

3. CHEMICAL AND PHYSICAL INFORMATION

3.1 CHEMICAL IDENTITY

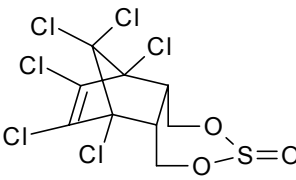
Technical-grade endosulfan contains at least 94% of two pure isomers, α - and β -endosulfan (Maier-Bode 1968; NRCC 1975). The α - and β -isomers of endosulfan are present in the ratio of 7:3, respectively. Technical-grade endosulfan may also contain up to 2% endosulfan alcohol and 1% endosulfan ether. Endosulfan sulfate is a reaction product found in technical endosulfan; it is also found in the environment due to photolysis and in organisms as a result of oxidation by biotransformation (EPA 1979; Coleman and Dolinger 1982). The chemical formula, structure, synonyms, and identification numbers for endosulfan, α -endosulfan, β -endosulfan, and endosulfan sulfate are listed in Tables 3-1, 3-2, 3-3, and 3-4, respectively.

3.2 PHYSICAL AND CHEMICAL PROPERTIES

Important physical and chemical properties of endosulfan, α -endosulfan, β -endosulfan, and endosulfan sulfate are listed in Tables 3-5, 3-6, 3-7, and 3-8, respectively. It should be noted that β -endosulfan is slowly converted to α -endosulfan (Hapeman et al. 1997; Rice et al. 1997).

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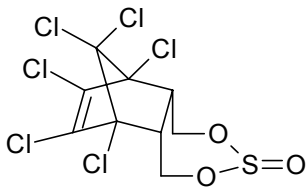
Table 3-1. Chemical Identity of Endosulfan

Characteristic	Information	Reference
Chemical name	Endosulfan	Budavari 1996
Synonym(s)	6,7,8,9,10,10-Hexachloro-1,5,5a,6,9,9a-hexahydro-6,9-methano-2,4,3-benzo(e)-dioxathiepin-3-oxide; Endosulfan technical; 5-Norbornene-2,3-dimethanol-1,4,5,6,7,7-hexachlorocyclic sulfite	HSDB 1999; IRIS 2000; Budavari 1996
Registered trade name(s)	Thiodan; Thionex; Thionate Malix; HOE 2671; FMC 5462; Cyclodan; Thifor; Beosit; Chlorthiepin; Endocide; Endosulphan	IRIS 1999; Suntio et al. 1988; Tomlin 1994; Budavari 1996
Chemical formula	$C_9H_6Cl_6O_3S$	Budavari 1996
Chemical structure		EPA 1984
Identification numbers:		
CAS registry	115-29-7	Budavari 1996
NIOSH RTECS	RB9275000	HSDB 1999
EPA hazardous waste	P050	HSDB 1999
OHM/TADS	7216559	HSDB 1999
DOT/UN/NA/IMCO shipping	2761	HCDB 1986
HSDB	390	HSDB 1999
NCI	C00566	HSDB 1999

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 Substance 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

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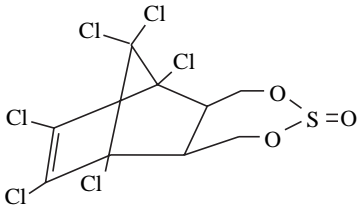
Table 3-2. Chemical Identity of α -Endosulfan

Characteristic	Information	Reference
Chemical name	α -Endosulfan	Tomlin 1994
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 (3 α , 5a β , 6 α , 9a α , 9 β)-	RTECS 1989; Tomlin 1994
Registered trade name(s)	α -Benzoepin; α -Thiodan; Thionex	RTECS 1989
Chemical formula	$C_9H_6Cl_6O_3S$	HSDB 1999
Chemical structure		EPA 1984
Identification numbers:		
CAS registry	959-98-8	Tomlin 1994
NIOSH RTECS	RB9275100	NIOSH 1997
EPA hazardous waste	No data	
OHM/TADS	No data	
DOT/UN/NA/IMCO shipping	No data	
HSDB	No data	
NCI	No data	

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 Substance 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

