4. CHEMICAL AND PHYSICAL INFORMATION

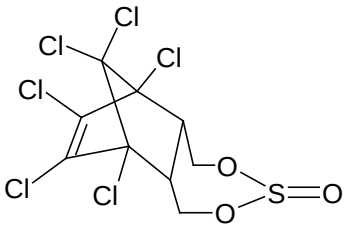
4.1 CHEMICAL IDENTITY

Technical-grade endosulfan contains at least 94% of two pure isomers, α- and β-endosulfan. The α- and β-isomers of endosulfan are present in the ratio of 7:3, respectively (FAO 2011a; Müller et al. 2009). Endosulfan sulfate is a reaction product found in technical endosulfan; it is also found in the environment due to oxidation by biotransformation (Dureja and Mukerjee 1982). The chemical formula, structure, synonyms, and identification numbers for endosulfan, α-endosulfan, β-endosulfan, and endosulfan sulfate are listed in Tables 4-1, 4-2, 4-3, and 4-4, respectively.

4.2 PHYSICAL AND CHEMICAL PROPERTIES

Important physical and chemical properties of endosulfan, α-endosulfan, β-endosulfan, and endosulfan sulfate are listed in Tables 4-5, 4-6, 4-7, and 4-8, respectively. It should be noted that β-endosulfan is slowly converted to α-endosulfan (Hapeman et al. 1997; Rice et al. 1997).

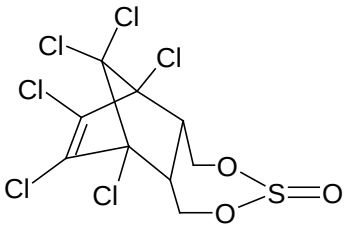
Table 4-1. Chemical Identity of Endosulfan

Characteristic	Information[a]
Chemical name	Endosulfan
Synonym(s)	6,7,8,9,10,10-Hexachloro-1,5,5a,6,9,9a-hexahydro-6,9-methano-2,4,3-benzodioxathiepin-3-oxide; Endosulfan technical; 5-Norbornene-2,3-dimethanol-1,4,5,6,7,7-hexachlorocyclic sulfit
Registered trade name(s)	Thiodan; Thionex; Thionate Malix; HOE 2671; FMC 5462; Cyclodan; Thifor; Beosit; Chlorthiepin; Endosulphan[b]
Chemical formula	$C_9H_6Cl_6O_3S$[c]
Chemical structure[e]	
Identification numbers:	
CAS registry	115-29-7[c]
NIOSH RTECS	RB9275000[c]
EPA hazardous waste	P050
OHM/TADS	7216559
DOT/UN/NA/IMDG shipping	2761[c]
HSDB	390
NCI	C00566

[a]All information obtained from HSDB 2010, except where noted.
[b]HSDB 2010; O'Neil et al. 2006
[c]NIOSH 2015

CAS = Chemical Abstracts Service; 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

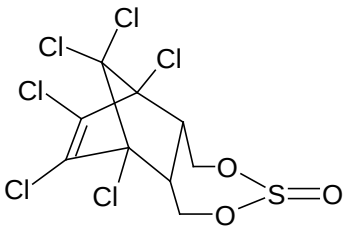
Table 4-2. Chemical Identity of α-Endosulfan

Characteristic	Information
Chemical name	α-Endosulfan[a]
Synonym(s)	Endosulfan I; Endosulfan A; 6,9-Methano-2,4,3-benzodioxathiepin, 6,7,8,9,10,10-hexachloro-1,5,5a,6,9,9a-hexahydro-, 3-oxide (3α, 5a β, 6α, 9a α, 9β)-; 5-Norbornene-2,3-dimethanol, 1,4,5,6,7,7-hexachloro-, cyclic sulfite, endo-[b]
Registered trade name(s)	α-Benzoepin; α-Thiodan; β-Thionex[c]
Chemical formula	$C_9H_6Cl_6O_3S$[b]
Chemical structure[e]	
Identification numbers:	
CAS registry	959-98-8[a]
NIOSH RTECS	RB9275100[c]
EPA hazardous waste	No data
OHM/TADS	No data
DOT/UN/NA/IMDG shipping	No data
HSDB	No data
NCI	No data

[a]Tomlin 2003
[b]RTECS 2012; Tomlin 2003
[c]RTECS 2012

CAS = Chemical Abstracts Service; 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

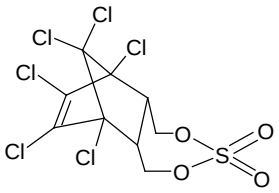
Table 4-3. Chemical Identity of β-Endosulfan

