CHLORDANE 88

## **CHAPTER 4. CHEMICAL AND PHYSICAL INFORMATION**

## 4.1 CHEMICAL IDENTITY

Data pertaining to the chemical identity of chlordane are listed in Table 4-1. Technical chlordane is a mixture of >140 related compounds, 120 of which have been identified by high resolution gas spectroscopy with electron capture, negative ionization mass spectroscopy (Dearth and Hites 1991c). Most of these compounds are minor or trace components. Sixty to 85% of technical chlordane consists of the stereoisomers *cis*- and *trans*-chlordane (Buchert et al. 1989; Worthing and Walker 1987). The ratio of the *cis* and *trans* isomers depends on the manufacturing process (Buchert et al. 1989). *cis*-Chlordane  $(1\alpha,2\alpha,3a\alpha,4\beta,7\beta,7a\alpha)$  is also known as  $\alpha$ -chlordane. *trans*-Chlordane  $(1\alpha,2\beta,3a\alpha,4\beta,7\beta,7a\alpha)$  is commonly known as  $\gamma$ -chlordane, although it is occasionally referred to as  $\beta$ -chlordane (CAS 1992; EPA 1984; Worthing and Walker 1987). This is particularly confusing because  $\gamma$ -chlordane is also the common name of the 2,2,4,5,6,7,8,8-octachloro isomer. This toxicological profile for chlordane uses the names *cis*- and *trans*-chlordane to avoid confusion.

Table 4-1. Chemical Identity of Chlordane				
Characteristic	Information		Reference	
Chemical name	1,2,4,5,6,7,8,8-Octachloro-2,3,3a,4,7,7a-hexahydro-4,7-methano-1H-indene		CAS 1987	
Synonym(s) and registered trade name(s)	1,2,4,5,6,7,8,9-Octachloro-3a,4,7,7a-tetrahydro-4,7-methanoinden; Chlordan; Velsicol 1068®; Octachlor®		Anonymous 1988; CAS 1987	
Chemical formula	C <sub>10</sub> H <sub>6</sub> Cl <sub>8</sub>		CAS 1988	
Chemical structure	trans CI CI H CI	CI CI H CI CI CI H	CAS 1988	
CAS Registry Number	12789-03-6 (technical) 57-74-9 (nonstereospecific) 5103-71-9 ( <i>cis</i> -chlordane or 5103-74-2 ( <i>trans-</i> chlordane or		CAS 1988; Worthing and Walker 1987	

CAS = Chemical Abstracts Service

Other major constituents of technical chlordane are chlordene; heptachlor; *cis*-, and *trans*-nonachlor;  $\alpha$ -,  $\beta$ -, and  $\gamma$ -chlordene; 3a,4,5,5a,6-exo-hexachloro-1a,2,3,3a,5a,5b-hexahydro-1,4-methano-

1H-cyclobuta[cd]pentalene; and 2,4,4,5,6,6,7,8-octachloro-2,3,3a,4,5,7a-hexahydro-1,4-methano-1H-indene (Miyazaki et al. 1985; Parlar et al. 1979).

## 4.2 PHYSICAL AND CHEMICAL PROPERTIES

The physical and chemical properties of chlordane are presented in Table 4-2. The physical and chemical properties of technical chlordane are difficult to specify since there are many components in the technical mixture. For example, technical chlordane is a viscous liquid made of a mixture of many compounds that are solids when pure (a eutectic mixture). The state of the technical product alone will determine the specific properties of the product. For example, the vapor pressure of individual components of chlordane will be lower than that of the technical product because individual components are solids and have crystal lattice energies that reduce their vapor pressures relative to a liquid (Bidleman and Foreman 1987). The vapor pressure of the mixture will also change over time since the more volatile components will be removed faster, changing the composition of the mixture. Compositional changes with time may also result from different rates of degradation and transport among the constituents of the mixture. Additionally, physical properties are not always available for the technical product, which makes comparing properties difficult and increases the uncertainty of any calculated properties. Finally, the overall effect of these differences cannot be evaluated since a complete set of physical properties for the components and technical product is not available.

