3. CHEMICAL AND PHYSICAL INFORMATION

3.1 CHEMICAL IDENTITY

Information regarding the chemical identity of endrin, endrin aldehyde, and endrin ketone is located in Table 3-l.

3.2 PHYSICAL AND CHEMICAL PROPERTIES

Information regarding the physical and chemical properties of endrin, endrin aldehyde, and endrin ketone is located in Table 3-2.

Table 3-1. Chemical Identity of Endrin, Endrin Aldehyde, and Endrin Ketone

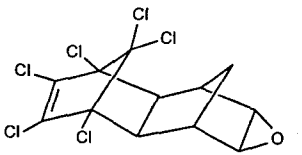
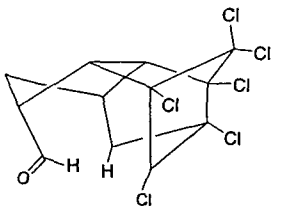
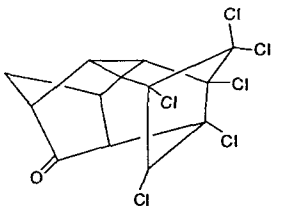
Characteristic	Endrin	Endrin Aldehyde	Endrin Ketone	Reference
Chemical name	2,7:3,6-Dimethanonapth(2,3-b)oxirene, 3,4,5,6,9,9-hexachloro-1a,2,2a,3,6,6a,7,7a-octahydro-, (1aα,2β,2aβ,3α,6α,6aβ,7β,7aα)-	1,2,4-Methenocyclopenta(cd)-pentalene-5-carboxaldehyde, 2,2a,3,3,4,7-hexachlorodeca-hydro-(1α,2β,2aβ,4β,4a β,5β,6aβ,6bβ,7R*)	2,5,7-Metheno-3H-cyclo-penta(a)pentalen-3-one,3b,4,5,6,6a-hexachlorodecahydro-(2α,3aβ,3bβ,4β,5β,6aβ,7α,7aβ,8R*)	EPA 1984a
Synonym(s)	Endrin; 1,2,3,4,10,10-hexachloro-6,7-epoxy-1,4,4A,5,6,7,8,8A- octahydro-endo, endo-1,4:5,8-dimethanonaphthalene, and others	Endrin aldehyde; 1,2,4-methanecyclopenta(c,d) pentalene-5-carboxaldehyde, 2,2a,3,3,4,7-hexachloro-decahydro	Endrin ketone	HSDB 1995
Registered trade name(s)	Mendrin, Hexadrin, Endrex experimental insecticide 269	No data	Delta-keto 153	NLM 1988 Sittig 1980
Chemical formula	$C_{12}H_8Cl_6O$	$C_{12}H_8Cl_6O$	$C_{12}H_8Cl_6O$	EPA 1984a
Chemical structure				EPA 1984a

Table 3-1. Chemical Identity of Endrin, Endrin Aldehyde, and Endrin Ketone (continued)

Characteristic	Endrin	Endrin Aldehyde	Endrin Ketone	Reference
Identification numbers:				
CAS registry	72-20-8	7421-93-4	53494-70-5	EPA 1984a
NIOSH RTECS	IO1575000	PC8580000	PC8600000	RTECS1994
EPA hazardous waste	P051; D012	No data	No data	HSDB 1994
OHM/TADS	7216522	8300215	No data	HSDB 1994
DOT/UN/NA/IMCO ship.	UN 2761; NA 2761; IMO 6.1	UN 2761; IMO 6.1	UN 2811; NA 2761; IMO 6.1	HSDB 1994, 1995
	198	6181	No data	HSDB 1995
HSDB	01565	No data	No data	HSDB 1994
NCI	C00157			

CAS = Chemical Abstracts Service; DOT/UN/NA/IMCO = Dept. 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 Endrin, Endrin Aldehyde, and Endrin Ketone

Characteristic	Endrin	Endrin Aldehyde	Endrin Ketone	Reference
Molecular weight	380.9	381.9	380.9	EPA 1984a
Color	White Colorless	No data	No data	HSDB 1995; IARC 1974 Worthington and Walker 1983
Physical state	Crystalline solid	Solid	Solid	EPA 1984a; HSDB 1995; IARC 1974
Melting point	235 °C 226–230 °C (decomp.)	145–149 °C, 235 °C (decomp.)	No data	EPA 1981a; HSDB 1995 Worthington and Walker 1983
Boiling point	Decomposes at 245 °C Decomposes above 200 °C	No data	No data	ACGIH 1986 HSDB 1995 IARC 1974
Density at 20 °C	No data	No data	No data	
Specific Gravity	1.7 at 20 °C	No data	No data	EPA 1980a, HSDB 1995
Odor	Mild; odorless	No data	No data	HSDB 1995
Odor threshold:				
Water	0.041 mg/L	No data	No data	Verschueren 1983
Air	1.8 x 10^{-2} ppm	No data	No data	Fazzalari, 1978
Solubility:				
Water at 25 °C	200 µg/L	50 mg/L, 0.25–0.26 ppm	No data	EPA 1981a
Organic solvents	acetone 17 g/100 mL benzene 13.8 g/100 mL carbon tet. 3.3 g/100 mL hexane 7.1 g/100 mL xylene 18.3 g/100 mL	No data	No data	HSDB 1995 Merck 1989

Table 3-2. Physical and Chemical Properties of Endrin, Endrin Aldehyde, and Endrin Ketone (continued)

Characteristic	Endrin	Endrin Aldehyde	Endrin Ketone	Reference
Partition coefficients:				
Log K_{ow}	5.6, 5.34 (calculated) 5.45 (calculated)	3.146, 4.7, 5.6 (calculated)	4.99 (calculated)	EPA 1981a, HSDB 1995
Log K_{oc}	4.532 (calculated) 5.195 (±0.005)	4.80 (calculated) 3.929–4.653 (calculated)	No data	SRC 1995 HSDB 1995, Kenaga 1980 de Bruijn et al. 1989
Vapor pressure at 25 °C	2.0×10^{-7} mm Hg	2.0×10^{-7} mm Hg	No data	EPA 1981a HSDB 1995 Worthington and Walker 1983
Henry's law constant	4.0×10^{-7} atm-m^3/mol (calculated) 5.41×10^{-7} atm-m^3/mol (calculated)	2×10^{-9} atm-m^3/mol 2.9×10^{-9} atm-m^3/mol 3.67×10^{-8} atm-m^3/mol (calculated)	2.02×10^{-8} atm-m^3/mol (calculated)	EPA 1981a,HSDB 1995 Thomas 1982 SRC 1994a
Autoignition temperature	No data	No data	No data	
Flashpoint	Non-flammable	Non-flammable	No data	HSDB 1995
Flammability limits	No data	No data	No data	
Explosive limits	No data	No data	No data	
Conversion factors	1 ppm = 15.6 mg/m^3 1 mg/m^3 = 0.06 ppm	1 ppm = 15.6 mg/m^3 1 mg/m^3 = 0.06 ppm	1 ppm = 15.6 mg/m^3 1 mg/m^3 = 0.06 ppm	

ACGIH = American Conference of Governmental and Industrial Hygienists; HSDB = Hazardous Substance Data Bank; SRC = Syracuse Research Corporation