-HPLC, Ellgehausen et al. 1981)

25 (20°C, Hartley & Kidd 1987; Herbicide Handbook 1989; Montgomery 1993)

22 (20–25°C, selected, Wauchope et al. 1992; Hornsby et al. 1996)

Vapor Pressure (Pa at 25°C or as indicated and reported temperature dependence equations):

0.00013 (20°C, Weber 1972; Worthing & Walker 1987; Worthing & Hance 1991)

0.00013 (20°C, Ashton & Crafts 1973; 1981)

0.00013 (20°C, Hartley & Kidd 1987; Herbicide Handbook 1989)

$2.20 \times 10^{-4}$ ,  $9.10 \times 10^{-3}$ , 0.22, 3.40, 38.0 (25, 50, 70, 100, 125°C, gas saturation-GC, Rordorf 1989)

$\log (P_s/\text{Pa}) = 17.151 - 6201.4/(T/\text{K})$ ; measured range 45–100°C (solid, gas saturation-GC, Rordorf 1989)

$\log (P_L/\text{Pa}) = 14.654 - 5297.1/(T/\text{K})$ ; measured range 109–139°C (liquid, gas saturation-GC, Rordorf 1989)

- 0.00128 (20°C, Montgomery 1993)  
 0.00028 (20–25°C, selected, Wauchope et al. 1992; Hornsby et al. 1996)

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

- 0.0013 (20°C, calculated-P/C, Suntio et al. 1988)  
 0.0012 (20°C, calculated-P/C, Muir 1991)  
 0.0120 (20°C, calculated-P/C, Montgomery 1993)  
 0.0014 (calculated-P/C, this work)

Octanol/Water Partition Coefficient, log K<sub>OW</sub>:

- 3.74 (shake flask-GC, Elkell & Walum 1979)  
 3.72, 3.74 (shake flask, Ellgehausen et al. 1981)  
 2.56 (RP-HPLC-k' correlation, Braumann et al. 1983)  
 3.34 (Worthing & Walker 1987)  
 3.43 (RP-HPLC-RT correlation, Finizio et al. 1991)  
 3.49 (Worthing & Hance 1991; Milne 1995)  
 3.43–3.73 (Montgomery 1993)  
 3.34 (RP-HPLC-RT correlation, Sicbaldi & Finizio 1993)  
 3.74 (recommended, Sangster 1993)  
 3.38, 3.36 (shake flask-UV, calculated-RP-HPLC-k' correlation, Liu & Qian 1995)  
 3.74 (recommended, Hansch et al. 1995)  
 3.44 (Pomona-database, Müller & Kördel 1996)  
 3.34 (RP-HPLC-RT correlation, Finizio et al. 1997)

Bioconcentration Factor, log BCF:

- 1.17 (*Daphnia magna*, wet wt. basis, Ellgehausen et al. 1980)  
 2.00, 2.00 (calculated-S, calculated-K<sub>OC</sub>, Kenaga 1980)  
 1.95 (catfish *Ictalurus melas*, wet wt basis, Wang et al. 1996)

Sorption Partition Coefficient, log K<sub>OC</sub>:

- 2.85 (soil, Colbert et al. 1975; Gaillardon et al. 1977; Kenaga 1980; Kenaga & Goring 1980)  
 2.87 (soil, calculated-S as per Kenaga & Goring 1980, Kenaga 1980)  
 2.85–2.87 (soil, quoted values, Bottoni & Funari 1992)  
 3.30 (soil, 20–25°C, selected, Wauchope et al. 1992; Hornsby et al. 1996)  
 2.68 (soil, HPLC-screening method, mean value from different stationary and mobile phases, Kördel et al. 1993, 1995b)  
 3.21–4.07 (Montgomery 1993)  
 3.30 (estimated-chemical structure, Lohninger 1994)  
 2.84 (calculated-K<sub>OW</sub>, Liu & Qian 1995)  
 2.85 (soil, calculated-MCI  $\chi$ , Sabljic et al. 1995)  
 2.68; 2.80 (HPLC-screening method; calculated-PCKOC fragment method, Müller & Kördel 1996)  
 4.62, 2.57, 2.90, 1.56, 3.55 soil, first generation Eurosoils ES-1, ES-2, ES-3, ES-4, ES-5, shake flask/batch equilibrium-HPLC/UV, Gawlik et al. 1998)  
 3.554, 2.878, 2.778, 2.505, 3.054 (soil, second generation Eurosoils ES-1, ES-2, ES-3, ES-4, ES-5, shake flask/batch equilibrium-HPLC/UV and HPLC-k' correlation, Gawlik et al. 2000)  
 2.85; 2.82, 2.74 (soil, quoted obs.; estimated-class-specific model, estimated-general model using molecular descriptors, Gramatica et al. 2000)  
 3.79 (3.28–4.30) (soil: organic carbon OC ≥ 0.5%, average, Delle Site 2001)  
 2.59, 2.86 (Kishon river sediments, sorption isotherm, Chefetz et al. 2004)

Environmental Fate Rate Constants, k, or Half-Lives, t<sub>1/2</sub>:

Volatilization:

Photolysis: 4 ppb contaminated water in the presence of TiO<sub>2</sub> and H<sub>2</sub>O<sub>2</sub> completely photodegraded after 15 h by solar irradiation (Muszkat et al. 1992).

Oxidation:

## Hydrolysis:

Biodegradation: aerobic  $t_{1/2} = 80\text{--}240$  d for  $1\text{ }\mu\text{g/mL}$  to biodegrade in sediment-water and anaerobic  $t_{1/2} > 650$  d for  $1\text{ }\mu\text{g/mL}$  to biodegrade in sediment-water both at  $25^\circ\text{C}$  (Muir & Yarechewski 1982; quoted, Muir 1991). biological degradation rate followed a first order kinetics, with  $t_{1/2} = 8.9\text{--}18.2$  d by raw water microflora from River Nile,  $t_{1/2} = 4.0\text{--}6.9$  d by raw water microflora + sewage (El-Dib & Abou-Waly 1998)

## Biotransformation:

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

$k_1 = 1.70\text{ h}^{-1}$  (*Chironomus tentans* larvae in pond sediment-water system, 96-h exposure, calculated by using first-order kinetic and concn factors, Muir et al. 1983)

$k_1 = 1.9\text{--}1.5\text{ h}^{-1}$  (*Chironomus tentans* larvae in river sediment-water system, 96-h exposure, calculated by using first-order kinetic and concn factors, Muir et al. 1983)

$k_1 = 3.6\text{--}2.7\text{ h}^{-1}$  (*Chironomus tentans* larvae in sediment (sand)-water system, 96-h exposure, calculated by using first-order kinetic and concn factors, Muir et al. 1983)

$k_1 = 3.6\text{--}4.4\text{ h}^{-1}$  (*Chironomus tentans* larvae in sediment (sand)-water system, 96-h exposure, calculated by using initial uptake data of 0–12 h, Muir et al. 1983)

$k_2 = 0.053\text{ h}^{-1}$  (*Chironomus tentans* larvae in pond sediment-water system, calculated by initial uptake data of 0–12 h, Muir et al. 1983)

$k_2 = 0.043\text{ h}^{-1}$  (*Chironomus tentans* larvae in river water system, calculated by concentration decay curve, Muir et al. 1983)

$k_2 = 0.040\text{ h}^{-1}$  (*Chironomus tentans* larvae in river sediment-water system, calculated by concentration decay curve, Muir et al. 1983)

$k_2 = 0.040\text{ h}^{-1}$  (*Chironomus tentans* larvae in sediment (sand)-water system, calculated by concentration decay curve, Muir et al. 1983)

$k_1 = 3.11\text{ h}^{-1}$ ,  $k_2 = 0.0346\text{ h}^{-1}$  (catfish *Ictalurus melas*, Wang et al. 1996)

## Half-Lives in the Environment:

## Air:

Surface water:  $t_{1/2} = 8.9\text{--}18.2$  d by raw water microflora from River Nile,  $t_{1/2} = 4.0\text{--}6.9$  d by raw water microflora + sewage (El-Dib & Abou-Waly 1998)

Ground water: reported half-lives or persistence,  $t_{1/2} = 14\text{--}28$  d (Bottoni & Funari 1992)

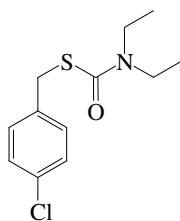
Sediment: aerobic  $t_{1/2} = 80\text{--}240$  d for  $1\text{ }\mu\text{g mL}^{-1}$  to biodegrade in sediment-water and anaerobic  $t_{1/2} > 650$  d for  $1\text{ }\mu\text{g mL}^{-1}$  to biodegrade in sediment-water both at  $25^\circ\text{C}$  (Muir & Yarechewski 1982; quoted, Muir 1991).

Soil: reported  $t_{1/2} = 14\text{--}28$  d (Worthing & Hance 1991; Bottoni & Funari 1992);

$t_{1/2} \sim 42$  d (estimated, Wauchope et al. 1992; Hornsby et al. 1996).

Biota: elimination  $t_{1/2} = 13.1$  h in pond sediment-water,  $t_{1/2} = 16.1$  h in river water,  $t_{1/2} = 17.3$  h in river sediment-water,  $t_{1/2} = 17.3$  in sand-water systems (*Chironomus tentans* larvae, Muir et al. 1983)

## 17.1.1.76 Thiobencarb



Common Name: Thiobencarb

Synonym: benthioncarb, Bolero, Saturn, Saturno, Siacarb

Chemical Name: *S*-(4-chlorophenyl)methyl diethylcarbamothioate

Pesticide Class: herbicide; Group: carbamate

Uses: herbicide

CAS Registry No: 28249-77-6

Molecular Formula:  $C_{12}H_{16}ClNOS$

Molecular Weight: 257.779

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

1.7 (Lide 2003)

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

126–129/0.008 mmHg (Ashton & Crafts 1981)

126–128/0.008 mmHg (Spencer 1982; Hartley & Kidd 1987; Herbicide Handbook 1989)

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

1.148–1.180 (Spencer 1982; Hartley & Kidd 1987; Herbicide Handbook 1989)

Molar Volume ( $cm^3/mol$ ):

Dissociation Constant  $pK_a$ :

Enthalpy of Fusion,  $\Delta H_{fus}$  (kJ/mol):

Entropy of Fusion,  $\Delta S_{fus}$  (J/mol K):

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

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

30 (Ashton & Crafts 1981)

30 (reported as 30 g/L, Spencer 1982)

30 ( $20^{\circ}C$ , Hartley & Kidd 1987; Herbicide Handbook 1989)

28 ( $20$ – $25^{\circ}C$ , recommended, Wauchope et al. 1992; Hornsby et al. 1996)

17.0 (Majewski & Capel 1995)

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

$1.96 \times 10^{-4}$  ( $20^{\circ}C$ , Ashton & Crafts 1981)

$4.21 \times 10^{-3}$  ( $20^{\circ}C$ , GC-RT correlation, Kim 1985)

$2.0 \times 10^{-4}$  ( $20^{\circ}C$ , Hartley & Kidd 1987)

$1.97 \times 10^{-4}$  (Herbicide Handbook 1989)

$2.93 \times 10^{-3}$  ( $20$ – $25^{\circ}C$ , selected, Wauchope et al. 1992; Hornsby et al. 1996)

$1.78 \times 10^{-3}$  (Majewski & Capel 1995)

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

0.027 (calculated-P/C, Majewski & Capel 1995)

0.0274 (quoted lit., Armbrust 2000)

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

3.42 ( $20^{\circ}C$ , shake flask-GC, Kanazawa 1981)

3.40 (shake flask-GC, Schimmel et al. 1983)

3.98 (HPLC-RT correlation, Kawamoto & Urano 1989)

3.42 (Gerstl 1990)

- 3.40 (recommended, Sangster 1993)
- 3.93 (HPLC-RT correlation, Scibaldi & Finizio 1993)
- 3.40 (LOGPSTAR or CLOGP data, Sabljic et al. 1995)
- 3.78 (RP-HPLC-RT correlation, Yu et al. 1997)
- 4.37 (RP-HPLC-RT correlation, Nakamura et al. 2001)

Bioconcentration Factor, log BCF or log  $K_B$ :

- 2.97 (Pait et al. 1992)
- 1.76, 1.77 (37.2, 18.6  $\mu\text{g/L}$  concn in water; carp, 3–5 d exposure, Wang et al. 1992)
- 1.38, 1.0 (20.0, 2.0  $\mu\text{g/L}$  concn in water; tilapia, 3–5 d exposure, Wang et al. 1992)
- 1.49, 1.13 (20.0, 2.0  $\mu\text{g/L}$  concn in water; loach, 3–5 d exposure, Wang et al. 1992)
- 0.92, 1.08 (15.0, 7.5  $\mu\text{g/L}$  concn in water; Grass carp, 3–5 d exposure, Wang et al. 1992)
- 1.20, 1.26 (10.0, 5.0  $\mu\text{g/L}$  concn in water; eel, 3–5 d exposure, Wang et al. 1992)
- 2.57, 1.94 (5.0, 1.4  $\mu\text{g/L}$  concn in water; black silver carp, 3–5 d exposure, Wang et al. 1992)
- 0.46, 0.86 (200, 20  $\mu\text{g/L}$  concn in water; freshwater clam, 3v5 d exposure, Wang et al. 1992)
- 1.82; 2.23 (*Gnathopogon aerulescens*; *Pseudorasbora parva*, flow-through condition, quoted, Devillers et al. 1996)

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

- 2.83 (soil, Gerstl 1990)
- 2.49, 3.02, 2.83 (soil, Bottoni & Funari 1992)
- 2.95 (soil, Wauchope et al. 1992; Hornsby et al. 1996)
- 3.43 (soil, calculated- $\chi$ , Meylan et al. 1992)
- 3.27 (calculated-QSAR MCI  $^1\chi$ , Sabljic et al. 1995)
- 2.95 (quoted lit., Armbrust 2000)
- 3.32, 2.75 (soil, estimated-class-specific model, estimated-general model using molecular descriptors, Gramatica et al. 2000)

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

Volatilization:

Photolysis:

Oxidation:

Hydrolysis: stable aqueous hydrolysis rates at pH 5, 7, 9; measured hydroxy radical rate constant  $k = 6.8 \times 10^{12} \text{ M}^{-1}/\text{h}$  (Armbrust 2000)

Biodegradation:  $t_{1/2} = 2\text{--}3$  wk in soil varies under aerobic conditions to  $t_{1/2} = 6\text{--}8$  months under anaerobic conditions (Hartley & Kidd 1987; Herbicide Handbook 1989)

aerobic degradation rate constant  $k = 0.057 \text{ d}^{-1}$  with  $t_{1/2} = 12 \text{ d}$  by aerobic activated sludge at  $20^\circ\text{C}$  (Kawamoto & Urano 1990)

aerobic rate constant,  $k = 1.38 \times 10^{-3} \text{ h}^{-1}$  (Armbrust 2000).