## 4. CHEMICAL AND PHYSICAL INFORMATION

Colorless	Table 4-2. P	hysical and Chemical Proper	ties of Chlordane
Color         Amber Colorless         Windholz 1983 Hawley 1981           Physical state         Viscous liquid (technical product)         Windholz 1983           Metting point cis-chlordane irans-chlordane irans-chlordane 104-1-5°C         Worthing and Walker 1987           Boiling point 175°C at 2 mmHg         Hawley 1981           Density at 25°C         1.59-1.63 g/cm³         Windholz 1983           Odor         Odorless Mild pungent         Hawley 1981           Odor threshold:         0.0084-0.0419 mg/m³         Ruth 1986           Solubility:³         Water at 25°C         0.056 mg/L for cis:trans (75:25)         Sanborn et al. 1976           Water at 25°C 1.850 mg/Lb         Whetstone 1964; Worthing and Walker 1987           Partition coefficients:         Whetstone 1964; Worthing and Walker 1987           Partition coefficients:         Log Kow 5.54 (estimated for pure chlordane)         EPA 1986b           Log Kow 3.49-4.64° clost for the color of the col	Property	Information	Reference
Colorless	Molecular weight	409.76 (pure chlordane)	Windholz 1983
Meliting point         cis-chlordane         106–107°C         Worthing and Walker 1987           Boiling point         175°C at 2 mmHg         Hawley 1981           Density at 25°C         1.59–1.63 g/cm³         Windholz 1983           Odor         Odorless Milid pungent         Hawley 1981 NRCC 1974           Odor threshold:         0.0084–0.0419 mg/m³         Ruth 1986           Solubility:³         Water at 25°C         0.056 mg/L for cis:trans (75:25) 1.850 mg/L³         Sanborn et al. 1976 Weil et al. 1974           Organic solvents         Miscible with hydrocarbon solvents         Whetstone 1964; Worthing and Walker 1987           Partition coefficients:         Log Kow         5.54 (estimated for pure chlordane)         EPA 1986b           Log Kow         3.49–4.64°         Lyman 1982           Log Koc         3.49–4.64°         Lyman 1982           Cis-chlordane         (supercooled liquid)         2.2x10° mmHg           (cry-stal)°         3.0x10° mmHg         Foreman and Bidleman 1987           trans-chlordane         (supercooled liquid)         2.9x10° mmHg           (crystal)°         3.9x10° mmHg         Suntio et al. 1988           8.31x10° atm-m³/mol         Fendinger et al. 1989           Cotham and Bidleman 1991         Autoignition temperature         No data	Color		
cis-chlordane         106-107°C         Worthing and Walker 1987           Boiling point         175°C at 2 mmHg         Hawley 1981           Density at 25°C         1.59-1.63 g/cm³         Windholz 1983           Odor         Odorless Mild pungent         Hawley 1981 NRCC 1974           Odor threshold:         0.0084-0.0419 mg/m³         Ruth 1986           Solubility:³         Water at 25°C         0.056 mg/L for cis:trans (75:25) Sanborn et al. 1976 Weil et al. 1974           Organic solvents         Miscible with hydrocarbon solvents         Whetstone 1964; Worthing and Walker 1987           Partition coefficients:         Log Kow         5.54 (estimated for pure chlordane)         EPA 1986b           Log Koo         3.49-4.64°         Lyman 1982           Lau et al. 1989         Lau et al. 1989           Vapor pressure: dischlordane         Foreman and Bidleman 1987           Cis-chlordane         (supercooled liquid)         2.2x10-5 mmHg           (crystal)*         3.0x10-6 mmHg           trans-chlordane         4.85x10-6 atm-m³/mol         Suntio et al. 1988           Fendinger et al. 1989         Fendinger et al. 1989           Henry's law constant at 25°C         4.85x10-6 atm-m³/mol (trans-)         Suntio et al. 1988           Fiashpoint         56°C (open cup)         OHM/TADS 1988     <	Physical state	Viscous liquid (technical product)	Windholz 1983