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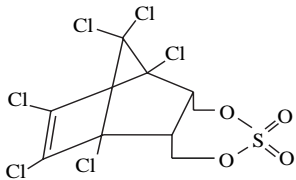
Table 3-3. Chemical Identity of β -Endosulfan

Characteristic	Information	Reference
Chemical name	β -Endosulfan	Tomlin 1994
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- benzodioxathiepin-3-oxide, (3 α , 5 α , 6 β , 9 β , 9 $\alpha\alpha$)-	CHEMLINE 1989; Tomlin 1994
Registered trade name(s)	α -Benzoepin; α -Thiodan; Thionex	CHEMLINE 1989
Chemical formula	$C_9H_6Cl_6O_3S$	HSDB 1999
Chemical structure		EPA 1984
Identification numbers:		
CAS registry	33213-65-9	Tomlin 1994
NIOSH RTECS	No data	
EPA hazardous waste	No data	
OHM/TADS	No data	
DOT/UN/NA/IMCO shipping	No data	
HSDB	No data	
NCI	No data	

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 Substance 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

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Table 3-4. Chemical Identity of Endosulfan Sulfate

Characteristic	Information	Reference
Chemical name	Endosulfan sulfate	Budavari 1996
Synonym(s)	6,7,8,9,10,10-Hexachloro-1,5,5a,6,9,9a-hexahydro-,6,9-methano-2,4,3-benzodioxathiepin-3,3-dioxide	HSDB 1999
Registered trade name(s)	No data	
Chemical formula	$C_9H_6Cl_6O_4S$	HSDB 1999
Chemical structure		EPA 1984
Identification numbers:		
CAS registry	1031-07-8	HSDB 1999
NIOSH RTECS	RB9150000	RTECS 1989
EPA hazardous waste	No data	
OHM/TADS	8300205	OHM/TADS 1989
DOT/UN/NA/IMCO shipping	No data	
HSDB	6180	HSDB 1999
NCI	No data	

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 Substance 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

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Table 3-5. Physical and Chemical Properties of Endosulfan

Property	Information	Reference
Molecular weight	406.95	Budavari 1996
Color	Cream to brown; mostly beige	Tomlin 1994
Physical state	Crystalline solid; Waxy solid	Budavari 1996; NIOSH 1997
Melting point		
Pure	106 EC	Budavari 1996
Technical	70–100 EC	Budavari 1996
Boiling point	No data	
Density at 20/4 EC	1.735 g/mL	HSDB 1999
Density for vapor	14	HCDB 1986
Odor		
α -Endosulfan	Terpene-like	HSDB 1999
Decomposition products	May have a slight odor of sulfur dioxide	HSDB 1999
Odor threshold:		
Water	No data	
Air	No data	
Solubility:		
Water at 25 EC	60–100 μ g/L	Sittig 1980
Organic solvents at 20 EC		
Dichloromethane	65 g/L	Coleman and Dolinger 1982; HSDB 1999; 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}	3.55 and 3.62	HSDB 1999
Log K_{oc}	3.5	EPA 1987b
Vapor pressure at 25 EC	1×10^{-5} mmHg	Coleman and Dolinger 1982; Mabey et al. 1982

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Table 3-5. Physical and Chemical Properties of Endosulfan (continued)

Property	Information	Reference
Vapor pressure at 20 EC	0.83 mPa	Tomlin 1997
Vapor pressure at 880 EC	9x10 ⁻³ mmHg	Maier-Bode 1968; NRCC 1975
Henry's law constant at 24.8 EC	1x10 ⁻⁵ atm m ³ /mol 1.01x10 ⁻⁴ atm m ³ /mol	Suntio et al. 1988 Montgomery 1993
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 1994
	α and β isomers are rapidly oxidized by peroxides or permanganate to endosulfan sulfate	HSDB 1999
	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 RL 1995
	Corrosive to iron	HSDB 1999
Conversion factors: ppm (v/v) to mg/m ³ in air at 25 EC	1 ppm=0.0601 mg/m ³	Verschueren 1977
mg/m ³ to ppm (v/v) in air at 25 EC	1 mg/m ³ =16.64 ppm	Verschueren 1977
Explosive limits	No data	

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Table 3-6. Physical and Chemical Properties of α -Endosulfan