Biotransformation:

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

Half-Lives in the Environment:

Air:

Surface water: lost from aqueous solution by volatility and photodegradation (Herbicide Handbook 1989)

biodegradation  $t_{1/2} = 12 \text{ d}$  by aerobic activated sludge at  $20^\circ\text{C}$  (Kawamoto & Urano 1990).

Ground water: reported half-lives or persistence,  $t_{1/2} = 6\text{--}7$ , 23–120, and 26–40 d (Bottoni & Funari 1992)

Sediment:

Soil: laboratory studies with Stockton adobe and Crowley silty clay loam gave  $t_{1/2} = 2\text{--}3$  wk under aerobic conditions to  $t_{1/2} = 6\text{--}8$  months under anaerobic conditions (Hartley & Kidd 1987; Herbicide Handbook 1989);

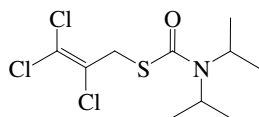
reported half-lives or persistence of 6–7 d, 23–120 d, 26–40 d (Bottoni & Funari 1992);

soil;  $t_{1/2} = 18 \text{ d}$  (Pait et al. 1992);

field  $t_{1/2} = 21 \text{ d}$  (Wauchope et al. 1992; Hornsby et al. 1996).

Biota:

## 17.1.1.77 Triallate



Common Name: Triallate

Synonym: Avadex BW, Buckle, CP 23426, Dipthal, Far-Go

Chemical Name: 2,3,3-trichloro-2-propene-1-thiol diisopropylcarbamate; *S*-(2,3,3-trichloro-allyl)diisopropyl-(thio-carbamate); *S*-(2,3,3-trichloro-2-propenyl) bis(1-methylethyl)-carbamothioate

Uses: herbicide to control wild oats in lentils, barley, peas, and winter wheat.

CAS Registry No: 2303-17-5

Molecular Formula: C<sub>10</sub>H<sub>16</sub>Cl<sub>3</sub>NOS

Molecular Weight: 304.664

Melting Point (°C):

29 (Lide 2003)

Boiling Point (°C):

148–149 (Khan 1980; Spencer 1982)

117 (at 40 mPa, Herbicide Handbook 1989; Montgomery 1993; Milne 1995)

Density (g/cm<sup>3</sup> at 20°C):

1.273 (25°C, Hartley & Kidd 1987; Herbicide Handbook 1989; Worthing & Hance 1991; Montgomery 1993; Tomlin 1994; Milne 1995)

Molar Volume (cm<sup>3</sup>/mol):

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

Dissociation Constant pK<sub>a</sub>:

Enthalpy of Vaporization, ΔH<sub>v</sub> (kJ/mol):

85.86 (Rordorf 1989)

Enthalpy of Fusion, ΔH<sub>fus</sub> (kJ/mol):

27.7 (Rordorf 1989)

Entropy of Fusion, ΔS<sub>fus</sub> (J/mol K):

Fugacity Ratio at 25°C (assuming ΔS<sub>fus</sub> = 56 J/mol K), F: 0.914 (mp at 29°C)

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

4.0 (20°C, Weber 1972; Weber et al. 1980)

4.0 (Ashton & Crafts 1973; Spencer 1973, 1982; Khan 1980)

4.0 (Martin & Worthing 1977, Worthing & Walker 1983, 1987; Worthing & Hance 1991; Herbicide Handbook 1978, 1989)

4.0 (Hartley & Graham-Bryce 1980; Hartley & Kidd 1987; Montgomery 1993; Tomlin 1994; Milne 1995)

< 1.0 (27°C, Ashton & Crafts 1981)

3.0 (20°C, selected, Suntio et al. 1988)

4.0 (20–25°C, selected, Wauchope et al. 1992; Hornsby et al. 1996)

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

0.016 (20°C, Weber 1972; Worthing & Walker 1987)

0.016 (Ashton & Crafts 1973; Spencer 1982; quoted, Suntio et al. 1988)

0.0276\* (gas saturation-GC, measured range 20–45°C, Grover et al. 1978)

log (P/mmHg) = 11.045 – 4401/(T/K); temp range 20–45°C (Antoine eq., gas saturation-GC, Grover et al. 1978)

0.0265 (29.5°C, Ashton & Crafts 1981)

0.0276 (gas saturation method, Spencer & Cliath 1983)

6.07 × 10<sup>-3</sup>, 4.81 × 10<sup>-3</sup> (20°C, GC-RT correlation, GC-RT correlation with mp correction, Kim 1985)

0.016 (Hartley & Kidd 1987; Worthing & Hance 1991; Tomlin 1994)

0.010 (20°C, selected, Suntio et al. 1988; quoted, Majewski & Capel 1995)



- 0.015 (Herbicide Handbook 1989)  
 0.017\* (gas saturation-GC, measured range 25–125°C, Rordorf 1989)  
 $\log (P_s/Pa) = 18.124 - 5932/(T/K)$ ; measured range 32.3–150°C (solid, gas saturation-GC, Rordorf 1989)  
 $\log (P_L/Pa) = 13.395 - 4485.1/(T/K)$ ; measured range 32.3–150°C (liquid, gas saturation-GC, Rordorf 1989)  
 0.026 (selected, Taylor & Spencer 1990)  
 0.0147 (20–25°C, selected, Wauchope et al. 1992; Hornsby et al. 1996)  
 0.016 (20°C, Montgomery 1993)

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

- 1.96 (calculated-P/C, Jury et al. 1983, 1984, 1987a, 1990; Jury & Ghodrati 1989)  
 1.02 (20°C, calculated-P/C, Suntio et al. 1988)  
 1.983 (calculated-P/C, Taylor & Glotfelty 1988)  
 1.226 (20°C, calculated-P/C, Muir 1991)  
 1.013 (20–25°C, calculated-P/C, Montgomery 1993)  
 0.762 (calculated-P/C, this work)

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

- 4.29 (Montgomery 1993)  
 4.53 (LOGPSTAR or CLOGP data, Sabljic et al. 1995)

Bioconcentration Factor,  $\log BCF$ :

- 2.45 (calculated-S, Kenaga 1980; quoted, Isensee 1991)  
 2.18 (calculated- $K_{oc}$ , Kenaga 1980)

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

- 3.56 (Guenzi & Beard 1974)  
 3.34 (soil, Grover 1974; Beestman & Demming 1976)  
 3.32 (soil, calculated-S as per Kenaga & Goring 1980, Kenaga 1980)  
 3.56 (soil, screening model calculations, Jury et al. 1987a,b; Jury & Ghodrati 1989)  
 3.22 (soil, calculated-MCI  $\chi$  and fragments contribution, Meylan et al. 1992)  
 3.38 (soil, 20–25°C, selected, Wauchope et al. 1992; Hornsby et al. 1996)  
 3.31 (calculated, Montgomery 1993)  
 3.38 (selected, Lohninger 1994)  
 3.35 (soil, calculated-MCI  $^1\chi$ , Sabljic et al. 1995)  
 3.60, 3.12 (soil, estimated-class-specific model, estimated-general model using molecular descriptors, Gramatica et al. 2000)  
 2.70, 2.64 (soils: organic carbon  $OC \geq 0.1\%$ ,  $OC \geq 0.5\%$ , average, Delle Site 2001)

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

Volatilization:  $t_{1/2} = 26$  d (Jury et al. 1983; quoted, Grover 1991); half-life of 100 d (Jury et al. 1984; quoted, Spencer & Cliath 1990);  
 estimated  $t_{1/2} \sim 8$  d from 1 m depth of water at 20°C (Muir 1991).

Photolysis:

Oxidation: calculated lifetime of 5 h for the vapor-phase reaction with OH radicals in the troposphere (Atkinson et al. 1992; Kwok et al. 1992).

Hydrolysis:  $t_{1/2} > 24$  wk for 1  $\mu\text{g/mL}$  to hydrolyze in aqueous buffer at pH 4, 7, and 9 in the dark at 25°C (Smith 1969; quoted, Muir 1991).

Biodegradation: estimated  $t_{1/2} = 680$  d at pH 6.8 and  $t_{1/2} = 1170$  d at pH 7.0, both at 25°C from biodegradation rate constants in aquatic systems (Smith 1969; quoted, Scow 1982);

$t_{1/2} = 100$  d for a 100 d leaching and screening test in 0–10 cm depth of soil (Jury et al. 1983, 1984, 1987a,b; 1990; Jury & Ghodrati 1989; Grover 1991).

Biotransformation:

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

## Half-Lives in the Environment:

Air: calculated life-time of 5 h for the vapor-phase reaction with OH radicals in the troposphere (Atkinson et al. 1992; Kwok et al. 1992).

Surface water:  $t_{1/2} = 680$  d at pH 6.8 and  $t_{1/2} = 1170$  d at pH 7.0, both at 25°C for biodegradation in aquatic systems (Smith 1969; quoted, Scow 1982).

Ground water:

Sediment:

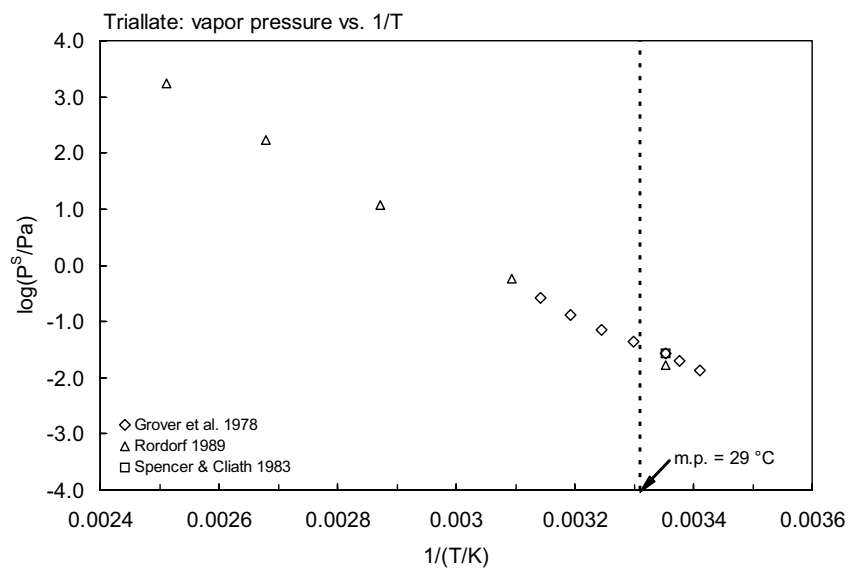
Soil: biodegradation  $t_{1/2} = 100$  d from screening model calculations (Jury et al. 1984, 1987a,b; 1990; Jury & Ghodrati 1989; quoted, Montgomery 1993);  
selected field  $t_{1/2} = 82$  d (Wauchope et al. 1992; Hornsby et al. 1996).

Biota: biochemical  $t_{1/2} = 100$  d from screening model calculations (Jury et al. 1987a,b; Jury & Ghodrati 1989).

**TABLE 17.1.1.77.1**

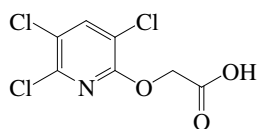
**Reported vapor pressures of triallate at various temperatures and the coefficients for the vapor pressure equations**

$\log P = A - B/(T/K)$	(1)	$\ln P = A - B/(T/K)$	(1a)
$\log P = A - B/(C + t/^{\circ}C)$	(2)	$\ln P = A - B/(C + t/^{\circ}C)$	(2a)
$\log P = A - B/(C + T/K)$	(3)		
$\log P = A - B/(T/K) - C \cdot \log (T/K)$	(4)		
<b>Grover et al. 1978</b>		<b>Rordorf 1989</b>	
<b>gas saturation method-GC</b>		<b>gas saturation-GC</b>	
<b>t/°C</b>	<b>P/Pa</b>	<b>t/°C</b>	<b>P/Pa</b>
20	0.0133	25	0.017
23	0.0202	50	0.59
25	0.0276	75	12.0
30	0.0446	100	170
35	0.0704	125	1700
40	0.131		for solid
45	0.267	eq. 1	P <sub>s</sub> /Pa
		A	18.124
eq. 1	P/mmHg	B	5932
A	11.045		for liquid
B	4401	eq. 1	P <sub>L</sub> /Pa
		A	13.395
mp/°C	33–33.5°C	B	4485.1



**FIGURE 17.1.1.77.1** Logarithm of vapor pressure versus reciprocal temperature for triallate.

## 17.1.1.78 Triclopyr



Common Name: Triclopyr

Synonym: Garlon, Truflon, Crossbow

Chemical Name: 3,5,6-trichloro-2-pyridinyloxyacetic acid

CAS Registry No: 56335-06-3

Uses: herbicide

Molecular Formula:  $C_7H_4Cl_3NO_3$

Molecular Weight: 256.471

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

148–150 (Spencer 1982; Hartley & Kidd 1987; Worthing & Walker 1987)

150.5 (Tomlin 1994)

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

290 (dec., Hartley & Kidd 1987; Tomlin 1994)

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

Dissociation Constant  $pK_a$ :

2.68 (Spencer 1982; Worthing & Walker 1987)

2.93 (Woodburn et al. 1993)

3.97 (Tomlin 1994)

Enthalpy of Vaporization,  $\Delta H_v$  (kJ/mol):

102.5 (Rordorf 1989)

Enthalpy of Fusion,  $\Delta H_{fus}$  (kJ/mol):

31.8 (Rordorf 1989)

Entropy of Fusion,  $\Delta S_{fus}$  (J/mol K):

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

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

430 (Kenaga 1980a,b)

440 (Spencer 1982; Hartley & Kidd 1987; Worthing & Walker 1987)

408 ( $20^{\circ}C$ , Tomlin 1994)

7690, 8100, 8220 ( $20^{\circ}C$ , at pH 5, 7, and 9, Tomlin 1994)

7618 ( $20$ – $25^{\circ}C$ , quoted as  $2.97E + 01$   $mol/m^3$ , Majewski & Capel 1995)

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

$1.6 \times 10^{-4}$  (Spencer 1982)

$1.68 \times 10^{-4}$  (Worthing & Walker 1987; Hartley & Kidd 1987; Tomlin 1994)

$1.90 \times 10^{-5}$ ,  $1.0 \times 10^{-3}$ , 0.031, 0.59, 7.80 (25, 50, 70, 100,  $125^{\circ}C$ , gas saturation-GC, Rordorf 1989)

$\log(P_s/Pa) = 17.65 - 6672.3/(T/K)$ ; measured range  $85.4$ – $145^{\circ}C$  (gas saturation-GC, Rordorf 1989)

$\log(P_L/Pa) = 14.445 - 5354.8/(T/K)$ ; measured range  $150$ – $186^{\circ}C$  (gas saturation-GC, Rordorf 1989)

$2.0 \times 10^{-4}$  (vapor pressure balance, Tomlin 1994)

$2.91 \times 10^{-3}$  ( $20$ – $25^{\circ}C$ , Majewski & Capel 1995)

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

$9.79 \times 10^{-5}$  ( $20$ – $25^{\circ}C$ , calculated-P/C, Majewski & Capel 1995)

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

–0.52 (Kenaga 1980a)

0.42, –0.45, –0.96 (pH 5, 7, and 9, Tomlin 1994)

1.30 (Isensee 1991)

2.53 (LOGPSTAR or CLOGP data, Sabljic et al. 1995)

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

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

- 1.49, -0.22 (fish: flowing water tests, static ecosystem tests, Kenaga 1980a)
- 1.30, 0 (fish: calculated-solubility,  $K_{OW}$ , Kenaga 1980b)

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

- 1.43 (soil, Kenaga 1980a)
- 1.43, 2.204 (soil: quoted, calculated, Kenaga 1980b)
- 1.43, 2.20 (soil, Bottoni & Funari 1992)
- 1.43 (quoted or calculated-MCI  $^1\chi$ , Sabljic et al. 1995)

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

Volatilization:

- Photolysis: photolysis  $t_{1/2} < 0.4$  d in sterile, pH 5-buffered water at 40°N latitude in midday, midsummer (McCall & Gavit 1986);
- photodecomposition  $t_{1/2} < 12$  h (Worthing 1987; Tomlin 1994);
- photodecomposition  $t_{1/2} < 24$  h (Hartley & Kidd 1987);
- aqueous photolysis pseudo-first order  $t_{1/2}(\text{average}) = 0.5$  and 1.3 d in pH 7-buffered water and natural river water, respectively, at 25°C under artificial lights and midsummer sunlight, 40°N latitude (Woodburn et al. 1993);
- aqueous photolysis rate constant,  $k = 8.3 \times 10^{-2} \text{ h}^{-1}$  (Armbrust 2000).