Characteristic	Information
Chemical name	β-Endosulfan[a]
Synonym(s)	Endosulfan II; Endosulfan B; 6,7,9,10,10-Hexachloro-1,5,5a,6,9,9a-hexahydro-6,9-methano-2,4,3-benzodiozathiepin-3-oxide, (3α, 5aα, 6β, 9β, 9aα)-; 5-Norbornene-2,3-dimethanol, 1,4,5,6,7,7-hexachloro-, cyclic sulfite, endo-[b]
Registered trade name(s)	β-Benzoepin; β-Thiodan; α -Thionex[c]
Chemical formula	$C_9H_6Cl_6O_3S$[b]
Chemical structure[e]	
Identification numbers:	
CAS registry	33213-65-9[a]
NIOSH RTECS	RB9875200[c]
EPA hazardous waste	No data
OHM/TADS	No data
DOT/UN/NA/IMDG shipping	No data
HSDB	No data
NCI	No data

[a]Tomlin 2003
[b]RTECS 2012; Tomlin 2003
[c]RTECS 2012

CAS = Chemical Abstracts Service; 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

Table 4-4. Chemical Identity of Endosulfan Sulfate

Characteristic	Information
Chemical name	Endosulfan sulfate[a]
Synonym(s)	6,7,8,9,10,10-Hexachloro-1,5,5a,6,9,9a-hexahydro-6,9-methano-2,4,3-benzodiozathiepin-3,3-dioxide; 5-Norbornene-2,3-dimethanol, 1,4,5,6,7,7-hexachloro-, cyclic Sulfate[a,b]
Registered trade name(s)	No data
Chemical formula	$C_9H_6Cl_6O_4S$[a]
Chemical structure[b]	
Identification numbers:	
CAS registry	1031-07-8[a]
NIOSH RTECS	RB9150000[b]
EPA hazardous waste	No data
OHM/TADS	8300205[c]
DOT/UN/NA/IMDG shipping	No data
HSDB	6180[a]
NCI	No data

[a]HSDB 2009
[b]RTECS 2012
[c]OHM/TADS 1989

CAS = Chemical Abstracts Service; 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

Table 4-5. Physical and Chemical Properties of Endosulfan

Property	Information	Reference
Molecular weight	406.93	O'Neil et al. 2006
Color	Cream to brown; mostly beige	Tomlin 2003
Physical state	Crystalline solid; waxy solid (commercial product)	NIOSH 2011; O'Neil et al. 2006
Melting point:		
Pure	106 °C	O'Neil et al. 2006
Technical	70–100 °C	O'Neil et al. 2006
Boiling point	106 °C	HSDB 2010
Density at 20/4 °C	1.745 g/mL	HSDB 2010
Density for vapor	14	HCDB 1986
Odor:		
α-Endosulfan	Terpene-like; Slight, sulfur dioxide odor	HSDB 2010
Decomposition products	May have a slight odor of sulfur dioxide	HSDB 2010
Odor threshold:		
Water	No data	
Air	No data	
Solubility:		
Water at 25 °C	0.53 mg/L	HSDB 2010
Organic solvents at 20 °C:		
Dichloromethane	200 g/L	Coleman and Dolinger 1982; HSDB 2010; Maier-Bode 1968
Ethanol	65 g/L	
Ethyl acetate	200 g/L	
Hexane	24 g/L	
Toluene	200 g/L	
Acetone	262 g/L	
Benzene	333 g/L	
Carbon tetrachloride	460 g/L	
Chloroform	746 g/L	
Ethanol	40 g/L	
Kerosene	164 g/L	
Methanol	89 g/L	
Xylene	388 g/L	
Partition coefficients:		
Log K_{ow}	3.83 (alpha) and 3.62 (beta)	HSDB 2010
Log K_{oc}	4.03 (alpha) and 4.13 (beta)	EPA 2010a
Vapor pressure at 25 ° C	$1x10^{-5}$ mmHg	Coleman and Dolinger 1982; EPA 1982
Vapor pressure at 25 °C	$1.73×10^{-7}$	HSDB 2010

Table 4-5. Physical and Chemical Properties of Endosulfan

Property	Information	Reference
Vapor pressure at 880 °C	$9x10^{-3}$ mmHg	Maier-Bode 1968; NRCC 1975
Henry's law constant at 20 °C	6.5×10^{-5} atm m^3/mol	HSDB 2010
Autoignition temperature	No data	
Flashpoint	No data	
Flammability limits in air	No data	
Reactivity	Both isomers are slowly hydrolyzed by aqueous acids and alkalis, with the formation of the diol and sulfur dioxide	Tomlin 2003
	α and β isomers are rapidly oxidized by peroxides or permanganate to endosulfan sulfate	HSDB 2010
	The β form is slowly converted to the more stable α form at high temperatures	Hapeman et al. 1997; Rice et al. 1997
	Both isomers slowly oxidize in air to endosulfan sulfate	Metcalf 1995
	Corrosive to iron	O'Neil et al. 2006
	Hydrolyzed rapidly by alkalies	O'Neil et al. 2006
Conversion factors:		
ppm (v/v) to mg/m^3 in air at 25 °C	1 ppm=0.0601 mg/m^3	Verschueren 1977
mg/m^3 to ppm (v/v) in air at 25 °C	1 mg/m^3=16.64 ppm	Verschueren 1977
Explosive limits	No data	

