

4. CHEMICAL AND PHYSICAL INFORMATION

4.1 CHEMICAL IDENTITY

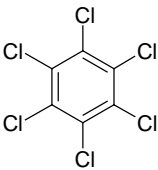
Hexachlorobenzene is a fully chlorinated hydrocarbon industrial chemical. Although hexachlorobenzene is not currently manufactured as a commercial end product in the United States, it is formed as a waste product in the production of several chlorinated hydrocarbons such as tetrachloroethylene and trichloroethylene, 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

Hexachloro-benzene is a white, crystalline solid (Verschueren 2001) that is practically insoluble in water (Haynes and Lide 2010). When heated to decomposition, hexachlorobenzene emits highly toxic fumes of hydrochloric acid, other chlorinated compounds, carbon monoxide, and carbon dioxide (NTP 2014). Dimethyl formamide and hexachloro-benzene react violently above 65 °C (HSBD 2012). Information regarding the physical and chemical properties of hexachloro-benzene is located in Table 4-2.

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Table 4-1. Chemical Identity of Hexachlorobenzene

Characteristics	Information ^a
Chemical name	Hexachlorobenzene ^b
Synonyms	Perchlorobenzene ^b ; HCB ^c ; pentachlorophenyl chloride
Trade names	AntiCarie; Ceku C. B.; No Bunt ^c
Chemical formula	C ₆ Cl ₆ ^b
Chemical structure	
Identification numbers:	
CAS Registry	118-74-1 ^c
NIOSH RTECs	DA2975000
EPA Hazardous Waste	U127 ^d
OHM/TADS	8100010
DOT/UN/NA/IMDG shipping	UN2729
HSDB	1724 ^e
NCI	No data

^aAll information obtained from HSDB 2012, except where noted

^bO'Neil et al. 2006

^cFarm Chemicals Handbook 2001

^dEPA 1999

^eHSDB 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

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Table 4-2. Physical and Chemical Properties of Hexachlorobenzene

Property	Information	Reference
Molecular weight	284.78	O'Neil et al. 2006
Color	White	Verschueren 2001
Physical state	Crystalline solid	Verschueren 2001
Melting point	231 °C	O'Neil et al. 2006
Boiling point	325 °C 323–326 °C	Haynes and Lide 2010 O'Neil et al. 2006
Density at 23 °C	2.044	O'Neil et al. 2006
Odor	No data	
Odor threshold:		
Water	No data	
Air	No data	
Solubility:		
Water at 25 °C	0.0062 mg/L 0.0047 mg/L	Farmer et al. 1976
Water at 20 °C	0.006 mg/L	Yalkowsky 1992
Organic solvents	Insoluble in water, slightly soluble in ethanol, soluble in diethyl ether and chloroform, and very soluble in benzene	Verschueren 2001 Haynes and Lide 2010
Partition coefficients:		
Log octanol/water	5.73	Hansch et al. 1995
Log K _{oc}	6.08 5.22 3.59	EPA 1981 Kenaga and Goring 1978
Vapor pressure at 20 °C	1.09x10 ⁻⁵ mmHg	O'Neil et al. 2006
Henry's law constant	5.8x10 ⁻⁴ atm·m ³ /mol	ten Hulscher et al. 1992
Hydroxyl radical constant at 25 °C	2.7x10 ⁻¹⁴ cm ³ /molecule-second	Brubaker and Hites 1998
Autoignition temperature	No data	
Flashpoint	242 °C	O'Neil et al. 2006
Flammability limits	No data	
Conversion factors	1 ppm = 11.8 mg/m ³ 1 mg/m ³ = 0.08 ppm	Verschueren 2001
Explosive limits	No data	