Oxidation:

- Hydrolysis: hydrolysis  $t_{1/2} > 3$  months in darkened, sterile, buffered water at pH of 5–9 and 25°C (Woodburn et al. 1993);
- stable aqueous hydrolysis rates at pH 5, 7, 9; measured hydroxy radical rate constant  $k = 4.3 \times 10^{12} \text{ M}^{-1} \cdot \text{h}^{-1}$  (Armbrust 2000).

- Biodegradation: in soil, fairly rapid degradation by microbial activity, with an average  $t_{1/2} = 46$  d depending on soil and climatic conditions (Spencer 1982; Tomlin 1994);
- aerobic rate constant,  $k = 9.03 \times 10^{-4} \text{ h}^{-1}$  (Armbrust 2000).

Biotransformation:

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

Half-Lives in the Environment:

Air:

- Surface water: stable to hydrolysis, but subject to photolysis with  $t_{1/2} < 12$  h (Spencer 1982; Worthing 1987; Tomlin 1994);
- photolysis  $t_{1/2} < 0.4$  d in sterile, pH 5 buffered water at 40°N latitude (McCall & Gavit 1986);
- $t_{1/2} \sim 3$  to 4 d in natural water during summer conditions (Solomon et al. 1988);
- pseudo-first order photolysis  $t_{1/2}(\text{ave.}) = 0.5$  and 1.3 d in pH-buffered water and natural river water, respectively; the photodegradation pseudo-first-order half-lives in sterile, pH 7 water, midsummer sunlight at 40°N latitude and 25°C calculated as  $k = 0.36$  (0.33–0.39) and 0.60 (0.50–0.70) d under artificial and natural sunlight, respectively;  $t_{1/2} = 0.71$  (0.70–0.73) and 1.86 (1.77–1.96) d in river water under artificial and natural sunlight conditions, respectively, in midsummer sunlight and approximately 40°N latitude and 25°C (Woodburn et al. 1993);
- photodecomposition  $t_{1/2} < 24$  h (Hartley & Kidd 1987).

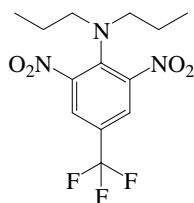
Ground water: reported half-lives or persistence,  $t_{1/2} = 40$  and 46 d (Bottoni & Funari 1992).

Sediment:

- Soil: fairly rapid degradation by microbial activity, with an average  $t_{1/2} = 46$  d depending on soil and climatic conditions (Spencer 1982; Tomlin 1994);

Biota:

## 17.1.1.79 Trifluralin



Common Name: Trifluralin

Synonym: Agreflan, Crisalin, Digermin, Elancolan, L-36352, Nitran, Nitrofor, Olitref, Treflan, Trifluoramine, Trifurex, Trikepin, Trim

Chemical Name: 2,6-dinitro-*N,N*-dipropyl-4-trifluoromethylaniline; 2,6-dinitro-*N,N*-dipropyl-4-(trifluoromethyl)-benzenamine

Uses: pre-emergence herbicide to control many grass and broadleaf weeds.

CAS Registry No: 1582-09-8

Molecular Formula:  $C_{13}H_{16}F_3N_3O_4$

Molecular Weight: 335.279

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

49 (Lide 2003)

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

362 (estimated, Grain 1982)

139–140 (at 4.2 mmHg, Hartley & Kidd 1987; Montgomery 1993; Milne 1995)

96–97 (at 0.18 mmHg, Herbicide Handbook 1989)

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

1.294 ( $25^{\circ}C$ , Montgomery 1993)

1.36 ( $22^{\circ}C$ , Tomlin 1994)

Molar Volume ( $cm^3/mol$ ):

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

Dissociation Constant  $pK_a$ :

Enthalpy of Vaporization,  $\Delta H_v$  ( $kJ/mol$ ):

8754 (Rordorf 1989)

Enthalpy of Fusion,  $\Delta H_{fus}$  ( $kJ/mol$ ):

23.85 (DSC method, Plato & Glasgow 1969)

23.5 (Rordorf 1989)

Entropy of Fusion,  $\Delta S_{fus}$  ( $J/mol K$ ):

Fugacity Ratio at  $25^{\circ}C$  (assuming  $\Delta S_{fus} = 56 J/mol K$ ), F: 0.581 (mp at  $49^{\circ}C$ )

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

24 ( $27^{\circ}C$ , Woodford & Evans 1963; Günther et al. 1968; Spencer 1973)

40 ( $29.5^{\circ}C$ , Melnikov 1971)

0.35 ( $20^{\circ}C$ , Weber 1972; Worthing & Walker 1987)

0.1–0.5 (Probst et al. 1975)

0.60 (Herbicide Handbook 1978; Kenaga 1980; Kenaga & Goring 1980)

0.05 (Wauchope 1978; Weber et al. 1980)

< 1.0 ( $20^{\circ}C$ , Khan 1980)

8.11 ( $20$ – $25^{\circ}C$ , Kanazawa 1981)

0.30 (Beste & Humburg 1983; Jury et al. 1984; Taylor & Glotfelty 1988; Herbicide Handbook 1989)

0.32 (generator column-HPLC-RI, Swann et al. 1983)

0.70 (HPLC-RT correlation, Swann et al. 1983)

4.0 ( $27^{\circ}C$ , Verschueren 1983; Montgomery 1993)

0.75 (shake flask-GC or LSC, Gerstl & Mingelgrin 1984)

< 1.0 ( $27^{\circ}C$ , Hartley & Kidd 1987; Worthing & Hance 1991; Milne 1995)

0.30 ( $20$ – $25^{\circ}C$ , selected, Wauchope et al. 1992; Hornsby et al. 1996)

0.184, 0.221, 0.189 (at pH 5, 7, 9, Tomlin 1994)

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

- 0.0265 (29.5°C, Probst et al. 1967; Khan 1980)
- 0.0292 (29°C, effusion method, Hamaker & Kerlinger 1971)
- 0.0138 (20°C, Weber 1972; Worthing & Walker 1987)
- 0.0323 (30°C, from Spencer & Cliath 1973 unpublished data, Spencer et al. 1973)
- 0.0065\* (20°C, gas saturation-GC, measured range 20–40°C, Spencer & Cliath 1974, Spencer 1976)
- $\log (P/\text{mmHg}) = 17.318 - 6344/(T/K)$ ; temp range 20–40°C (Antoine eq., Spencer 1976)
- 0.0262 (30°C, effusion method-pressure gauge, DePablo 1976)
- 0.0137 (Worthing & Walker 1979, Worthing & Hance 1991; Hartley & Kidd 1987)
- 0.0029 (20–25°C, Weber et al. 1980)
- 0.0173 (Herbicide Handbook 1983)
- 0.015 (20°C, Jury et al. 1983)
- 0.0147 (Herbicide Handbook 1989)
- 0.010\* (gas saturation-GC, measured range 25–125°C, Rordorf 1989)
- $\log (P_s/\text{Pa}) = 17.46 - 5800.6/(T/K)$ ; measured range 48.8–124°C (solid, gas saturation-GC, Rordorf 1989)
- $\log (P_L/\text{Pa}) = 13.65 - 4573.1/(T/K)$ ; measured range 48.8–124°C (liquid, gas saturation-GC, Rordorf 1989)
- 0.015 (20°C, selected, Taylor & Spencer 1990)
- 0.0147 (20–25°C, selected, Wauchope et al. 1992; Hornsby et al. 1996)
- 0.0147 (20°C, Montgomery 1993)
- 0.0095 (Tomlin 1994)
- 0.0363 (liquid  $P_L$ , GC-RT correlation; Donovan 1996)

Henry's Law Constant ( $\text{Pa}\cdot\text{m}^3/\text{mol}$  at 25°C or as indicated and reported temperature dependence equations):

- 16.61 (calculated-P/C, Jury et al. 1983, 1984, 1987a,b; Jury & Ghodrati 1989)
- 4.02 (20°C, calculated-P/C, Suntio et al. 1988)
- 16.36 (calculated-P/C, Taylor & Glotfelty 1988)
- 5.206 (fog chamber-GC/ECD, Fendinger et al. 1989)
- 5.95 (wetted-wall column-GC/ECD, Fendinger et al. 1989)
- 16.0 (calculated-P/C, Nash 1989)
- 13.27 (20°C, calculated-P/C, Muir 1991)
- 4.903 (23°C, calculated-P/C, Montgomery 1993)
- 15.2, 6.67, 4.02 (quoted literature values, Grover et al. 1997)
- 10.31, 15.06 (20°C, distilled water, salt water 33.3% NaCl, wetted wall column-GC, Rice et al. 1997b)
- $\log K_{AW} = -1546/(T/K) + 2.87$ ; temp range 8.3–43.5°C, (distilled water, wetted-wall column-GC, Rice et al. 1997b)
- $\log K_{AW} = -1232/(T/K) + 1.94$ ; temp range 8.3–43.5°C, (salt water solution, 33.3% NaCl, wetted-wall column-GC, Rice et al. 1997b)
- 11.16, 11.04; 12.50 (20°C, microlayer, subsurface natural water of salinity 17% and TOC 0.4–1.0 ppm, from Pt. Lookout, Chesapeake Bay; estimated value adjusted to salinity, Rice et al. 1997b)
- 10.97, 10.72; 12.38 (20°C, microlayer, subsurface natural water of salinity 16% and TOC 0.5–0.6 ppm, from Solomons, Chesapeake Bay; estimated adjusted to salinity, Rice et al. 1997b)
- 10.40, 10.06; 11.82 (20°C, microlayer, subsurface natural water of salinity 12%, TOC 0.6 ppm, from Sandy Point, Chesapeake Bay; estimated value adjusted to salinity, Rice et al. 1997b)
- 12.43, 12.70; 14.84 (20°C, microlayer, subsurface water of salinity 32%, TOC 2.2–46 ppm, ocean water from Bering/Chukchi Sea; estimated value adjusted to salinity, Rice et al. 1997b)
- 9.49, 13.14, 19.67 (8.3, 20, 43.5°C, subsurface water from Bering Sea, TOC 2.14 ppm, wetted-wall column-GC, Rice et al. 1997b)
- 8.504, 12.80; 19.61 (8.3, 20, 43.5°C, surface microlayer water from Bering Sea, TOC 3.14 ppm, wetted-wall column-GC, Rice et al. 1997b)
- 8.87, 12.26, 19.69 (8.3, 20, 43.5°C, subsurface water from Chukchi Sea, TOC 3.3 ppm, wetted-wall column-GC, Rice et al. 1997b)
- 7.95, 12.04; 19.40 (8.3, 20, 43.5°C, surface microlayer water from Chukchi Sea, TOC 45.5 ppm, wetted-wall column-GC, Rice et al. 1997b)

6.99, 9.94, 15.85 (8.3, 20, 43.5°C, melted surface ice from the Arctic Ocean, TOC 48.8 ppm, wetted-wall column-GC, Rice et al. 1997b)

$\log K_{AW} = -786/(T/K) + 0.307$ ; temp range: 8.3–43.5°C, (ocean water from the Chukchi Sea, wetted-wall column-GC, Rice et al. 1997b)

$\log K_{AW} = -1232/(T/K) + 1.900$ ; temp range: 8.3–43.5°C, (subsurface microlayer of ocean water from the Chukchi Sea, wetted-wall column-GC, Rice et al. 1997b)

4.026 (calculated-P/C, this work)

9.63 (20°C, selected from literature experimentally measured data, Staudinger & Roberts 2001)

$\log K_{AW} = 2.870 - 1546/(T/K)$ , (van't Hoff eq. derived from literature data, Staudinger & Roberts 2001)

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

5.34 (Kenaga & Goring 1980)

3.06 (Rao & Davidson 1980)

5.34 (shake flask-UV, Briggs 1981)

5.28 (shake flask, Brown & Flagg 1981)

3.97 (shake flask-GC, Kanazawa 1981)

4.94 (HPLC-k' correlation, McDuffie 1981)

4.86 (shake flask, Dubelman & Bremer 1983)

4.19 (shake flask-GC or LSC, Gerstl & Mingelgrin 1984)

5.07 (Herbicide Handbook 1989; Worthing & Hance 1991; Milne 1995)

5.07, 5.28, 5.34 (Montgomery 1993)

4.88 (RP-HPLC-RT correlation, Saito et al. 1993)

4.82 (RP-HPLC-RT correlation, Sicbaldi & Finizio 1993)

5.34 (recommended, Sangster 1993; Hansch et al. 1995)

5.27 (pH 7.7–8.9, Tomlin 1994)

5.13 (Pomona-database, Müller & Kördel 1996)

4.82 (RP-HPLC-RT correlation, Finizio et al. 1997)

4.98 (RP-HPLC-RT correlation using short ODP column, Donovan & Pescatore 2002)

#### Bioconcentration Factor, $\log BCF$ :

3.97, 3.66 (measured, Metcalf & Sanborn 1975)