Table 4-6. Physical and Chemical Properties of α-Endosulfan

Property	Information	Reference
Molecular weight	406.93	O'Neil et al. 2006
Color:		
Pure	Colorless	HSDB 2010
Technical	Cream to brown, mostly beige	Tomlin 2003
Physical state	Crystalline solid	HSDB 2010
Melting point	108–110 °C	O'Neil et al. 2006
Boiling point	No data	
Density at 20/4 °C Density for vapor	No data	
Odor:	No data	
Odor threshold:		
Water	No data	
Air	No data	
Solubility:		
Water at 22 °C (pH 7.2)	0.15 mg/L	HSDB 2010
Water at 25 °C	0.53 mg/L	HSDB 2010
Organic solvents at 20 °C	No data	
Partition coefficients:		
Log K_{ow}	3.83	HSDB 2010
Log K_{oc}	3.55	HSDB 1999
Vapor pressure at 25 °C	$1x10^{-5}$ mmHg	EPA 1982
Henry's law constant at 25 °C	$1x10^{-5}$ atm m^3/mol $1.01x10^{-4}$ atm m^3/mol	EPA 1982 Montgomery 1993
Autoignition temperature	No data	
Flashpoint	No data	
Flammability limits in air	No data	
Conversion factors:		
ppm (v/v) to mg/m^3 in air at 25 °C	1 ppm=0.0601 mg/m^3	Verschueren 1977
mg/m^3 to ppm (v/v) in air at 25 °C	1 mg/m^3=16.64 ppm	Verschueren 1977
Explosive limits	No data	

Table 4-7. Physical and Chemical Properties of β-Endosulfan

Property	Information	Reference
Molecular weight	406.93	O'Neil et al. 2006
Color	Cream or tan	Tomlin 2003
Physical state	Crystalline solid	Budavari 1996
Melting point	208–210 °C	O'Neil et al. 2006
Boiling point	No data	
Density at 20/4 °C Density for vapor	No data	
Odor	No data	
Odor threshold:		
Water	No data	
Air	No data	
Solubility:		
Water at 22 °C (pH 7.2)	0.33	HSDB 2010
Water at 25 °C	0.28	HSDB 2010
Organic solvents at 20 °C	Soluble in most organic solvents	O'Neil et al. 2006
Partition coefficients:		
Log K_{ow}	3.62	HSDB 2010
Log K_{oc}	4.1	Verschueren 2001
Vapor pressure at 25 °C	$1x10^{-5}$ mmHg	EPA 1982
Henry's law constant at 25 °C	$1.91x10^{-5}$ atm m^3/mol	EPA 1982
Autoignition temperature	No data	
Flashpoint	No data	
Flammability limits in air	No data	
Reactivity	Both isomers are slowly hydrolysed by aqueous acids and alkalis, with the formation of the diol and sulfur dioxide	Tomlin 2003
	The β form is slowly converted to the more stable α form at high temperatures	Hapeman et al. 1997; Rice et al. 1997
Conversion factors:		
ppm (v/v) to mg/m^3 in air at 25 °C	1 ppm=0.0601 mg/m^3	Verschueren 1977
mg/m^3 to ppm (v/v) in air at 25 °C	1 mg/m^3=16.64 ppm	Verschueren 1977
Explosive limits	No data	

Table 4-8. Physical and Chemical Properties of Endosulfan Sulfate

Property	Information	Reference
Molecular weight	422.95	HSDB 2009
Color	Brown	HSDB 2009
Physical state	Crystalline solid	HSDB 2009
Melting point	181–182 °C 198–201 °C	EPA 1982; HSDB 2012; White-Stevens 1971
Boiling point	No data	
Density at 20/4 °C Density for vapor	No data	
Odor	Pungent	HSDB 2009
Odor threshold:		
Water	No data	
Air	No data	
Solubility:		
Water at 22 °C (pH 7.2)	0.22	EPA 1982; NRCC 1975; OHM/TADS 1989
Water at 25 °C	0.117; 0.22	
Organic solvents at 20 °C	No data	
Partition coefficients:		
Log K_{ow}	3.66	EPA 1979
Log K_{oc}	No data	
Vapor pressure at 25 °C	$1.0X10^{-11}$ mmHg	HSDB 2009
Henry's law constant at 25 °C	$2.61x10^{-5}$ atm m^3/mol	EPA 1982
Autoignition temperature	No data	
Flashpoint	No data	
Flammability limits in air	No data	
Conversion factors:		
ppm (v/v) to mg/m^3 in air at 25 °C	1 ppm=0.058 mg/m^3	Verschueren 1977
mg/m^3 to ppm (v/v) in air at 25 °C	1 mg/m^3=17.29 ppm	Verschueren 1977
Explosive limits	No data	