Property	Information	Reference
Molecular weight	406.93	Budavari 1996
Color:		Tomlin 1994
Pure	Colorless	
Technical	Cream to brown, mostly beige	
Physical state	Crystalline solid	Tomlin 1994
Melting point	108–110 EC	Budavari 1996
Boiling point	No data	
Density at 20/4 EC	No data	
Odor	No data	
Odor threshold:		
Water	No data	
Air	No data	
Solubility:		
Water at 22 EC (pH 7.2)	0.15 mg/L	HSDB 1999
	0.32 mg/L	Tomlin 1994
Water at 25 EC	0.53 mg/L	EPA 1982c; Weil et al. 1974
Organic solvents at 20 EC	No data	
Partition coefficients:		
Log K_{ow}	3.83	Hansch et al. 1995
Log K_{oc}	3.55	HSDB 1999
Vapor pressure at 25 EC	1×10^{-5} mmHg	EPA 1982c
Henry's law constant at 25 EC	1×10^{-5} atm m ³ /mol 1.01×10^{-4} atm m ³ /mol	EPA 1982c 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 EC	1 ppm=0.0601 mg/m ³	Verschueren 1977
mg/m ³ to ppm (v/v) in air at 25 EC	1 mg/m ³ =16.64 ppm	Verschueren 1977
Explosive limits	No data	

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Table 3-7. Physical and Chemical Properties of β -Endosulfan

Property	Information	Reference
Molecular weight	406.93	Budavari 1996
Color	Cream or tan	Tomlin 1994
Physical state	Crystalline solid	Budavari 1996
Melting point	207–209 EC 208–210 EC 212 EC	EPA 1979; Coleman and Dolinger 1982; EPA 1982c; Budavari 1996
Boiling point	No data	
Density at 20/4 EC	No data	
Odor	No data	
Odor threshold:		
Water	No data	
Air	No data	
Solubility:		
Water at 22 EC (pH 7.2)	0.33	Tomlin 1994
Water at 25 EC	0.28	EPA 1982c; Weil et al. 1974
Organic solvents at 20 EC	Soluble in most organic solvents	Budavari 1996
Partition coefficients:		
Log K_{ow}	3.52	Hansch and Leo 1995
Log K_{oc}	No data	
Vapor pressure at 25 EC	1×10^{-5} mmHg	EPA 1982c
Henry's law constant at 25 EC	1.91×10^{-5} atm m ³ /mol	EPA 1982c
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 1994
	The β form is slowly converted to the more stable α form at high temperatures	Hapeman et al. 1997; Rice et al. 1997

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Table 3-7. Physical and Chemical Properties of β -Endosulfan (*continued*)

Property	Information	Reference
Conversion factors: ppm (v/v) to mg/m ³ in air at 25 EC	1 ppm=0.0601 mg/m ³	Verschueren 1977
mg/m ³ to ppm (v/v) in air at 25 EC	1 mg/m ³ =16.64 ppm	
Explosive limits	No data	

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Table 3-8. Physical and Chemical Properties of Endosulfan Sulfate

Property	Information	Reference
Molecular weight	422.9	EPA 1982c
Color	Brown	HSDB 1999
Physical state	Crystalline solid	HSDB 1999
Melting point	181 EC 198–201EC	EPA 1982c; White-Stevens 1971
Boiling point	No data	
Density at 20/4 EC	No data	
Odor	Pungent	HSDB 1999
Odor threshold:		
Water	No data	
Air	No data	
Solubility:		
Water at 22 EC (pH 7.2)	0.22	EPA 1982c; NRCC 1975;
Water at 25 EC	0.117; 0.22	OHM/TADS 1989
Organic solvents at 20 EC	No data	
Partition coefficients:		
Log K_{ow}	3.66	EPA 1979
Log K_{oc}	No data	
Vapor pressure at 25 EC	1×10^{-5} mmHg	EPA 1979; EPA 1982c
Henry's law constant at 25 EC	2.61×10^{-5} atm m ³ /mol	EPA 1982c
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 EC	1 ppm=0.058 mg/m ³	Verschueren 1977
mg/m ³ to ppm (v/v) in air at 25 EC	1 mg/m ³ =17.29 ppm	Verschueren 1977
Explosive limits	No data	

