CHAPTER 4. CHEMICAL AND PHYSICAL INFORMATION

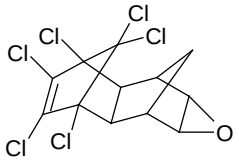
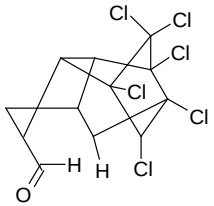
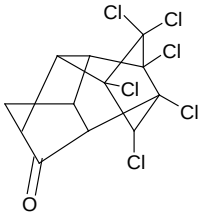
4.1 CHEMICAL IDENTITY

Information regarding the chemical identity of endrin, endrin aldehyde, and endrin ketone is located in Table 4-1.

4.2 PHYSICAL AND CHEMICAL PROPERTIES

Information regarding the physical and chemical properties of endrin, endrin aldehyde, and endrin ketone is located in Table 4-2.

Table 4-1. Chemical Identity of Endrin, Endrin Aldehyde, and Endrin Ketone

Characteristic	Endrin	Endrin aldehyde	Endrin ketone	Reference
Chemical name	2,7:3,6-Dimethanonaphth(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)-entalene-5-carboxaldehyde, 2,2a,3,3,4,7-hexachlorodecahydro- (1α,2β,2aβ,4β,4aβ,5β,6aβ,6bβ,7R*)	2,5,7-Metheno-3H-cyclopenta(a)entalen-3-one,3b,4,5,6,6a-hexachlorodecahydro-(2α,3aβ,3bβ,4β,5β,6aβ, 7α,7aβ,8R*)	EPA 1984b
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-hexachlorodecahydro	Endrin ketone	NLM 2020
Registered trade name(s)	*Mendrin, Hexacrin, Endrex* experimental insecticide 269	No data	Delta-keto 153	NLM 2020; Sittig 1980
Chemical formula	$C_{12}H_8Cl_6O$	$C_{12}H_8Cl_6O$	$C_{12}H_8Cl_6O$	EPA 1984b
Chemical structure				EPA 1984b
CAS registry	72-20-8	7421-93-4	53494-70-5	EPA 1984b

CAS = Chemical Abstracts Services

Table 4-2. Physical and Chemical Properties of Endrin, Endrin Aldehyde, and Endrin Ketone

Property	Endrin	Endrin aldehyde	Endrin ketone	Reference
Molecular weight	380.9	381.9	380.9	EPA 1984b
Color	White, colorless	No data	No data	IARC 1974; NLM 2020; Worthing and Walker 1983
Physical state	Crystalline solid	Solid	Solid	EPA 1984b; IARC 1974; NLM 2020
Melting point	235°C; 226–230°C (decomposes)	145–149°C; 235°C (decomposes)	No data	EPA 1981; NLM 2020; Worthing and Walker 1983
Boiling point	Decomposes at 246°C; decomposes above 200°C	No data	No data	ACGIH 1986; IARC 1974; NLM 2020
Density at 20°C	No data	No data	No data	
Odor	1.7 at 20°C	No data	No data	EPA 1980; NLM 2020
Odor threshold:				
Water	0.041 mg/L			Verschueren 1983
Air	$1.8x10^{-2}$ ppm	No data	No data	Fazzalari 1978
Solubility:				
Water	200 µg/L at 20°C	50 mg/L; 0.25–0.26 ppm	No data	EPA 1981
Organic solvents	Acetone:17 g/100 mL; benzene 13.8 g/100 mL; carbon tetrachloride: 3.3 g/100 mg/L; hexane: 7.1 g/100 mL; xylene: 18.3 g/100 mL	No data	No data	Budavari 1989; NLM 2020
Partition coefficients:				
Log K_{ow}	5.6, 5.34 (calculated), 5.45 (calculated)	3.146, 4.7, 5.6 (calculated)	4.99 (calculated)	EPA 1981, 1995a; NLM 2020
K_{oc}	4.532 (calculated); 5.195 (±0.005)	4.80 (calculated); 3.929–4.653 (calculated)	No data	De Bruijin et al. 1989; Kenaga 1980; NLM 2020
Vapor pressure	$2.0x10^{-7}$ mmHg	$2.0x10^{-7}$ mmHg	No data	EPA 1981; NLM 2020; Worthing and Walker 1983

Table 4-2. Physical and Chemical Properties of Endrin, Endrin Aldehyde, and Endrin Ketone

Property	Endrin	Endrin aldehyde	Endrin ketone	Reference
Henry's law constant	$4.0x10^{-7}$ atm-m^3/mol (calculated); $5.4x10^{-7}$ atm-m^3/mol (calculated)	$2x10^{-9}$ atm-m^3/mol; $2.9x10^{-9}$ atm-m^3/mol; $3.67x10^{-8}$ atm-m^3/mol (calculated)	$2.02x10^{-8}$ atm-m^3/mol	EPA 1981; NLM 2020; EPA 1994; Thomas 1982
Autoignition temperature	No data	No data	No data	
Flashpoint	Non-flammable	Non-flammable	No data	NLM 2020
Flammability 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	
Explosive limits	No data	No data	No data	