3. CHEMICAL AND PHYSICAL INFORMATION

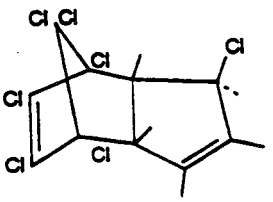
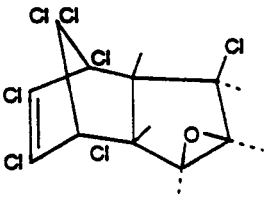
3.1 CHEMICAL IDENTITY

Information regarding the chemical identities of heptachlor and heptachlor epoxide is located in Table 3-l.

3.2 PHYSICAL AND CHEMICAL PROPERTIES

Information regarding the physical and chemical properties of heptachlor and heptachlor epoxide is located in Table 3-2.

TABLE 3-1. Chemical Identity of Heptachlor and Heptachlor Epoxide[a]

Characteristic	Heptachlor	Heptachlor epoxide
Chemical name	Heptachlor	Heptachlor epoxide
Synonym(s)	2-Chlorochlordene; 1,4,5,6,7,8,8a-heptachloro-3a,4,7,7a-tetrahydro-4,7-methanoindene; 1,4,5,6,6a-heptachloro-dicyclopentadiene; and others	Epoxyheptachlor; 1,4,5,6,7,8,8a-hepta-chloro-2,3-epoxy-3a,4,7,7a-tetra-hydro-4,7-methanoindene
Registered trade name(s)	Heptagran; Heptamul; Heptagranox; Heptamak; Basaklor; Drinox[b]; Soleptax; Gold Crest H-60; Termide; Velsicol 104	Velsicol 53-CS-17
Chemical formula	$C_{10}H_5Cl_7$	$C_{10}H_5Cl_7O$
Chemical structure		
Identification numbers:		
CAS registry	76-44-8	1024-57-3
NIOSH RTECS	PC0700000	PB9450000[c]
EPA hazardous waste	P059	No data
OHM/TADS	7216526	833300216
DOT/UN/NA/IMCO shipping	NA 2761	No data
HSDB	554	6182
NCI	C00180	

[a]All information obtained from HSDB 1990a for heptachlor or 1990b for heptachlor epoxide unless otherwise noted.
[b]OHM/TADS 1985a
[c]OHM/TADS 1985b

CAS = Chemical Abstracts Services; DOT/UN/NA/IMCO = 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

TABLE 3-2. Physical and Chemical Properties of Heptachlor and Heptachlor Epoxide[a]

Property	Heptachlor	Heptachlor epoxide
Molecular weight	373.35	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
Density:		
at 9°C	1.57 g/cm^3	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}	5.44[e]	5.40[f]
Log K_{oc}	4.34[e]	3.34–4.37[g]
Vapor pressure		
at 20°C	3x10^{-4} mmHg[h]	2.6x10^{-6} mmHg[i]
at 25°C	3x10^{-4} mmHg	No data
Henry's law constant:		
at 25°C	1.48x10^{-3} atm-m^3/mol[d]	3.2x10^{-5} atm-m^3/mol[d]
Autoignition temperature	No data	No data
Flashpoint	No data	No data
Flammability limits	Noncombustible but may be dissolved in flammable liquids	No data
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	Stable[j]	Stable[i]

[a]All information obtained from HSDB 1990a for heptachlor or 1990b for heptachlor epoxide unless otherwise noted
[b]IARC 1974
[c]Worthing and Walker 1987
[d]EPA 1987a
[e]Chapman 1989
[f]MacKay 1982
[g]Estimated from Lyman et al. 1982
[h]ACGIH 1986
[i]OHM/TADS 1985b
[j]OHM/TADS 1985a