3.51, 3.03 (fathead minnow, kinetic test, chronic exposure, Spacie & Hamelink 1979)

3.11 (mosquito fish, correlated-S, Spacie & Hamelink 1979)

3.01 (rainbow trout, correlated- $K_{OW}$ , Spacie & Hamelink 1979)

3.26–3.76 (Spacie & Hamelink 1979)

3.66, 3.04 (quoted exptl., calculated- $K_{OC}$ , Kenaga 1980)

2.92 (calculated-S, Kenaga 1980)

2.95 (calculated- $K_{OW}$ , Briggs 1981)

3.50 (*Pseudorasbora parva*, Kanazawa 1981)

3.26–3.76 (selected, Schnoor & McAvoy 1981; Schnoor 1992)

2.67, 5.02 (dry leaf, wet leaf, Bacci et al. 1990)

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

4.14 (soil, Harvey 1974; Kenaga 1980; Kenaga & Goring 1980)

3.76 (soil, calculated-S as per Kenaga & Goring 1980, Kenaga 1980)

3.64 (av. 3 soils, McCall et al. 1980)

4.49 (Georgia's Hickory Hill pond sediment, Brown & Flagg 1981)

2.70 (selected, sediment/water, Schnoor & McAvoy 1981; Schnoor 1992)

3.78 (soil, Thomas 1982)

3.87 (soil average, Jury et al. 1983)

3.63 (soil slurry method, Swann et al. 1983)

3.98 (RP-HPLC-RT correlation, Swann et al. 1983)

3.86 (screening model calculations, Jury et al. 1987a,b; Jury & Ghodrati 1989)

5.13 (RP-HPLC-k' correlation, cyanopropyl column, Hodson & Williams 1988)

3.59 (Nash 1988)



- 2.94 (average of 2 soils, Kanazawa 1989)  
 3.64–4.15, 3.76–4.14 (soil, quoted values, Bottoni & Funari 1992)  
 4.71, 4.44, 4.59 (No. 1 and 2 soil, No. 3 soil and No. 4 soil; Francioso et al. 1992)  
 3.90 (soil, 20–25°C, selected, Wauchope et al. 1992)  
 4.37 (selected, Lohninger 1994)  
 3.94 (soil, HPLC-screening method, mean value from different stationary and mobile phases, Kördel et al. 1993, 1995a,b)  
 3.93 (soil, calculated-MCI  $\chi$ , Sabljic et al. 1995)  
 3.94; 3.99 (HPLC-screening method; calculated-PCKOC fragment method, Müller & Kördel 1996)  
 3.86 (soil, estimated-general model using molecular descriptors, Gramatica et al. 2000)  
 3.53, 3.45, 3.96 (soils: organic carbon  $OC \geq 0.1\%$ ,  $OC \geq 0.5\%$ ,  $0.1 \leq OC < 0.5\%$ , average, Delle Site 2001)  
 4.42 (average values for sediments with  $OC \geq 0.5\%$ , Delle Site 2001)

#### Sorption Partition Coefficient, $\log K_{OM}$ :

- 3.87 (Grover et al. 1978)  
 3.63 (experimental, Grover et al. 1979)  
 4.14 (av. soils/sediments, Kenaga & Goring 1980)  
 3.90 (sorption isotherm-GC, Briggs 1981)  
 1.36, 2.08, 2.98 ( $\log K_p$ : with first-order rate 0.52, 0.2,  $8.3 \times 10^{-3} \text{ h}^{-1}$ , Karickhoff & Morris 1985)  
 4.14, 3.75 (selected, estimated, Magee 1991)  
 2.94–4.49 (Montgomery 1993)  
 4.37 (selected, Lohninger 1994)  
 3.90 (soil, 20–25°C, selected, Hornsby et al. 1996)

#### Adsorption Coefficient $K_d$ ( $\text{L kg}^{-1}$ ):

- 8.1 (homoionic  $K^+$ -montmorillonite clay minerals, Haderlein et al. 1996)

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

Volatilization: initial rate constant  $k = 2.6 \times 10^{-2} \text{ h}^{-1}$  and predicted rate constant  $k = 6.6 \times 10^{-2} \text{ h}^{-1}$  from soil with  $t_{1/2} = 10.5 \text{ h}$  (Thomas 1982);

$t_{1/2} = 18 \text{ d}$  (Jury et al. 1983; quoted, Grover 1991);

measured rate constant  $k = 2\text{--}6 \text{ d}^{-1}$  (Glottfelty et al. 1984; quoted, Glottfelty 1989);

estimated rate constant  $k = 0.7 \text{ d}^{-1}$  (Glottfelty et al. 1989);

estimated  $t_{1/2} \sim 1.6 \text{ d}$  from 1 m depth of water at 20°C (Muir 1991).

Photolysis:  $t_{1/2} < 1 \text{ h}$  under acidic conditions in aqueous methanolic solution (Crosby & Leitis 1973)

$k = 2.0 \text{ d}^{-1}$  with  $t_{1/2} = 22 \text{ min}$  for direct sunlight photolysis near surface water at 40°N in the summer (Zepp & Cline 1977; Zepp 1980; Zepp et al. 1984)

$t_{1/2}(\text{calc}) = 0.94 \text{ h}$  for disappearance via direct sunlight photolysis in aqueous media (Zepp & Baughman 1978; quoted, Harris 1982)

$k = 0.03 \text{ d}^{-1}$  with  $t_{1/2} = 22 \text{ d}$  for direct sunlight near surface (Schnoor & McAvoy 1981)

$k = 0.028\text{--}0.012 \text{ min}^{-1}$  corresponding to  $t_{1/2} = 25\text{--}60 \text{ min}$  for July, midday sunlight in an outdoor chamber (Mongar & Miller 1988)

$t_{1/2} = 0.5 \text{ h}$  estimated from photolysis reaction rate by direct sunlight of midday in mid-summer at 40°N near surface water (Zepp 1991)

$t_{1/2} \sim$  minutes to several months depending on the substrate under sunlight in all media (summary of literature data, Grover et al. 1997)

#### Oxidation:

Hydrolysis:  $t_{1/2}(\text{calc}) > 1 \text{ yr}$  buffered at pH 4, 7, 9 and incubated at 50°C (Grover et al. 1997)

Abiotic Transformations: Degradation by abiotic reductive transformations:

$k = 1.79 \times 10^{-3} \text{ min}^{-1}$  at pH 6.5,  $1.08 \times 10^{-2} \text{ min}^{-1}$  at pH 6.72–6.75,  $1.64 \times 10^{-2} \text{ min}^{-1}$  at pH 6.84,  $4.90 \times 10^{-2} \text{ min}^{-1}$  at pH 6.94,  $7.09 \times 10^{-2} \text{ min}^{-1}$  at pH 6.97,  $0.141 \text{ min}^{-1}$  at pH 7.14,  $0.390 \text{ min}^{-1}$  at pH 7.46,  $0.566 \text{ min}^{-1}$  at pH 7.53, and  $0.727 \text{ min}^{-1}$  at pH 7.73 covering half-lives of 1–400 min., in reaction mixture of 0.5 mM Fe(II) and 100 mg/L goethite solutions (Klupinski & Chin 2003)

$k = 1.88 \text{ M}^{-1} \text{ s}^{-1}$  in  $\text{H}_2\text{S}$  with (mecapto)juglone (hydroquinone moiety, an abiotic reductant found in natural systems) solution at pH 6.65 (Wang & Arnold 2003)

Aqueous solutions with surface-bound Fe(II) species and their first-order rate constants as:

$k = 1.13 \times 10^{-3} \text{ h}^{-1}$  at pH 6.5,  $k = 1.11 \times 10^{-2} \text{ h}^{-1}$  at pH 7.0,  $k = 0.0251 \text{ h}^{-1}$  at pH 7.4, and  $k = 3.40 \text{ h}^{-1}$  at pH 7.8 for aqueous ferrous ion system;

$k = 0.361 \text{ h}^{-1}$  at pH 6.5,  $k = 0.750 \text{ h}^{-1}$  at pH 6.7,  $k = 2.57 \text{ h}^{-1}$  at pH 7.0, and  $k = 6.66 \text{ h}^{-1}$  at pH 7.3 for Fe(II)/goethite system; and

$k = 4.23 \times 10^{-3} \text{ h}^{-1}$  at pH 6.5,  $k = 5.38 \times 10^{-3} \text{ h}^{-1}$  at pH 7.0,  $k = 1.10 \times 10^{-2} \text{ h}^{-1}$  at pH 7.4 and  $k = 2.36 \times 10^{-2} \text{ h}^{-1}$  at pH 7.8 for Fe(II)/clay system, all with total dissolved Fe(II) = 1 mM (Wang & Arnold 2003)

#### Biodegradation:

$t_{1/2} = 4\text{--}5 \text{ d}$  for 4  $\mu\text{g/mL}$  to biodegrade in flooded soils at 24.5°C and  $t_{1/2} > 21 \text{ d}$  at 3.3°C (Probst et al. 1967; quoted, Means et al. 1983; Muir 1991);

$t_{1/2} > 20 \text{ d}$  for 0.33  $\mu\text{g/mL}$  to biodegrade in soil suspension at 25°C (Willis et al. 1974; quoted, Muir 1991);

$t_{1/2} = 20 \text{ d}$  for 0.5  $\mu\text{g/mL}$  to biodegrade in flooded soil with 0.5–1.0 cm of water on top of the soil at 20–42°C (Savage 1978; quoted, Muir 1991);

Degradation  $t_{1/2} < 1$  month in three soils, Goldsborol loamy sand, Cecil loamy sand Drummer clay loam treated with 1 ppm trifluralin) for 4 month under aerobic conditions, no degradation in sterile controls. (shake flask-TLC, Camper et al. 1980)

$t_{1/2} < 1$  month for 1.0  $\mu\text{g/mL}$  to biodegrade in flooded soils at 25°C (derived from Camper et al. 1980; Muir 1991)

$k = 0.008 \text{ d}^{-1}$  by soil incubation die-away test and  $k = 0.025 \text{ d}^{-1}$  by flooded soil incubation die-away test (Rao & Davidson 1980; quoted, Scow 1982);

$t_{1/2} = 132 \text{ d}$  for a 100 d leaching and screening test in 0–10 cm depth of soil (Rao & Davidson 1980; quoted, Jury et al. 1983, 1984, 1987a,b; Jury & Ghodrati 1989; Grover 1991);

$t_{1/2} = 46 \text{ wk}$  for 2.0  $\mu\text{g/mL}$  to biodegrade in flooded soils at 25°C (Brewer et al. 1982; quoted, Muir 1991);

$t_{1/2} = 20 \text{ h}$  for 0.36  $\mu\text{g/mL}$  to biodegrade in sediment-water microcosm at 20°C (Spain & Van Veld 1983; quoted, Muir 1991);

$k = -0.00504$  to  $-0.00730 \text{ h}^{-1}$  in nonsterile sediment,  $k = -0.00160$  to  $-0.00651 \text{ h}^{-1}$  in sterile sediment by shake-tests at Range Point;  $k = -0.00827$  to  $-0.01140 \text{ h}^{-1}$  in nonsterile water, and  $k = -0.00499$  to  $-0.00712 \text{ h}^{-1}$  in sterile water by shake-tests at Range Point (Walker et al. 1988)

$k = -0.00621$ ,  $-0.0121 \text{ h}^{-1}$  in nonsterile sediment,  $k = -0.00476$ ,  $-0.00409 \text{ h}^{-1}$  in sterile sediment by shake-tests at Davis Bayou and  $k = -0.00439$ ,  $-0.00349 \text{ h}^{-1}$  in nonsterile water, and  $k = -0.00299$ ,  $-0.00598 \text{ h}^{-1}$  in sterile water by shake-tests at Davis Bayou (Walker et al. 1988).

#### Biotransformation:

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

#### Half-Lives in the Environment:

Air: mean  $t_{1/2} = 42 \text{ min}$  under August conditions in California range from 21–63 min (Woodrow et al. 1978)

$t_{1/2} = 25\text{--}60 \text{ min}$  for July, midday sunlight in an outdoor chamber (Mongar & Miller 1988)

$t_{1/2} = 182\text{--}193 \text{ min}$  under fall sunlight conditions in October (Woodrow et al. 1983)

Surface water: calculated  $t_{1/2} = 21 \text{ min}$  from midday direct sunlight photolysis rate constant of  $2.0 \text{ h}^{-1}$  (Zepp 1978; Zepp & Cline 1977; quoted, Zepp et al. 1984);

calculated  $t_{1/2} = 0.94 \text{ h}$  for disappearance via direct sunlight photolysis in aqueous media (Zepp & Baughman 1978; quoted, Harris 1982);

$t_{1/2} < 20 \text{ d}$  for 2.5–5 cm water over flooded soils,  $t_{1/2} \sim 20 \text{ h}$  in water above sediment in estuarine sediment-water microcosm (Muir 1991);

$t_{1/2} < 9 \text{ h}$  in buffered aqueous solution of pH 7 under Xenon lamp (quoted, Grover et al. 1997)

$t_{1/2} = 1\text{--}400 \text{ min}$  in reaction mixture of 0.5 mM and 100 mg/L goethite solution for pHs from 6.5 to 7.73 (Klupinski & Chin 2003).

Ground water: reported  $t_{1/2} = 4\text{--}67$ , 57–126, 70, 83, and 105–132 d (Bottoni & Funari 1992)

Sediment: degradation  $t_{1/2} = 9 \text{ d}$  in estuarine sediment ( $18^\circ/\infty$ ) system (Means et al. 1983).

