

3. CHEMICAL AND PHYSICAL INFORMATION

3.1 CHEMICAL IDENTITY

Table 3-1 lists common synonyms, trade names, and other pertinent identification information for hexachloroethane.

3.2 PHYSICAL AND CHEMICAL PROPERTIES

Table 3-2 lists important physical and chemical properties of hexachloroethane.

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TABLE 3-1. Chemical Identity of Hexachloroethane

Characteristic	Information	Reference
Chemical name	Hexachloroethane	HSDB 1995
Synonym(s)	Perchloroethane; carbon hexachloride; 1,1,1,2,2,2-hexachloroethane; hexachloroethylene; HCE; and others	ACGIH 1991; Gordon et al. 1991; HSDB 1995
Registered trade name(s)	Avlothane; Distokal; Distopan; Distopin; Egitol; Falkitol; Fasciolin; Mottenhexe; Phenohep	IARC 1979
Chemical formula	C ₂ Cl ₆	HSDB 1995
Chemical structure	$ \begin{array}{c} \text{Cl} \quad \text{Cl} \\ \quad \\ \text{Cl} - \text{C} - \text{C} - \text{Cl} \\ \quad \\ \text{Cl} \quad \text{Cl} \end{array} $	Howard 1989
Identification numbers:		
CAS registry	67-72-1	HSDB 1995
NIOSH RTECS	KI 4025000	HSDB 1995
EPA hazardous waste	U131	
OHM/TADS	No data	HSDB 1995
DOT/UN/NA/IMCO shipping	NA 9037	HSDB 1995
HSDB	2033	HSDB 1995
NCI	C04604	HSDB 1995

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

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TABLE 3-2. Physical and Chemical Properties of Hexachloroethane

Property	Information	Reference
Molecular weight	236.74	Weast 1986
Color	Colorless	HSDB 1995
Physical state	Solid	HSDB 1995
Melting point	Sublimes	ACGIH 1991; Budavari et al. 1989
Boiling point	186.8°C (triple point)	Budavari et al. 1989
Density:		
at 20°C	2.091 g/mL	Weast 1986
Odor	Camphoraceous	Budavari et al. 1989
Odor threshold:		
Water	0.010 mg/L	Amoore and Hautala 1983
Air	0.15 ppm (1.5 mg/m ³)	Amoore and Hautala 1983
Solubility:		
Water at 22°C	50 mg/L	Verschueren 1983
Water at 25°C	14 mg/L	Spanggard et al. 1985
Organic solvent(s)	Soluble in alcohol, benzene, chloroform, ether, oils	Budavari et al. 1989
Partition coefficients:		
Log K _{ow}	3.82	Howard 1989
Log K _{oc}	3.34	Callahan et al. 1979
Log K _{oc}	4.3	Mabey et al. 1982
Vapor pressure:		
at 20°C	0.4 mmHg	Verschueren 1983
at 30°C	0.8 mmHg	Verschueren 1983
Henry's law constant:		
at 25°C:	2.237×10 ⁻² atm m ³ /mole	Yaws et al. 1991
	6,100 L-torr/mol	Spanggard et al. 1985
	(8.0×10 ⁻³ atm m ³ /mol	
	2.8×10 ⁻³ atm m ³ /mole	Howard 1989
Autoignition temperature	Nonflammable	IARC 1979
Flashpoint	Nonflammable	IARC 1979
Flammability limits	Nonflammable	IARC 1979
Conversion factors	1 ppm = 9.68 mg/m ³	Verschueren 1983
	1 mg/m ³ = 0.10 ppm	
Explosive limits	No data	

