

4. CHEMICAL AND PHYSICAL INFORMATION

4.1 CHEMICAL IDENTITY

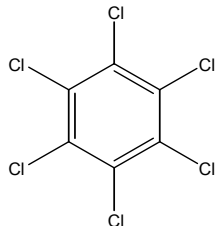
Hexachlorobenzene is a chlorinated hydrocarbon industrial chemical. Although hexachlorobenzene is not currently manufactured as a commercial end product in the United States, it is formed as a waste product in the production of several chlorinated hydrocarbons such as tetrachloroethylene, trichloroethylene, and carbon tetrachloride, and is a contaminant in some pesticides such as pentachloronitrobenzene and pentachlorophenol. Its presence in the environment is also due to its previous use as a fungicide. Hexachlorobenzene is a very persistent environmental chemical due to its chemical stability and resistance to biodegradation. Information regarding the chemical identity of hexachlorobenzene is located in Table 4-1.

4.2 PHYSICAL AND CHEMICAL PROPERTIES

Hexachlorobenzene is a white, crystalline solid (Verschueren 1996) that is practically insoluble in water (Lide 1998). When heated to decomposition, it emits toxic fumes of chlorides (Sax 1984). Dimethyl formamide and hexachlorobenzene react violently above 65 EC (NFPA 1986). Information regarding the physical and chemical properties of hexachlorobenzene is located in Table 4-2.

4. CHEMICAL AND PHYSICAL INFORMATION

Table 4-1. Chemical Identity of Hexachlorobenzene

Characteristics	Information	Reference
Chemical name	Hexachlorobenzene	Budavari 1996
Synonyms	Perchlorobenzene; HCB; pentachlorophenyl chloride	Budavari 1996 Farm Chemicals Handbook 2001 HSDB 2001
Trade names	AntiCarie; Ceku C. B.; No Bunt	Farm Chemicals Handbook 2001
Chemical formula	C ₆ Cl ₆	Budavari 1996
Chemical structure		
Identification numbers:		
CAS Registry	118-74-1	Farm Chemicals Handbook 2001
NIOSH RTECs	DA2975000	HSDB 2001
EPA Hazardous Waste	U127	EPA 1999e (40 CFR 261.33)
OHM/TADS	8100010	HSDB 2001
DOT/UN/NA/IMCO	UN2729	HSDB 2001
Shipping		
HSDB	1724	NLM 2001
NCI	No data	

CAS = Chemical Abstracts Service; DOT/UN/NA/IMO = 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

4. CHEMICAL AND PHYSICAL INFORMATION

Table 4-2. Physical and Chemical Properties of Hexachlorobenzene

Property	Information	Reference
Molecular weight	284.78	Budavari 1996
Color	White	Verschueren 1996
Physical state	Crystalline solid	Verschueren 1996
Melting point	231 EC	Budavari 1996
Boiling point	325 EC 323–326 EC	Lide 1998 Budavari 1996
Density at 23 EC	2.044	Budavari 1996
Odor	No data	
Odor threshold: Water	No data	
Air	No data	
Solubility: Water at 25 EC	0.006 mg/L	Farmer et al. 1976
Water at 20 EC	0.005815 mg/L	Yalkowsky 1992
	0.006 mg/L	Verschueren 1996
Organic solvents	Insoluble in water, slightly soluble in ethanol, soluble in ethyl ether, and very soluble in benzene	Lide 1998
Partition coefficients: Log octanol/water	5.73	Hansch et al. 1995
Log K _{oc}	6.08 5.22 3.59	EPA 1981a Kenaga and Goring 1978
Vapor pressure at 20 EC	1.09x10 ⁻⁵ mmHg	Budavari 1996
Henry's law constant	5.8x10 ⁻⁴ atm-m ³ /mol	Ten Hulscher et al. 1992
Hydroxyl radical constant at 25 EC	2.7x10 ⁻¹⁴ cm ³ /molecule-second	Brubaker and Hites 1998
Autoignition temperature	No data	
Flashpoint	242 EC	Budavari 1996
Flammability limits	No data	
Conversion factors	1 ppm = 11.8 mg/m ³ 1 mg/m ³ = 0.08 ppm	Verschueren 1996
Explosive limits	No data	