$t_{1/2} = 18.5 \text{ d}$  in flooded sediment (quoted, Grover et al. 1997)

Soil:  $t_{1/2} = 4\text{--}5 \text{ d}$  for 4  $\mu\text{g/mL}$  to biodegrade in flooded soils at 24.5°C and  $t_{1/2} > 21 \text{ d}$  at 3.3°C (Probst et al. 1967; quoted, Means et al. 1983; Muir 1991);

estimated persistence of 6 months in soil (Kearney et al. 1969; Edwards 1973; quoted, Morrill et al. 1982; Jury et al. 1987a);

degradation  $t_{1/2} = 93 \text{ d}$  in soil (Parr & Smith 1973; quoted, Means et al. 1983);

- $t_{1/2} > 20$  d for  $0.33 \mu\text{g mL}^{-1}$  to biodegrade in soil suspension at  $25^\circ\text{C}$  (Willis et al. 1974; quoted, Muir 1991);  
 degradation  $t_{1/2} = 1$  d (Kearney et al. 1976; quoted, Means et al. 1983); and  $t_{1/2} = 54$  d in soil (Zimdahl & Gwynn 1977; quoted, Means et al. 1983);  
 $t_{1/2} = 20$  d for  $0.5 \mu\text{g/mL}$  to biodegrade in flooded soil with 0.5–1.0 cm of water on top of the soil at  $20\text{--}42^\circ\text{C}$  (Savage 1978; quoted, Muir 1991);  
 persistence of more than 6 months (Wauchope 1978);  
 $t_{1/2} < 21$  d in flooded soil at  $20\text{--}25^\circ\text{C}$  (Golab et al. 1979)  
 biodegradation  $t_{1/2} < 1$  month in 3 flooded soils at  $25^\circ\text{C}$  (Camper et al. 1980);  
 estimated first-order  $t_{1/2} \sim 86.6$  d in soil from biodegradation rate constant  $k = 0.008 \text{ d}^{-1}$  by soil incubation die-away test and  $t_{1/2} = 27.7$  d in anaerobic systems from rate constant  $k = 0.025 \text{ d}^{-1}$  by flooded soil incubation die-away test (Rao & Davidson 1980; quoted, Scow 1982);  
 $t_{1/2} = 2$  d on Bosket silt loam,  $t_{1/2} = 2$  d on Sharkey clay for the first 3 to 5 days when sprayed onto soil surface, rate of loss much slower for the remainder of the 7- or 12-d sampling period with  $t_{1/2} = 70$  d on Bosket silt loam,  $t_{1/2} = 50$  d on Sharkey clay (Savage & Jordon 1980)  
 $t_{1/2} = 30$  d flooded soil in aquatic ecosystem (Yockim et al. 1980)  
 field  $t_{1/2} = 0.1\text{--}0.3$  d in moist fallow soil (Glottfelty 1981; quoted, Nash 1983);  
 Field studies:  $t_{1/2} = 9.5$  wk - 1978 first study;  $t_{1/2} = 11.8$  wk -1978 second study;  $t_{1/2} = 12.2$  wk -1979, in a Crowley silt loam at Stuttgart, Arkansas (Brewer et al. 1982)  
 Laboratory studies:  $t_{1/2} = 19.6$  wk at  $4^\circ\text{C}$ ,  $t_{1/2} = 7.1$  wk at  $25^\circ\text{C}$  for soil of field capacity moisture (27% w/w for Crowley silt),  $t_{1/2} = 16.2$  wk at  $4^\circ\text{C}$ ,  $t_{1/2} = 3.9$  wk at  $25^\circ\text{C}$  for flooded soils, Crowley silt loam; and  $t_{1/2} = 27.0$  wk at  $4^\circ\text{C}$ ,  $t_{1/2} = 8.1$  wk at  $25^\circ\text{C}$  for soil of field capacity moisture (34% w/w for Sharkey silty clay),  $t_{1/2} = 18.6$  wk at  $4^\circ\text{C}$  and  $t_{1/2} = 5.4$  wk at  $25^\circ\text{C}$  for flooded soils, Sharkey silty clay (Brewer et al. 1982)  
 microagroecosystem  $t_{1/2} = 3\text{--}4$  d in moist fallow soil (Nash 1983);  
 $t_{1/2} = 46$  wk for  $2.0 \mu\text{g/mL}$  to biodegrade in flooded soils at  $25^\circ\text{C}$  (derived from Brewer et al. 1982, Muir 1991);  
 very persistent in soils with  $t_{1/2} > 100$  d (Willis & McDowell 1982);  
 $t_{1/2} = 20$  h for  $0.36 \mu\text{g/mL}$  to biodegrade in sediment-water microcosm at  $20^\circ\text{C}$  (Spain & Van Veld 1983; quoted, Muir 1991);  
 measured dissipation rate  $k = 0.69 \text{ d}^{-1}$  (Nash 1983; quoted, Nash 1988);  
 estimated dissipation rate  $k = 1.6$  and  $0.24 \text{ d}^{-1}$  (Nash 1988);  
 first-order adsorption rate constants:  $k = 0.52, 0.2, 8.3 \times 10^{-3} \text{ h}^{-1}$  (Karickhoff & Morris 1985; quoted, Brusseau & Rao 1989);  
 $t_{1/2} \sim 22$  d in submerged soils in a model ecosystem (Muir 1991);  
 reported  $t_{1/2} = 4\text{--}67$  d,  $57\text{--}126$  d,  $70$  d,  $83$  d,  $105\text{--}132$  d (Bottoni & Funari 1992);  
 selected field  $t_{1/2} = 60$  d (Wauchope et al. 1992; Hornsby et al. 1996; quoted, Halfon et al. 1996)  
 Estimated  $t_{1/2} \sim 25$  to  $> 201$  d under a variety of agronomic conditions in agriculture soils depending on depth of incorporation, soil moisture, soil temperature, soil air, and soil organic matter content (summary of literature data, Grover et al. 1997)  
 Biota:  $t_{1/2} = 22\text{--}31$  d in river saugers,  $t_{1/2} = 17\text{--}57$  d in river shorthead redhorse,  $t_{1/2} = 23$  d in river golden redhorse,  $t_{1/2} = 3$  d in lab. fathead minnow (Spacie & Hamelink 1979);  
 biochemical  $t_{1/2} = 132$  d (Jury et al. 1987a,b; Jury & Ghodrati 1989).

TABLE 17.1.1.79.1

Reported vapor pressures of trifluralin at various temperatures and the coefficients for the vapor pressure equations

$\log P = A - B/(T/K)$	(1)	$\ln P = A - B/(T/K)$	(1a)
$\log P = A - B/(C + t/^{\circ}\text{C})$	(2)	$\ln P = A - B/(C + t/^{\circ}\text{C})$	(2a)
$\log P = A - B/(C + T/K)$	(3)		
$\log P = A - B/(T/K) - C \cdot \log (T/K)$	(4)		
<b>Spencer &amp; Cliath 1974</b>		<b>Rordorf 1989</b>	
<b>gas saturation method</b>		<b>gas saturation-GC</b>	
<b>t/°C</b>	<b>P/Pa</b>	<b>t/°C</b>	<b>P/Pa</b>
20	0.0065	25	0.010
30	0.0323	50	0.32
40	0.155	75	6.30
		100	82.0
		125	780
			for solid
		eq. 1	$P_s/\text{Pa}$
		A	17.46
		B	5800.6
			for liquid
		eq. 1	$P_L/\text{Pa}$
		A	13.65
		B	4573.1

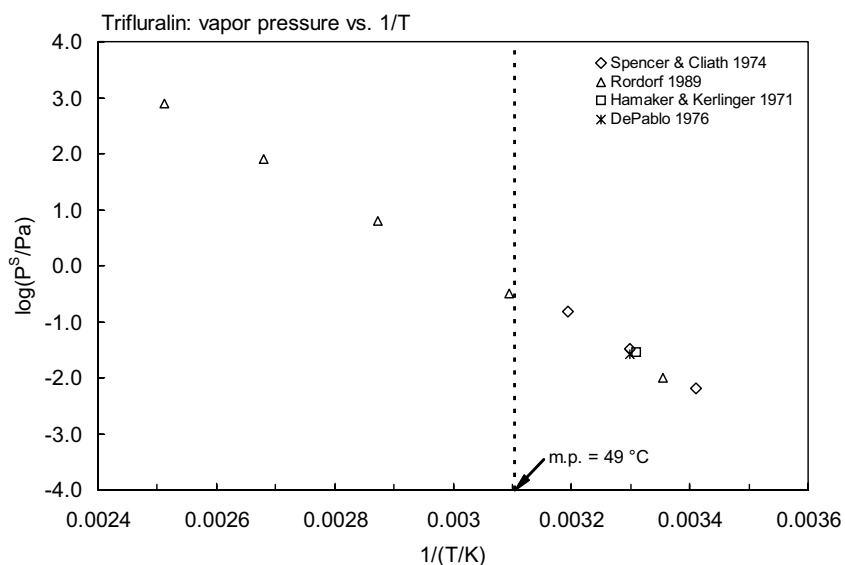
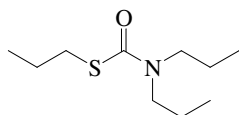


FIGURE 17.1.1.79.1 Logarithm of vapor pressure versus reciprocal temperature for trifluralin.

## 17.1.1.80 Vernolate



Common Name: Vernolate

Synonym: PPTC, R1607, Vanalate, Vernam, Vernnolaolate

Chemical Name: *S*-propyldipropylthiocarbamate; *S*-propyldipropylcarbamothioate

Uses: herbicide incorporated with soil for pre-planting or pre-emergence control of broadleaf and grass weeds in groundnuts, soybeans, maize, tobacco, and sweet potatoes.

CAS Registry No: 1929-77-7

Molecular Formula:  $C_{10}H_{21}NOS$

Molecular Weight: 203.345

Melting Point (C): liquid

Boiling Point (°C):

150 (at 30 mmHg, Herbicide Handbook 1989; Worthing & Hance 1991; Tomlin 1994; Milne 1995)

149–150 (at 30 mmHg, Budavari 1989)

Density (g/cm<sup>3</sup> at 20°C):

0.954 (Ashton & Crafts 1981; Herbicide Handbook 1989; Worthing & Hance 1991)

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

Molar Volume (cm<sup>3</sup>/mol):

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

Dissociation Constant  $pK_a$ :

Enthalpy of Fusion,  $\Delta H_{fus}$  (kJ/mol):

Entropy of Fusion,  $\Delta S_{fus}$  (J/mol K):

Fugacity Ratio at 25°C (assuming  $\Delta S_{fus} = 56$  J/mol K), F: 1.0

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

107 (Martin & Worthing 1977)

90 (20°C, Khan 1980; Spencer 1982; Ashton & Crafts 1981; Herbicide Handbook 1989)

107 (21°C, Verschueren 1983)

90 (20°C, Hartley & Kidd 1987; Worthing & Walker 1987, Worthing & Hance 1991)

107 (Budavari 1989; Milne 1995)

95 (Wauchope 1989)

108 (20–25°C, selected, Wauchope et al. 1992; Hornsby et al. 1996)

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

0.84 (20°C, Hartley & Graham-Bryce 1980)

1.386 (Khan 1980; Spencer 1982; Herbicide Handbook 1989)

1.333 (Ashton & Crafts 1981)

0.244 (20°C, GC-RT correlation, Kim 1985)

1.39 (Hartley & Kidd 1987)

0.9 (20°C, selected, Suntio et al. 1988)

1.386 (Budavari 1989)

1.39 (Worthing & Hance 1991; Tomlin 1994)

1.293 (20–25°C, selected, Wauchope et al. 1992; Hornsby et al. 1996)

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

2.05 (20°C, calculated-P/C, Suntio et al. 1988)

2.034 (calculated-P/C, this work)

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

3.84 (20°C, Worthing & Hance 1991; Tomlin 1994)

- 3.84 (20°C, Milne 1995)
- 3.84 (recommended, Hansch et al. 1995)
- 3.86 (RP-HPLC-RT correlation, Finizio et al. 1997)

Bioconcentration Factor, log BCF:

- 1.64 (calculated-S, Kenaga 1980)
- 1.70 (calculated, Pait et al. 1992)

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

- 2.52 (calculated-S, Kenaga 1980)
- 2.41 (soil, 20–25°C, selected, Wauchope et al. 1992; Hornsby et al. 1996)
- 2.03, 1.93 (quoted exptl.; calculated-MCI and fragment contribution method, Meylan & Howard 1992)
- 2.41 (estimated-chemical structure, Lohninger 1994)
- 2.33 (soil, calculated-MCI  $\chi$ , Sabljic et al. 1995)
- 2.33; 2.40, 2.11 (soil, quoted exptl.; estimated-class-specific model, estimated-general model using molecular descriptors, Gramatica et al. 2000)

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

Biodegradation: microbial degradation  $t_{1/2} = 8\text{--}16$  d at 27°C,  $t_{1/2} > 64$  d at 4°C in soil (Tomlin 1994).

Half-Lives in the Environment:

Soil:  $t_{1/2} \sim 1.5$  wk in moist loam soil at 21–27°C (Herbicide Handbook 1989);  
selected field  $t_{1/2} = 12$  d (Wauchope et al. 1992; Hornsby et al. 1996);  
soil  $t_{1/2} = 11$  d (Pait et al. 1992);  
microbial degradation  $t_{1/2} = 8\text{--}16$  d at 27°C,  $t_{1/2} > 64$  d at 4°C (Tomlin 1994).

Biota:

## 17.2 SUMMARY TABLES

TABLE 17.2.1

Common names, chemicals names and physical properties of herbicides

Compound	Synonym	Chemical name	Molecular formula	Molecular weight, MW g/mol	m.p. °C	Fugacity ratio, F at 25°C*	pK <sub>a</sub>	pK <sub>b</sub>
Alachlor [15972-60-8]	Lasso, Metachlor	$\alpha$ -chloro-2,6-diethyl- <i>N</i> -methoxy-methylacetanilide	C <sub>14</sub> H <sub>20</sub> ClNO <sub>2</sub>	269.768	40	0.713	0.62	
Ametryn [834-12-8]	Evik, Gesapax	2-methylthio-4-(ethylamino)-6-(isopropylamino)- <i>s</i> -triazine	C <sub>9</sub> H <sub>17</sub> N <sub>5</sub> S	227.330	88	0.241	4.00 4.10	10.07
Amitrole [61-82-5]	Amerol, Aminotriazole	3-amino-1 <i>H</i> -1,2,4-triazole	C <sub>2</sub> H <sub>4</sub> N <sub>4</sub>	84.080	159	0.0484		9.83
Atrazine	Gesaprim	2-chloro-4-(ethylamino)-6-(isopropylamino)- <i>s</i> -triazine	C <sub>8</sub> H <sub>14</sub> ClN <sub>5</sub>	215.684	173	0.0353	1.68 1.70	12.32
Barban [101-27-9]	Carbyne	4-chlorobut-2-ynyl-3-chlorocarbamate	C <sub>11</sub> H <sub>9</sub> Cl <sub>2</sub> NO <sub>2</sub>	258.101	75	0.323		
Benefin [1861-40-1]	Balan, Bonalan Benfluralin	<i>N</i> -butyl- <i>N</i> -ethyl- $\alpha,\alpha,\alpha$ -trifluoro-2,6-di-nitro- <i>p</i> -toluidine	C <sub>13</sub> H <sub>16</sub> N <sub>3</sub> O <sub>4</sub> F <sub>3</sub>	335.279	66	0.396		
Bifenox [42576-02-3]	Modown	methyl-5-(2,4-dichlorophenoxy)-2-nitrobenzoate	C <sub>14</sub> H <sub>9</sub> Cl <sub>2</sub> NO <sub>5</sub>	342.131	85	0.258		
Bromacil [314-40-9]	Borea, Hyvar X	5-bromo-3- <i>sec</i> -butyl-6-methyl-uracil	C <sub>9</sub> H <sub>13</sub> BrN <sub>2</sub> O <sub>2</sub>	261.115	158	0.0496	9.10 < 7.0	
Bromacil lithium salt			C <sub>9</sub> H <sub>12</sub> N <sub>2</sub> O <sub>3</sub> Li	267.0			9.27	
Bromoxynil [1689-84-5]	Brominal, Buctril	3,5-dibromo-4-hydroxybenzonitrile	C <sub>7</sub> H <sub>3</sub> Br <sub>2</sub> NO	276.913	190	0.0241	4.06 4.20	
Bromoxynil butyrate ester [3861-41-4]			C <sub>13</sub> H <sub>9</sub> BrNO <sub>3</sub>	307.119			4.10	
Bromoxynil octanoate [1689-99-2]		2,6-dibromo-4-cyanophenyl octanoate	C <sub>15</sub> H <sub>17</sub> Br <sub>2</sub> NO <sub>2</sub>	403.109	45–46	0.629	4.08	
<i>sec</i> -Bumeton [26259-45-0]	Etazine, Sumitol	<i>N</i> -ethyl-6-methoxy- <i>N'</i> -(1-methyl-propyl)-1,3,5-triazine-2,4-diamine	C <sub>10</sub> H <sub>19</sub> N <sub>5</sub> O	225.291	87	0.246	4.40	
Butachlor [23184-66-9]	Machete	<i>N</i> -butoxymethyl-2-chloro-2',6'-diethylacetanilide	C <sub>17</sub> H <sub>26</sub> ClNO <sub>2</sub>	311.847	< –5	1		
Butralin [33629-47-9]	Amex, Tamex	<i>N</i> - <i>sec</i> -butyl-4- <i>tert</i> -butyl-2',6'- dinitroaniline	C <sub>14</sub> H <sub>21</sub> N <sub>3</sub> O <sub>4</sub>	295.335	60	0.454		
Butylate [2008-41-5]	Sutan	<i>S</i> -ethyl bis(2-methylpropyl) carbamothioate	C <sub>11</sub> H <sub>23</sub> NOS	217.372	liquid	1		
Chloramben [133-90-4]	Amiben, Amoben	3-amino-2,5-dichlorobenzoic acid	C <sub>7</sub> H <sub>5</sub> Cl <sub>2</sub> NO <sub>2</sub>	206.027	200	0.0192	3.40	