Density at 25°C         1.59–1.63 g/cm³         Windholz 1983           Odor         Odorless Mild pungent         Hawley 1981 NRCC 1974           Odor threshold:         0.0084–0.0419 mg/m³         Ruth 1986           Solubility:³         Ruth 1986           Water at 25°C         0.056 mg/L for cis:trans (75:25) (Meil et al. 1976)           Organic solvents         Miscible with hydrocarbon solvents         Whetstone 1964; Worthing and Walker 1987           Partition coefficients:         Log Kow         5.54 (estimated for pure chlordane)         EPA 1986b           Log Koc         3.49–4.64°         Lyman 1982         Lau et al. 1989           Vapor pressure: <sup>d</sup> cis-chlordane (supercooled liquid) (crystal)°         2.2x10-5 mmHg         Foreman and Bidleman 1987           cis-chlordane (supercooled liquid) (crystal)°         2.9x10-5 mmHg         Suntio et al. 1988           Henry's law constant at 25°C         4.85x10-5 atm-m³/mol b (trans-) (trans-) (cotham and Bidleman 1991         Suntio et al. 1988 (Cotham and Bidleman 1991           Autoignition temperature         No data         No data           Flammability limits         No data         HSDB 1988           Conversion factors         1 ppm (v/v) = 16.75 mg/m³ in air 1 mg/m³ = 0.0597 ppm (v/v) in air         HSDB 1988			
Odor         Odorless Mild pungent         Hawley 1981 NRCC 1974           Odor threshold:         0.0084–0.0419 mg/m³         Ruth 1986           Solubility:³         Ruth 1986           Water at 25°C         0.056 mg/L for cis:trans (75:25)         Sanborn et al. 1976 Weil et al. 1974           Organic solvents         Miscible with hydrocarbon solvents         Whetstone 1964; Worthing and Walker 1987           Partition coefficients:         Log Kow         5.54 (estimated for pure chlordane)         EPA 1986b           Log Koc         3.49–4.64°         Lyman 1982           Log Koc         3.49–4.64°         Lyman 1982           Lau et al. 1989         Lau et al. 1989           Vapor pressure: <sup>d</sup> cis-chlordane (supercooled liquid) (crystal)°         2.2x10-5 mmHg         Foreman and Bidleman 1987           cis-chlordane (supercooled liquid) (crystal)°         2.9x10-5 mmHg         Suntio et al. 1988           trans-chlordane (supercooled liquid) (crystal)°         2.9x10-5 mmHg         Suntio et al. 1988           Henry's law constant at 25°C         4.85x10-5 atm-m³/mol (trans-) 4.8x10-5 atm-m³/mol (trans-) 4.8x10-5 atm-m³/mol (trans-)         Cotham and Bidleman 1991           Autoignition temperature         No data           Flammability limits         No data           Conversion factors         1 ppm (v/v) = 16.75 mg/m³ in air 1 mg/m³ = 0.0597 ppm (	Boiling point	<del>_</del>	
Mild pungent         NRCC 1974           Odor threshold:         0.0084–0.0419 mg/m³         Ruth 1986           Solubility:³         Water at 25°C         0.056 mg/L for cis:trans (75:25)	·		Windholz 1983
