

4. CHEMICAL AND PHYSICAL INFORMATION

4.1 CHEMICAL IDENTITY

Information regarding the chemical identity of heptachlor and heptachlor epoxide is located in Table 4-1.

4.2 PHYSICAL AND CHEMICAL PROPERTIES

Information regarding the physical and chemical properties of heptachlor and heptachlor epoxide is located in Table 4-2.

4. CHEMICAL AND PHYSICAL INFORMATION

Table 4-1. Chemical Identity of Heptachlor and Heptachlor Epoxide^a

Characteristic	Heptachlor	Heptachlor epoxide
Synonym(s)	3-Chlorochlordene; 1,4,5,6,7,8,8a-hepta- chloro-3a,4,7,7a-tetrahydro- 4,7-methanoindene; 1,4,5,6,7,8,8-heptachloro- 3A,4,5,5a tetrahydro; alpha- dicyclopentadiene, 3,4,5,6,8,8a heptachloro, and others	Epoxyheptachlor; 1,4,5,6,7,8,8a-hepta- chloro-2,3-epoxy-3a,4,7,7a-tetra- hydro-4,7-methanoindene; 4,7-methanoindan, 1,4,5,6,7,8, 8-heptachloro-2,3-epoxy- 3a,4,7,7a-tetrahydro-; 2,5-methano-2h-indeno (1,2-b)oxirene, 2,3,4,5,6,7, 7-heptachloro-1a,1b, 5,5a,6,6a-hexahydro-, (1aalpha,1bbeta,2alpha,5alpha, 5abeta,6beta,6aalpha)-
Registered trade name(s)	Basaklor; Gold Crest H-60; Termide; Heptagran; Heptagranox; Heptamak; Heptamul; Soleptax; Velsicol 104	Velsicol 53-CS-17
Chemical formula	C ₁₀ H ₅ Cl ₇	C ₁₀ H ₅ Cl ₇ O
Chemical structure		
Identification numbers:		
CAS registry	76-44-8	1024-57-3
NIOSH RTECS	PC0700000	
EPA hazardous waste	P059	D031
OHM/TADS	7216526	833300216
DOT/UN/NA/IMDG shipping	UN 2761, UN2782, UN 2995, UN2996, IMO 3.0, IMO 6.1	UN 2761, UN2782, UN 2995, UN2996, IMO 3.0, IMO 6.1
HSDB	554	6182
NCI	C00180	

^aAll information obtained from HSDB 2007a for heptachlor or HSDB 2007b for heptachlor epoxide unless otherwise noted.

CAS = Chemical Abstracts Services; DOT/UN/NA/IMDG = Department of Transportation/United Nations/North America/International Maritime Dangerous Goods Code; EPA = Environmental Protection Agency; HSDB = Hazardous Substances Data Bank; NCI = National Cancer Institute; NIOSH = National Institute for Occupational Safety and Health; OHM/TADS = Oil and Hazardous Materials/Technical Assistance Data System; RTECS = Registry of Toxic Effects of Chemical Substances

4. CHEMICAL AND PHYSICAL INFORMATION

Table 4-2. Physical and Chemical Properties of Heptachlor and Heptachlor Epoxide^a

Property	Heptachlor	Heptachlor epoxide
Molecular weight	373.32	389.40
Color	White (pure); tan (technical grade) ^b	White ^b
Physical state	Crystalline solid	Crystalline solid ^b
Melting point	95–96 °C (pure); 46–74 °C (technical grade) ^c	160–161.5 °C
Boiling point	145 °C	No data
Specific Gravity:		
at 9 °C	1.57	No data
Odor	Camphor-like	No data
Odor threshold:		
Water	No data	No data
Air	0.3 mg/m ³	0.3 mg/m ³
Solubility:		
Water at 25 °C	0.05 mg/L ^d	0.275 mg/L ^d
Organic solvent(s)	Soluble in most organic solvents	Soluble in most organic solvents ^b
Partition coefficients:		
Log K _{ow}	6.10	5.40
Log K _{oc}	4.34 ^e	3.34–4.37 ^f
Vapor pressure		
	3x10 ⁻⁴ mmHg ^g at 20 °C	1.95x10 ⁻⁵ mmHg at 30 °C ^h
	3x10 ⁻⁴ mmHg at 25 °C	No data
Henry's law constant:		
at 25 °C	2.94x10 ⁻⁴ atm-m ³ /mol	3.2x10 ⁻⁵ atm-m ³ /mol
Autoignition temperature	No data	No data
Flashpoint	No data	No data
Flammability limits	Highly flammable	Non-combustible
Conversion factors	1 ppm=15.27 mg/m ³ at 25 °C, 1 atm	1 ppm=15.93 mg/m ³ at 25 °C, 1 atm
Explosive limits	Non-combustible	Containers may explode when heated

^aAll information obtained from HSDB 2007a for heptachlor or HSDB 2007b for heptachlor epoxide unless otherwise noted

^bIARC 1974

^cWorthing and Walker 1987

^dEPA 1987

^eChapman 1989

^fEstimated from Lyman et al. 1982

^gACGIH 1986

^hNash 1983