(Continued)

TABLE 17.2.1 (Continued)

Compound	Synonym	Chemical name	Molecular formula	Molecular weight, MW g/mol	m.p. °C	Fugacity ratio, F at 25°C*	pK <sub>a</sub>	pK <sub>b</sub>
Chloramben salts [133-90-4]	Amiben	ammonium or sodium salt of chloramben	C <sub>7</sub> H <sub>5</sub> Cl <sub>2</sub> NO <sub>2</sub>	206.027				
Chlorazine [580-48-3]		6-chloro- <i>N,N,N'</i> -tetraethyl-1,3,5-triazine-2,4-diamine	C <sub>11</sub> H <sub>20</sub> ClN <sub>5</sub>	257.764	27	0.956		
Chlorbromuron [13360-45-7]	Maloran	3-(4-bromo-3-chlorophenyl)-1-methoxy-1-methylurea	C <sub>9</sub> H <sub>10</sub> BrClN <sub>2</sub> O <sub>2</sub>	293.544	96	0.201		
Chlorfenac [85-34-7]	Fenac	(2,3,6-trichlorophenyl)acetic acid	C <sub>8</sub> H <sub>5</sub> Cl <sub>3</sub> O <sub>2</sub>	239.484	161	0.046		
Chlorpropham [101-21-3]	Furloe	isopropyl 3-chlorocarbanilate	C <sub>10</sub> H <sub>12</sub> ClNO <sub>2</sub>	213.661	41	0.697		
Chlorsulfuron [64902-72-3]	Glean, Telar	1-(2-chlorophenylsulfonyl)-3-(4-methoxy-6-methyl-1,3,5-triazin-2-yl)urea	C <sub>12</sub> H <sub>12</sub> ClN <sub>5</sub> O <sub>4</sub> S	357.773	176	0.0330	3.60	
Chlortoluron [15545-48-9]	Dicuran	3-(3-chloro- <i>p</i> -tolyl)-1,1-dimethylurea	C <sub>10</sub> H <sub>13</sub> ClN <sub>2</sub> O	212.675	147	0.0635		
Cyanazine [21725-46-2]	Bladex, Fortrol	2-(4-chloro-6-ethylamino-1,3,5-triazin-2-ylamino)-2-methylpropionitrile	C <sub>9</sub> H <sub>13</sub> ClN <sub>6</sub>	240.692	168	0.0395	1 0.63	12.9
2,4-D [94-75-7]	Agratect, Farmco, Weed Tox	2-(2,4-dichlorophenoxy)acetic acid	C <sub>8</sub> H <sub>6</sub> Cl <sub>2</sub> O <sub>3</sub>	221.038	140.5	0.0736	2.64 3.31	
2,4-D dimethylamine salt [2008-39-1]			C <sub>10</sub> H <sub>13</sub> Cl <sub>2</sub> NO <sub>3</sub>	266.121	85-87	0.252		
2,4-D esters			C <sub>8</sub> H <sub>6</sub> Cl <sub>2</sub> O <sub>3</sub> (a)	221.038			2.80	
Dalapon [75-99-0]	Dowpon, Radapon	2,2-dichloropropionic acid	C <sub>3</sub> H <sub>4</sub> Cl <sub>2</sub> O <sub>2</sub>	142.969	liquid	1	1.74 1.84	
Dalapon sodium salt [120-20-8]		sodium 2,2-dichloropropionate	C <sub>3</sub> H <sub>3</sub> Cl <sub>2</sub> Na	164.95	166.5 dec			
2,4-DB [94-82-6]	Embutox	4-(2,4-dichlorophenoxy)butyric	C <sub>10</sub> H <sub>10</sub> Cl <sub>2</sub> O <sub>3</sub>	249.090	118	0.122	4.80	
2,4-DB butoxyethyl ester			C <sub>16</sub> H <sub>22</sub> O <sub>4</sub> Cl <sub>2</sub>	349.249			4.80	
Diallate [2303-16-4]	Avadex	<i>S</i> -(2,3-dichloroallyl)diisopropylthiocarbamate	C <sub>10</sub> H <sub>17</sub> Cl <sub>2</sub> NOS	270.219				
Dicamba [1918-00-9]	Banvel, Dianat, Mediben	3,6-Dichloro- <i>o</i> -anisic acid	C <sub>8</sub> H <sub>6</sub> Cl <sub>2</sub> O <sub>3</sub>	221.038	115	0.131	1.91 1.95	
Dichlobenil [1194-65-6]	Casoron	2,6-dichlorobenzonitrile	C <sub>7</sub> H <sub>3</sub> Cl <sub>2</sub> N	172.012	144.5	0.0672		
Dichlorophen (F.A.B) [97-23-4]	Super Mosstox	4,4'-dichloro-2,2'-methylenediphenol	C <sub>13</sub> H <sub>10</sub> Cl <sub>2</sub> O <sub>2</sub>	269.123	177.5	0.0320		
Dichloroprop [120-36-5]	2,4-DP	( <i>RS</i> )-2-(2,4-dichlorophenoxy)-propionic acid	C <sub>9</sub> H <sub>8</sub> Cl <sub>2</sub> O <sub>3</sub>	235.064	117.5	0.124	3.0	



Dichlorprop-P [15165-67-0]	Cornox RK	( <i>R</i> )-2-(2,4-dichlorophenoxy)propionic acid	C <sub>9</sub> H <sub>8</sub> Cl <sub>2</sub> O <sub>3</sub>	235.064	122	0.112	3.0 2.86
Dichlorprop ester	Weedone	butoxyethyl ester of	C <sub>9</sub> H <sub>8</sub> Cl <sub>2</sub> O <sub>3</sub>	335.3			2.85
Diclofop [40843-25-2]		( <i>R</i> -2-(2,4-dichloro-2-(4-aryloxyphenoxy)propionic acid	C <sub>15</sub> H <sub>12</sub> Cl <sub>2</sub> O <sub>4</sub>	327.159			
Diclofop-methyl [51338-27-3]	Hoelon	2-(4-(2,4-dichlorophenoxy)phenoxy)-propanoic acid methyl ester	C <sub>16</sub> H <sub>14</sub> Cl <sub>2</sub> O <sub>4</sub>	341.186	40	0.713	3.10
Dinitramine [29091-05-2]	Cobexo	<i>N,N</i> -diethyl-2,6-dinitro-4-trifluoro-methyl- <i>m</i> -phenylenediamine	C <sub>11</sub> H <sub>13</sub> N <sub>4</sub> O <sub>4</sub> F <sub>3</sub>	322.241	98	0.192	
Dinoseb [88-85-7]	Antox, Aretit, BNP 30, DNBP	2- <i>sec</i> -butyl-4,6-dinitrophenol	C <sub>10</sub> H <sub>12</sub> N <sub>2</sub> O <sub>5</sub>	240.212	40	0.713	4.62
Dinoseb salts [88-85-7]	Premerge, Dinitro	2- <i>sec</i> -butyl-4,6-dinitrophenyl ammonium, amine, acetate salts					4.50
Diphenamid [957-51-7]	Dymid, Enide	<i>N,N</i> -dimethyldiphenylacetamide	C <sub>16</sub> H <sub>17</sub> NO	239.312	135	0.0833	
Diquat [2764-72-9]	Reglone, Pathclear Cleasweep, Weedol	1,1'-ethylene-2,2'-dipyridine	C <sub>12</sub> H <sub>14</sub> N <sub>2</sub>	186.236			
Diquat dibromide salt [85-00-7]			C <sub>12</sub> H <sub>12</sub> Br <sub>2</sub> N <sub>2</sub>	344.1			10
Diuron [330-54-1]	DMU, Karmex DCMU	3-(3,4-dichlorophenyl)-1,1-dimethylurea	C <sub>9</sub> H <sub>10</sub> Cl <sub>2</sub> N <sub>2</sub> O	233.093	158	0.0496	
EPTC [759-94-4]	Eptam, Eradicane	<i>S</i> -ethyl dipropylthiocarbamate	C <sub>9</sub> H <sub>19</sub> NOS	189.318	liquid	1	
Ethalfuralin [55283-68-6]	Benzenamine, Somilan, Sonalan, Sonalen	<i>N</i> -ethyl- <i>N</i> -(2-methyl-2-propenyl)-2,6-dinitro-(trifluoromethyl)-benzenamine	C <sub>13</sub> H <sub>14</sub> F <sub>3</sub> N <sub>3</sub> O <sub>4</sub>	333.263	57	0.485	
Fenoprop (G.R.) [93-72-1]	Silvex, 2,4,5-TP	(±)-2-(2,4,5-trichlorophenoxy)-propionic acid	C <sub>9</sub> H <sub>7</sub> Cl <sub>3</sub> O <sub>3</sub>	269.509	181.6	0.0291	
Fenuron [101-42-8]	Dybar, Urab	1,1-dimethyl-3-phenylurea	C <sub>9</sub> H <sub>12</sub> N <sub>2</sub> O	164.203	132	0.0892	
Fenuron-TCA [4482-55-7]		1,1-dimethyl-3-phenyluronium trichloroacetate	C <sub>11</sub> H <sub>13</sub> Cl <sub>3</sub> N <sub>2</sub> O <sub>3</sub>	327.592	65-68	0.392	
Fluchloralin [33245-39-5]	Basalin Basalin, BAS-392H	<i>N</i> -(2-chloroethyl) α,α,α-trifluoro-2,6-dinitro- <i>N</i> -propyl- <i>p</i> -toluidine	C <sub>12</sub> H <sub>13</sub> ClF <sub>3</sub> N <sub>3</sub> O <sub>4</sub>	355.697	42	0.681	
Fluometuron [2164-17-2]	Cotoran, Cottonex, Meturon	<i>N,N</i> -dimethyl- <i>N'</i> -[3-(trifluoromethyl)-phenyl]urea	C <sub>10</sub> H <sub>11</sub> F <sub>3</sub> N <sub>2</sub> O	232.201	164	0.0433	
Fluorodifen [15457-05-3]	Soyex	4-nitrophenyl α,α,α-trifluoro-2-nitro- <i>p</i> -tolyl ether	C <sub>13</sub> H <sub>7</sub> F <sub>3</sub> N <sub>2</sub> O <sub>5</sub>	328.200	94	0.210	
Fluridone [59756-60-4]	Fluridon, Pride, Sonar	1-methyl-3-phenyl-5-[3-(trifluoromethyl)phenyl]-4-(1 <i>H</i> )-pyridinone	C <sub>19</sub> H <sub>14</sub> F <sub>3</sub> NO	329.315	155	0.0530	12.3

(Continued)

TABLE 17.2.1 (Continued)

Compound	Synonym	Chemical name	Molecular formula	Molecular weight, MW g/mol	m.p. °C	Fugacity ratio, F at 25°C*	pK <sub>a</sub>	pK <sub>b</sub>
Glyphosate [1071-83-6]	Roundup, Polado	<i>N</i> -(phosphoromethyl)glycine	C <sub>3</sub> H <sub>8</sub> NO <sub>5</sub> P	169.074	230 dec	0.0097	5.70	
Glyphosate-mono( <i>iso</i> -propylammonium) [38641-94-0]			C <sub>6</sub> H <sub>17</sub> N <sub>2</sub> O <sub>5</sub> P	228.2	200	0.0190		
Ioxynil [1689-83-4]	Actril, Totril	4-hydroxy-3,5-di-iodobenzonitrile	C <sub>7</sub> H <sub>3</sub> I <sub>2</sub> NO	370.914	201 dec	0.0190	3.96	
Ioxynil-octanoate [3681-47-0]		4-cyano-2,6-iodophenyl octanoate	C <sub>15</sub> H <sub>17</sub> I <sub>2</sub> NO <sub>2</sub>	497.1	59–60	0.459		
Ioxynil-sodium salt [2961-62-8]			C <sub>7</sub> H <sub>2</sub> I <sub>2</sub> NNaO	392.9	360	0.00052		
Isopropalin [33820-53-0]	Paralan	4-isopropyl-2,6-dinitro- <i>N</i> -dipropylaniline	C <sub>15</sub> H <sub>23</sub> N <sub>3</sub> O <sub>4</sub>	309.362	liquid	1		
Isoproturon [34123-59-6]	Alon, Arelon, Graminon	3- <i>p</i> -cumenyl-1,1-dimethylurea	C <sub>12</sub> H <sub>18</sub> N <sub>2</sub> O	206.284	155–156	0.0520		
Linuron [330-55-2]	Afalon, Lorox	3-(3,4-dichlorophenyl)-1-methoxy-1-methylurea	C <sub>9</sub> H <sub>10</sub> Cl <sub>2</sub> N <sub>2</sub> O <sub>2</sub>	249.093	93	0.215		
MCPA (G.R., H) [94-74-6]	Metaxon, Agroxone, Agritox	4-chloro- <i>o</i> -tolylxyacetic acid	C <sub>9</sub> H <sub>9</sub> ClO <sub>3</sub>	200.618	120	0.117	3.05 3.13	
MCPA dimethylamine salt [94-74-6]			C <sub>11</sub> H <sub>16</sub> ClNO <sub>3</sub>	243.7			3.12	
MCPA ester	Weedone, Weedar		C <sub>9</sub> H <sub>9</sub> ClO <sub>3</sub>	200.6				
MCPA sodium salt			C <sub>9</sub> H <sub>8</sub> ClNaO <sub>3</sub>	222.6				
MCPA-thioethyl [25319-90-8]		<i>S</i> -ethyl 4-chloro- <i>o</i> -tolylxythioacetate	C <sub>11</sub> H <sub>13</sub> ClO <sub>2</sub> S	244.7	41–42	0.689		
MCPB [94-81-5]	Tropotox	4-(4-chloro-2-methylphenoxy)butyric acid	C <sub>11</sub> H <sub>13</sub> ClO <sub>3</sub>	228.672	100	0.184	4.84 4.80	
MCPB sodium salt [6062-26-6]			C <sub>11</sub> H <sub>12</sub> ClNaO <sub>2</sub>	250.7				
Mecoprop [7085-19-0]	Iso-Cornox, MCPP	(±)-2-(4-chloro- <i>o</i> -tolylxy)-propionic acid	C <sub>10</sub> H <sub>11</sub> ClO <sub>3</sub>	214.645	94-95	0.208	3.78 3.75	
Mecoprop-P [16484-77-8]		( <i>R</i> )-2-(4-chloro- <i>o</i> -tolylxy)propionic acid	C <sub>10</sub> H <sub>11</sub> ClO <sub>3</sub>	214.645	95	0.206	3.78	
Metobromuron [3060-89-7]	Patoran	3-(4-bromophenyl)-1-methoxy-1-methyl urea	C <sub>9</sub> H <sub>11</sub> BrN <sub>2</sub> O <sub>2</sub>	259.099	95	0.206		