Solubility:a   Water at 25°C   0.056 mg/L for <i>cis:trans</i> (75:25)   Sanborn et al. 1976   Weil et al. 1974   Weil et al. 1987   Weil et al. 1987   Partition coefficients:  Log Kow   5.54 (estimated for pure chlordane)   EPA 1986b   Lyman 1982   Lau et al. 1989   EPA 1986b   Lyman 1982   Lau et al. 1989   EPA 1986b   Lyman 1982   Lau et al. 1989   EPA 1986b   Lyman 1987   EPA 1986b   Lyman 1982   Lau et al. 1989   EPA 1986b   EPA 1986b   Lyman 1987   EPA 1986b   Lyman 1982   Lau et al. 1989   EPA 1986b   EPA 1986b	Odor		
Water at 25°C         0.056 mg/L for cis:trans (75:25)         Sanborn et al. 1976           Organic solvents         Miscible with hydrocarbon solvents         Whetstone 1964; Worthing and Walker 1987           Partition coefficients:         User the partition of the partiti	Odor threshold:	0.0084–0.0419 mg/m <sup>3</sup>	Ruth 1986
Organic solvents       1.850 mg/Lb       Weil et al. 1974         Organic solvents       Miscible with hydrocarbon solvents       Whetstone 1964; Worthing and Walker 1987         Partition coefficients:       Log K₀w       5.54 (estimated for pure chlordane)       EPA 1986b         Log K₀c       3.49–4.64°       Lyman 1982         Lau et al. 1989       Lau et al. 1989         Vapor pressure:d cis-chlordane       Foreman and Bidleman 1987         (supercooled liquid)       2.2x10-5 mmHg         (crystal)e       3.0x10-6 mmHg         trans-chlordane       2.9x10-5 mmHg         (supercooled liquid)       2.9x10-5 mmHg         (crystal)e       3.9x10-6 mmHg         Henry's law constant at 25°C       4.85x10-5 atm-m³/mol (trans-) 4.8x10-5 atm-m³/mol (trans-) 4.8x10-5 atm-m³/mol (trans-) 4.8x10-5 atm-m³/mol       Suntio et al. 1988 Fendinger et al. 1989 Cotham and Bidleman 1991         Autoignition temperature       No data         Flashpoint       56°C (open cup)       OHM/TADS 1988         Flammability limits       No data         Conversion factors       1 ppm (v/v) = 16.75 mg/m³ in air 1 mg/m³ = 0.0597 ppm (v/v) in air       HSDB 1988	Solubility: <sup>a</sup>		
Partition coefficients:  Log K₀w  Log K₀c  3.49–4.64°  6.3 (trans-) suspended solids  Vapor pressure:d  (supercooled liquid) (crystal)e  trans-chlordane (supercooled liquid) (crystal)e  (supercooled liquid) (crystal)e  trans-chlordane (supercooled liquid) (crystal)e  3.9x10-5 mmHg  trans-chlordane (supercooled liquid) (crystal)e  3.9x10-5 atm-m³/mol (trans-) 4.8x10-5 atm-m³/mol (trans-) 4.8x10-5 atm-m³/mol Cotham and Bidleman 1991  Autoignition temperature  No data  Flashpoint  56°C (open cup)  OHM/TADS 1988  Flammability limits  No data  Conversion factors  1 ppm (v/v) = 16.75 mg/m³ in air 1 mg/m³ = 0.0597 ppm (v/v) in air  HSDB 1988	Water at 25°C		
Log K₀w         5.54 (estimated for pure chlordane)         EPA 1986b           Log K₀c         3.49–4.64°         Lyman 1982           6.3 (trans-) suspended solids         Lau et al. 1989           Vapor pressure:dosic-chlordane (supercooled liquid) (crystal)es         2.2x10-5 mmHg           (supercooled liquid) (crystal)es         3.0x10-6 mmHg           Henry's law constant at 25°C (supercooled liquid) (crystal)es         2.9x10-5 mmHg           Henry's law constant at 25°C (supercooled liquid) (crystal)es         3.9x10-6 mmHg           Henry's law constant at 25°C (supercooled liquid) (crystal)es         4.85x10-5 atm-m³/mol (trans-) Fendinger et al. 1988 Fendinger et al. 1989 Cotham and Bidleman 1991           Autoignition temperature         No data           Flashpoint         56°C (open cup)         OHM/TADS 1988           Flammability limits         No data           Conversion factors         1 ppm (v/v) = 16.75 mg/m³ in air mg/m³ = 0.0597 ppm (v/v) in air         HSDB 1988	Organic solvents	Miscible with hydrocarbon solvents	