Metolachlor [51218-45-2]	Codal, Dual, Primagram	2-chloro-6'-ethyl- <i>N</i> -(2-methoxy- 1-methylethyl)acet- <i>o</i> -toluidide	C <sub>15</sub> H <sub>22</sub> ClNO <sub>2</sub>	283.795	liquid	1	
Metoxuron [19937-59-8]	Dosanex	3-(3-chloro-4-methoxyphenyl)- 1,1-dimethylurea	C <sub>10</sub> H <sub>13</sub> ClN <sub>2</sub> O <sub>2</sub>	228.675	126-127	0.101	
Metribuzin [21087-64-9]	Metribuzine, Lexone, Preview, Sencor	4-amino-6-( <i>t</i> -butyl)-3-(methylthio)- 1,2,4-triazin-5-(4 <i>H</i> )-one	C <sub>8</sub> H <sub>14</sub> N <sub>4</sub> OS	214.288	126	0.102	
Molinate [2212-67-1]	Ordram	<i>S</i> -ethyl azepane-1-carbothioate	C <sub>9</sub> H <sub>17</sub> NOS	187.302	liquid	1	
Monolinuron [1746-81-2]	Aresin	3-(4-chlorophenyl)-1-methoxy- 1-methylurea	C <sub>9</sub> H <sub>11</sub> ClN <sub>2</sub> O <sub>2</sub>	214.648	77	0.309	
Monuron [150-68-5]	Telvar, Urox	1,1-dimethyl-3-( <i>p</i> -chloro-phenyl)-urea	C <sub>9</sub> H <sub>11</sub> ClN <sub>2</sub> O	198.648	170.5	0.0374	
Napropamide [15299-99-7]	Devrinol	2-( $\alpha$ -naphthloxy)- <i>N,N</i> - diethylpropionamide	C <sub>17</sub> H <sub>21</sub> NO <sub>2</sub>	271.355	75	0.323	2.93
Neburon [555-37-3]	Kloben	1-butyl-3-(3,4-dichlorophenyl)-1-methyl urea	C <sub>12</sub> H <sub>16</sub> Cl <sub>2</sub> N <sub>2</sub> O	275.174	102-103	0.174	
Nitralin [4726-14-1]	Planavin	4-(methylsulfonyl)-2,6-dinitro- <i>N,N</i> -dipropylaniline	C <sub>13</sub> H <sub>19</sub> N <sub>3</sub> O <sub>6</sub> S	345.371	150	0.0594	
Nitrofen [1836-75-5]	nitrophen, Tok, Tokkron	2,4-dichloro-1-(4-nitrophenoxy)benzene	C <sub>12</sub> H <sub>7</sub> Cl <sub>2</sub> NO <sub>3</sub>	284.095	70	0.362	
Norfluorazon [27314-13-2]			C <sub>12</sub> H <sub>9</sub> ClF <sub>3</sub> N <sub>3</sub> O	303.666	184	0.0275	
Oryzalin [19044-88-3]	Ryccelan, Ryccelon, Surflan	4-(dipropylamino)-3,5-dinitro- benzenesulfonamide	C <sub>12</sub> H <sub>18</sub> N <sub>4</sub> O <sub>6</sub> S	346.359	141	0.0728	9.40 8.60
Paraquat [4685-14-7]	Cyclone, Gramoxone	1,1'-dimethyl-4,4'-pyridinium	C <sub>12</sub> H <sub>14</sub> N <sub>2</sub>	186.252	dec.		
Paraquat dichloride salt [1910-42-5]			C <sub>12</sub> H <sub>14</sub> Cl <sub>2</sub> N <sub>2</sub>	257.2			< 4
Pebulate [1114-71-2]	Tillam	<i>s</i> -propyl butylethylcarbamothioate	C <sub>10</sub> H <sub>21</sub> NOS	203.345	liquid	1	
Pendimethalin [40487-42-1]	penoxalin	<i>N</i> -(1-ethylpropyl-3,4-dimethyl- 2,6-dinitrobenzenamine	C <sub>13</sub> H <sub>19</sub> N <sub>3</sub> O <sub>4</sub>	281.308	56	0.496	
Pentachlorophenol [87-86-5]	PCP	pentachlorophenol	C <sub>6</sub> Cl <sub>5</sub> OH	266.336	174	0.0350	4.74
Pentachlorophenol sodium salt (Pentacon)							
Pentachlor	Solan	3'-chloro-2-methylvaler- <i>p</i> -toluidide	C <sub>13</sub> H <sub>18</sub> ClNO	239.741	85-86	0.255	
[2307-68-8]							
Picloram [1918-02-1]	Tordon	4-amino-3,5,6-trichloro-picolinic acid	C <sub>6</sub> H <sub>3</sub> Cl <sub>3</sub> N <sub>2</sub> O <sub>2</sub>	241.459	218.5	0.0126	1.90 3.60

(Continued)

TABLE 17.2.1 (Continued)

Compound	Synonym	Chemical name	Molecular formula	Molecular weight, MW g/mol	m.p. °C	Fugacity ratio, F at 25°C*	pK <sub>a</sub>	pK <sub>b</sub>
Picloram-potassium salt [2425-60-0]			C <sub>6</sub> H <sub>2</sub> Cl <sub>3</sub> KN <sub>2</sub> O <sub>2</sub>	279.6				
Profluralin [26399-36-0]	Pregard	<i>N</i> -(cyclopropylmethyl)-2,6-dinitro- <i>N</i> -propyl-4-(trifluoromethyl)-benzenamine	C <sub>14</sub> H <sub>16</sub> F <sub>3</sub> N <sub>3</sub> O <sub>4</sub>	347.290	34	0.816		
Prometon [1610-18-0]	Primatol, Gesagram	2,4-bis(isopropylamino)-6-methoxy- <i>s</i> -triazine	C <sub>10</sub> H <sub>19</sub> N <sub>5</sub> O	225.291	91.5	0.223	4.28 4.30	9.73
Prometryn [7287-19-6]	Caparol, Gesagard	<i>N,N</i> -1,3,5-triazine-2,4-diamine-bis(isopropylamino)-6-(methylthio)	C <sub>10</sub> H <sub>19</sub> N <sub>5</sub> S	241.357	119	0.120	4.05 4.10	9.95
Pronamide [23950-58-5]	Kerb, Promamide	3,5-dichloro- <i>N</i> -(1,1-dimethyl-propynyl)-benzamide	C <sub>12</sub> H <sub>11</sub> Cl <sub>2</sub> NO	256.127	155	0.0530		
Propachlor [1918-16-7]	Ramrod	2-chloro- <i>N</i> -(1-methylethyl)- <i>N</i> -phenylacetamide	C <sub>11</sub> H <sub>14</sub> ClNO	211.688	77	0.309		
Propanil [709-98-8]	Propanex, Riselect, Stampede 3E	<i>N</i> -(3,4-dichlorophenyl)-propionamide	C <sub>9</sub> H <sub>9</sub> Cl <sub>2</sub> NO	218.079	92	0.220		
Propazine [139-40-2]	Gesamil, Milogard	2-chloro-4,6-bis(isopropylamino)- <i>s</i> -triazine	C <sub>9</sub> H <sub>16</sub> ClN <sub>5</sub>	229.710	213	0.0143	1.85 1.80	12.15
Propham [122-42-9]	IPC	isopropyl carbanilate	C <sub>10</sub> H <sub>13</sub> NO <sub>2</sub>	179.216	90	0.230		
Pyrazon [1698-60-8]	Chloridazon	5-amino-4-chloro-2-phenyl-3(2 <i>H</i> )-pyridazinone	C <sub>10</sub> H <sub>8</sub> ClON <sub>3</sub>	221.643	205	0.0171		
Simazine [122-34-9]	Gesatop, Weedex, Aquazine	2-chloro-4,6-di(ethylamino)- <i>s</i> -triazine	C <sub>7</sub> H <sub>12</sub> ClN <sub>5</sub>	201.657	226	0.0107	1.65 1.60	12.35
Simetryne [1014-70-6]	Gy-bon	<i>N,N'</i> -diethyl-6-methylthio-1,3,5-triazine-2,4-diyl-diamine	C <sub>8</sub> H <sub>15</sub> N <sub>2</sub> S	171.283	82-83	0.273		11
2,4,5-T [93-76-5]	Gesatop	2,4,5-trichlorophenoxyacetic acid	C <sub>8</sub> H <sub>5</sub> Cl <sub>3</sub> O <sub>3</sub>	255.483	153	0.0555	2.80 2.88	
2,3,6-TBA [50-31-7]	Trysben, Cambilene	2,3,6-trichlorobenzoic acid	C <sub>7</sub> H <sub>3</sub> Cl <sub>3</sub> O <sub>2</sub>	225.457	124.5	0.106		
Terbacil [5902-51-2]	Sinbar	3- <i>tert</i> -butyl-5-chloro-6-methyluracil	C <sub>9</sub> H <sub>13</sub> ClN <sub>2</sub> O <sub>2</sub>	216.664	176	0.0330	9.0	
Terbumeton [33693-04-8]	Caragard	<i>N-tert</i> -butyl- <i>N'</i> -ethyl-6-methoxy-1,3,5-triazine	C <sub>10</sub> H <sub>19</sub> N <sub>5</sub> O	225.290	123-124	0.108		9.41
Terbuthylazine [5915-41-3]	Gardoprim	<i>N-tert</i> -butyl-6-chloro- <i>N'</i> -ethyl-1,3,5-triazine-2,4-diamine	C <sub>9</sub> H <sub>16</sub> ClN <sub>5</sub>	229.710	178	0.0320		12
Terbutryn [886-50-0]	Igran, Clarosan, Prebane	<i>N-tert</i> -butyl- <i>N'</i> -ethyl-6-methyl-thio-1,3,5-triazine-2,4-diamine	C <sub>10</sub> H <sub>19</sub> N <sub>5</sub> S	241.357	104	0.168	4.30 4.07	9.7

Thiobencarb [28249-77-6]	Benthiocarb, Bolero, Saturno	<i>S</i> -4-chlorobenzyl-diethyl-thiocarbamate	C <sub>12</sub> H <sub>16</sub> ClNOS	257.779	1.7	1	
Triallate [2303-17-5]	Avadex BW, Far-Go	<i>S</i> -(2,3,3-trichloro-2-propenyl)- bis(1-methylethyl)carbamothioate	C <sub>10</sub> H <sub>16</sub> Cl <sub>3</sub> NOS	304.664	29	0.914	
Triclopyr [55335-06-3]	Garlon, Truflon, Crossbow	3,5,6-trichloro-2-pyridinyloxyacetic acid	C <sub>7</sub> H <sub>4</sub> Cl <sub>3</sub> NO <sub>3</sub>	256.471	148–150	0.0607	2.68
Trifluralin [1582-09-8]	Treflan, Triflurex, Elancolan	2,6-dinitro- <i>N,N</i> -dipropyl- 4-trifluoromethylaniline	C <sub>13</sub> H <sub>16</sub> F <sub>3</sub> N <sub>3</sub> O <sub>4</sub>	335.279	49	0.581	
Vernolate [1929-77-7]	Surpass, Vernam	<i>S</i> -propyldipropylthiocarbamate	C <sub>10</sub> H <sub>21</sub> NOS	203.345	liquid	1	

Note: F.A.B. – fungicide algicide bactericide; G.R. – growth regulator

pK<sub>a</sub> – acid dissociation constant; pK<sub>b</sub> – basicity constant

(a) ester is quickly converted to parent acid.

\* Assuming ΔS<sub>fus</sub> = 56 J/mol K.