Log K₀c         3.49–4.64° (6.3 (trans-) suspended solids         Lyman 1982 Lau et al. 1989           Vapor pressure:d cis-chlordane (supercooled liquid) (crystal)e (supercooled liquid) (sup	Partition coefficients:		
Vapor pressure:d	Log Kow	5.54 (estimated for pure chlordane)	EPA 1986b
cis-chlordane(supercooled liquid) $2.2x10^{-5}$ mmHg(crystal)e $3.0x10^{-6}$ mmHg $trans$ -chlordane $2.9x10^{-5}$ mmHg(supercooled liquid) $2.9x10^{-5}$ mmHg(crystal)e $3.9x10^{-6}$ mmHgHenry's law constant at $25^{\circ}$ C $4.85x10^{-5}$ atm-m³/mol $(trans$ -) $4.8x10^{-5}$ atm-m³/mol $(trans$ -) $4.8x10^{-5}$ atm-m³/molSuntio et al. 1988 Fendinger et al. 1989 Cotham and Bidleman 1991Autoignition temperatureNo dataFlashpoint $56^{\circ}$ C (open cup)OHM/TADS 1988Flammability limitsNo dataConversion factors1 ppm (v/v) = 16.75 mg/m³ in air 1 mg/m³ = 0.0597 ppm (v/v) in airHSDB 1988	Log K <sub>oc</sub>		•
(crystal)e trans-chlordane (supercooled liquid) (crystal)e $2.9 \times 10^{-6}$ mmHgHenry's law constant at $25^{\circ}$ C $4.85 \times 10^{-6}$ atm-m³/mol b $8.31 \times 10^{-5}$ atm-m³/mol (trans-) $4.8 \times 10^{-5}$ atm-m³/molSuntio et al. 1988 Fendinger et al. 1989 Cotham and Bidleman 1991Autoignition temperatureNo dataFlashpoint $56^{\circ}$ C (open cup)OHM/TADS 1988Flammability limitsNo dataConversion factors1 ppm (v/v) = 16.75 mg/m³ in air 1 mg/m³ = 0.0597 ppm (v/v) in airHSDB 1988	Vapor pressure:d cis-chlordane		Foreman and Bidleman 1987
(supercooled liquid) (crystal)e $2.9 \times 10^{-5}$ mmHgHenry's law constant at 25°C $4.85 \times 10^{-5}$ atm-m³/mol b $8.31 \times 10^{-5}$ atm-m³/mol (trans-) $4.8 \times 10^{-5}$ atm-m³/molSuntio et al. 1988 Fendinger et al. 1989 Cotham and Bidleman 1991Autoignition temperatureNo dataFlashpoint $56$ °C (open cup)OHM/TADS 1988Flammability limitsNo dataConversion factors $1 \text{ ppm (v/v)} = 16.75 \text{ mg/m³ in air} \\ 1 \text{ mg/m³} = 0.0597 \text{ ppm (v/v) in air}$ HSDB 1988	(crystal) <sup>e</sup>		
$8.31 \times 10^{-5} \text{ atm-m}^3/\text{mol } (\textit{trans-}) \\ 4.8 \times 10^{-5} \text{ atm-m}^3/\text{mol} & \text{Cotham and Bidleman 1991}$ Autoignition temperature No data	(supercooled liquid)		
Flashpoint 56°C (open cup) OHM/TADS 1988  Flammability limits No data  Conversion factors 1 ppm (v/v) = 16.75 mg/m³ in air HSDB 1988 1 mg/m³ = 0.0597 ppm (v/v) in air	Henry's law constant at 25°C	8.31x10 <sup>-5</sup> atm-m <sup>3</sup> /mol ( <i>trans-</i> )	Fendinger et al. 1989
Flammability limits  No data  Conversion factors  1 ppm $(v/v) = 16.75 \text{ mg/m}^3 \text{ in air}$ HSDB 1988  1 mg/m³ = 0.0597 ppm $(v/v)$ in air	Autoignition temperature	No data	
Conversion factors 1 ppm (v/v) = 16.75 mg/m <sup>3</sup> in air HSDB 1988 1 mg/m <sup>3</sup> = 0.0597 ppm (v/v) in air	Flashpoint	56°C (open cup)	OHM/TADS 1988
1 mg/m³ = 0.0597 ppm (v/v) in air	Flammability limits	No data	
Explosive limits No data	Conversion factors	11 \ /	HSDB 1988
	Explosive limits	No data	

<sup>&</sup>lt;sup>a</sup>The solubility of the components of technical chlordane may differ from the solubility of the technical product. <sup>b</sup>Study did not specify whether test substance was technical grade or a mixture.

<sup>&</sup>lt;sup>c</sup>Estimated for pure chlordane using Equations 4-5 and 4-8 in Lyman (1982).

<sup>&</sup>lt;sup>d</sup>Vapor pressure for technical chlordane may differ from that of individual components of technical chlordane.

<sup>&</sup>lt;sup>e</sup>Calculated from the supercooled value.