**TABLE 17.2.2**  
**Summary of selected physical-chemical properties of herbicides at 25°C**

Compound	Selected properties						Henry's law constant H/(Pa·m <sup>3</sup> /mol) calcd P/C	log K <sub>OC</sub> reported
	Vapor pressure		Solubility			log K <sub>OW</sub>		
	P <sup>S</sup> /Pa	P <sub>L</sub> /Pa	S/(g/m <sup>3</sup> )	C <sup>S</sup> /(mol/m <sup>3</sup> )	C <sub>L</sub> /(mol/m <sup>3</sup> )			
Alachlor	0.0020	2.88 × 10 <sup>-3</sup>	240	0.890	1.281	2.8	0.0022	2.23
Ametryn	0.0001	3.92 × 10 <sup>-4</sup>	185	0.814	3.191	2.58	1.23 × 10 <sup>-4</sup>	2.59
Amitrole	5.50 × 10 <sup>-7*</sup>	1.14 × 10 <sup>-5</sup>	280000	3330	68850	0.52	1.65 × 10 <sup>-10</sup>	2.04
Atrazine	4.00 × 10 <sup>-5</sup>	1.19 × 10 <sup>-3</sup>	30	0.139	4.140	2.75	2.88 × 10 <sup>-4</sup>	2.00
Barban	5.00 × 10 <sup>-5*</sup>	1.60 × 10 <sup>-4</sup>	11	0.043	0.1362	2.68	1.17 × 10 <sup>-3</sup>	2.66
Benefin	0.0088	0.0226	0.1	0.003	0.0077	5.29	29.4	3.95
Bifenox	3.20 × 10 <sup>-4</sup>	1.25 × 10 <sup>-3</sup>	0.35	0.0010	0.0040	4.48	0.313	
Bromacil	4.00 × 10 <sup>-5</sup>	8.46 × 10 <sup>-4</sup>	815	3.121	66.018	2.11	1.28 × 10 <sup>-5</sup>	1.86
Bromacil lithium salt	4.13 × 10 <sup>-5</sup>							1.51
Bromoxynil	6.40 × 10 <sup>-4</sup>	0.0307	130	0.469	22.54	< 2.0	1.36 × 10 <sup>-3</sup>	
Bromoxynil octanoate	6.40 × 10 <sup>-4</sup>	1.03 × 10 <sup>-3</sup>				5.4		4.25
<i>sec</i> -Bumeton	0.00097	3.98 × 10 <sup>-3</sup>	620	2.756	11.31		3.52 × 10 <sup>-4</sup>	2.30
Butachlor	6.0 × 10 <sup>-4</sup>	6.00 × 10 <sup>-4</sup>	23	0.074	0.074	4.50	8.14 × 10 <sup>-3</sup>	2.8
Butralin	0.0017	3.86 × 10 <sup>-3</sup>	1	0.0034	7.69 × 10 <sup>-3</sup>	4.54	0.502	3.75
Butylate	1.73	1.73	45	0.182	0.182	4.15	8.36	2.60
Chloramben	0.93	51.19	700	3.398	187.05	1.11	0.274	1.32
Chloramben salts	0		900000					1.18
Chlorbromuron	5.33 × 10 <sup>-5</sup>	2.69 × 10 <sup>-4</sup>	50	0.170	0.858		3.13 × 10 <sup>-4</sup>	2.7
Chlorfenac	1	19.75	200	0.835	16.50		1.20	
Chlorpropham	0.001	0.001	89*	0.417	0.600	3.51	2.40 × 10 <sup>-3</sup>	2.85, 2.8
Chlorsufuron	6.13 × 10 <sup>-4*</sup>	0.019	7000	19.56	609.4	-1.0	3.13 × 10 <sup>-5</sup>	1.6
Chlortoluron	1.70 × 10 <sup>-5</sup>	2.80 × 10 <sup>-4</sup>	70	0.329	5.418	2.38	5.17 × 10 <sup>-5</sup>	2.81
Cyanazine	2.13 × 10 <sup>-7</sup>	5.41 × 10 <sup>-6</sup>	171	0.710	18.03	2.22	3.00 × 10 <sup>-7</sup>	2.3
2,4-D	8.0 × 10 <sup>-5*</sup>	1.11 × 10 <sup>-3</sup>	400	1.810	25.12	2.81	4.42 × 10 <sup>-5</sup>	1.68-2.73
2,4-D (a)	0.001	0.0139	890	4.026	55.92	2.81	2.48 × 10 <sup>-4</sup>	
2,4-D DMA salt	0		796000	2991	12000			1.3
2,4-D esters			100					2.00
Dalapon	1.0 × 10 <sup>-5*</sup>	1.0 × 10 <sup>-5</sup>	502000	3510	3510	0.78	2.85 × 10 <sup>-9</sup>	0.48, 2.13
Dalapon sodium salt			900000	5455			0	
2,4-DB	0		46	0.185	1.539	3.53		2.64
2,4-DB butoxyethyl ester	0.00001		8					2.7
2,4-DB DMA salt	0		709000					1.30

Diallate	0.02	0.0224	50*	0.185	0.207	5.23	0.108	2.70
Dicamba	0.0045*	0.0349	4500	20.36	158.1	2.21	$2.21 \times 10^{-4}$	0.342, -0.4
Dicamba salt			400000	1646				0.301
Dichlobenil	0.07*	1.076	18	0.105	1.609	2.74	0.669	2.91
Dichlorophen (F.A.B)	$1.30 \times 10^{-8}$	$4.24 \times 10^{-7}$	30	0.111	3.635		$1.17 \times 10^{-7}$	
Dichloroprop	0.0004	$3.25 \times 10^{-3}$	350	1.489	12.099	3.43	$2.69 \times 10^{-4}$	3.0
Dichloroprop-P	$6.20 \times 10^{-5}$	$5.65 \times 10^{-4}$	590	2.510	22.855	1.95	$2.47 \times 10^{-5}$	2.23
Dichloroprop(2,4-DP)ester	$1.0 \times 10^{-5}$		50	0.149				3.00
Diclofop-methyl	$4.67 \times 10^{-4*}$	$6.57 \times 10^{-4}$	0.8	$2.34 \times 10^{-3}$	$3.30 \times 10^{-3}$	4.58	0.199	4.2
Dinitramine	0.00048	$2.59 \times 10^{-3}$	1	0.0031	0.017	4.30	0.155	3.6
Dinoseb	0.01*	0.0141	50	0.208	0.293	3.56	0.048	2.85
Diphenamid	$4.0 \times 10^{-6*}$	$4.95 \times 10^{-5}$	260	1.087	13.46	1.92	$3.68 \times 10^{-6}$	2.31
Diquat	$1.30 \times 10^{-5}$	0.0170	700000	3800	$4.96 \times 10^6$	-3.05*	$3.42 \times 10^{-9}$	
Diquat dibromide	0		718000	2087				
Diuron	$9.2 \times 10^{-5*}$	$1.9 \times 10^{-3}$	40	0.172	3.630	2.78	$6.83 \times 10^{-4}$	2.6
EPTC	2*	2.0	370	1.954	1.954	3.2	1.023	2.3
Fenopro (H., G.R.)	$1.33 \times 10^{-5*}$	$4.54 \times 10^{-4}$	140	0.519	17.73		$2.56 \times 10^{-5}$	2.48
Fenuron	0.0267	0.305	3800	23.14	264.7	0.98	$1.15 \times 10^{-3}$	1.43
Fenuron-TCA			4800	14.65	38.13			
Fluchloralin	0.004	$6.03 \times 10^{-3}$	1	0.00281	0.0042	4.60*	1.343	3.50
Fluometuron	$6.70 \times 10^{-5}$	$1.61 \times 10^{-3}$	90	0.388	9.292	2.42	$1.73 \times 10^{-4}$	2.24
Fluridone	$1.3 \times 10^{-5}$	$2.5 \times 10^{-4}$	12	0.036	0.7039	2.98	0.357	2.544-3.04
Fluorodifen	$9.5 \times 10^{-6}$	$4.47 \times 10^{-6}$	2	0.0061	0.0293	3.65		3.13
Glyphosate	$4.0 \times 10^{-5*}$	$2.15 \times 10^{-3}$	12000	70.96	3818.4	-1.6	$5.64 \times 10^{-7}$	3.43-3.69
Ioxynil	0.001	0.066	50	0.135	8.904		$7.42 \times 10^{-3}$	
Ioxynil-octanoate	0.0037	$8.21 \times 10^{-3}$						
Isopropalin	0.0019	0.0019	0.11	$3.56 \times 10^{-4}$	$3.56 \times 10^{-4}$	4.71	5.34	4.0
Isoproturon	$3.30 \times 10^{-6}$	$6.52 \times 10^{-5}$	55	0.267	5.266	2.25	$1.24 \times 10^{-5}$	1.86
Linuron	0.023*	$6.74 \times 10^{-2}$	75	0.301	1.449	3.0	$7.54 \times 10^{-2}$	2.91
MCPA (H., G.R.)	0.0002	$1.70 \times 10^{-3}$	1605	8.001	68.05	2.69*	$2.50 \times 10^{-5}$	2.03-2.07
MCPA dimethylamine salt							1.30	
MCPA ester	0.0002		5.0					3.00
MCPA-thioethyl	0.021	0.0309	2.3	0.0094	0.0138		2.234	
MCPB	$5.77 \times 10^{-5*}$	$3.18 \times 10^{-4}$	41	0.179	0.989	3.43	$3.22 \times 10^{-4}$	
MCPB sodium salt	0		200000	798				1.30
Mecoprop	$3.1 \times 10^{-4}$	$1.53 \times 10^{-3}$	620	2.89	14.23	3.94	$7.43 \times 10^{-5}$	
Mecoprop-P	$4.0 \times 10^{-4}$	$1.97 \times 10^{-3}$	860	4.007	19.73		$9.98 \times 10^{-5}$	
Metobromuron	$4.0 \times 10^{-4}$	$2.02 \times 10^{-3}$	330	1.274	6.416	2.41	$3.14 \times 10^{-4}$	

(Continued)

TABLE 17.2.2 (Continued)

Compound	Selected properties					log K <sub>OW</sub>	Henry's law constant H/(Pa·m <sup>3</sup> /mol) calcd P/C	log K <sub>OC</sub> reported
	Vapor pressure		Solubility					
	P <sup>S</sup> /Pa	P <sub>L</sub> /Pa	S/(g/m <sup>3</sup> )	C <sup>S</sup> /(mol/m <sup>3</sup> )	C <sub>L</sub> /(mol/m <sup>3</sup> )			
Metolachlor	0.0042*	4.20 × 10 <sup>-3</sup>	430	1.80	1.80	3.13	2.33 × 10 <sup>-3</sup>	2.26
Metoxuron	0.0043	0.0439	678	2.965	30.26	1.6	1.45 × 10 <sup>-3</sup>	
Molinate	0.75	0.750	970	5.179	5.179	3.21	0.145	1.92
Monolinuron	0.02	0.0732	735	3.425	12.54	2.30	5.84 × 10 <sup>-3</sup>	2.3
Monuron	6.66 × 10 <sup>-5</sup>	2.12 × 10 <sup>-3</sup>	230	1.007	32.08	1.94	6.62 × 10 <sup>-5</sup>	2.00
Neburon			4.8	0.017	0.1031	3.8		3.36
Nitralin	0.2	3.526	0.5	0.0014	0.0255		138.2	
Oryzalin	1.30 × 10 <sup>-6</sup>	1.87 × 10 <sup>-5</sup>	2.4	0.0069	0.0995	3.73	1.88 × 10 <sup>-4</sup>	2.78
Paraquat	< 0.0001		~700000					
Paraquat dichloride salt	0		620000					6.0
Pebulate	1.2*	1.20	92*	0.452	0.452	3.84	2.653	2.63
Pentanochlor			8	0.033	0.134			
Picloram	6.0 × 10 <sup>-5</sup> *	4.98 × 10 <sup>-3</sup>	430	1.781	147.7	0.3	3.37 × 10 <sup>-5</sup>	1.23
Picloram-potassium salt			1430.6				1.20	
Profluralin	0.009	0.0116	0.10	2.88 × 10 <sup>-4</sup>	3.7 × 10 <sup>-4</sup>	6.34	31.35	4.0
Prometon	0.0003	1.38 × 10 <sup>-3</sup>	750	3.329	15.31	2.99	9.01 × 10 <sup>-5</sup>	2.54
Prometryn	0.0001	8.70 × 10 <sup>-4</sup>	48	0.199	1.730	3.51	5.03 × 10 <sup>-4</sup>	2.60
Pronamide	0.011	0.208	15	0.059	1.105	3.26	0.188	2.90
Propachlor	0.03	0.0958	600	2.834	9.055	2.18	0.011	1.90
Propanil	0.005*	0.0230	200	0.917	4.218	3.07	5.45 × 10 <sup>-3</sup>	2.17
Propazine	3.90 × 10 <sup>-6</sup>	2.89 × 10 <sup>-4</sup>	8.6	0.037	2.766	2.90	1.04 × 10 <sup>-3</sup>	2.19
Propham	sublime		250	1.395	5.804	2.60		1.71
Propyzamide	5.80 × 10 <sup>-5</sup>	1.15 × 10 <sup>-3</sup>	15	0.059	1.157	3.28	9.90 × 10 <sup>-4</sup>	2.90
Pyrazon (chloridazon)	7*	441.8	360	1.625	102.5	1.14	4.309	2.08
Simazine	8.50 × 10 <sup>-6</sup>	8.27 × 10 <sup>-4</sup>	5	0.025	2.412	2.18	3.43 × 10 <sup>-4</sup>	2.11
Simetryne	9.47 × 10 <sup>-5</sup>	3.55 × 10 <sup>-4</sup>	450	2.110	7.904		4.49 × 10 <sup>-5</sup>	2.30
2,4,5-T	0.005*	0.0922	220	0.861	15.89	3.13	5.81 × 10 <sup>-3</sup>	1.72
2,3,6-TBA			7700	34.15	340.6	4.34		
Terbacil	5.0 × 10 <sup>-5</sup>	1.56 × 10 <sup>-3</sup>	710	3.277	102.1	1.89	1.53 × 10 <sup>-5</sup>	1.74
Terbumeton	2.70 × 10 <sup>-4</sup>	2.57 × 10 <sup>-3</sup>	130	0.577	5.500	3.04	4.68 × 10 <sup>-4</sup>	
Terbuthylazine	1.50 × 10 <sup>-4</sup>	4.89 × 10 <sup>-3</sup>	8.5	0.037	1.206	3.04	4.05 × 10 <sup>-3</sup>	2.21-2.44
Terbutryn	0.00013*	8.04 × 10 <sup>-4</sup>	22	0.091	0.564	3.74	1.43 × 10 <sup>-3</sup>	2.85
Thiobencarb	2.2	2.20	19.1	0.074	0.0741	3.42	29.69	



Triallate	0.015	0.0164	4	0.013	0.0144	4.29	1.14	3.38
Trifluralin	0.026*	0.0259	0.5*	$1.49 \times 10^{B3}$	$2.57 \times 10^{B3}$	5.34	10.08	4.14
Vernolate	0.90	0.90	90	0.443	0.443	3.84	2.034	2.414

Note: F.A.B. – fungicide algicide bactericide; G.R. – growth regulator, H - herbicide

2,4-D(a) physical-chemical properties modified from values used in Vol. IV.

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

**TABLE 17.2.3****Suggested half-life classes of herbicides in various environmental compartments 25°C**

Compound	Air class	Water class	Soil class	Sediment class
Atrazine	1	8	6	6
2,4-D	2	3	5	6
Dalapon	5	6	6	6
2,4-DB	3	4	4	5
Diallate	2	6	6	7
Dicamba	3	5	5	6
Diuron	2	5	6	7
EPTC	2	4	4	6
Glyphosate	4	6	6	7
Isopropalin	2	5	6	7
Linuron	2	5	6	7
Mecoprop	2	4	4	6
Metolachlor	4	6	6	7
Simazine	3	5	6	7
2,4,5-T	3	5	5	6
Triallate	4	6	4	5
Trifluralin	4	6	6	7

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

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