

3. CHEMICAL AND PHYSICAL INFORMATION

3.1 CHEMICAL IDENTITY

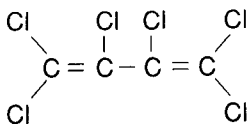
Information regarding the chemical identity of hexachlorobutadiene is located in Table 3-1.

3.2 PHYSICAL AND CHEMICAL PROPERTIES

Information regarding the physical and chemical properties of hexachlorobutadiene is located in Table 3-2.

3. CHEMICAL AND PHYSICAL INFORMATION

TABLE 3-1. Chemical Identity of Hexachlorobutadiene

Characteristic	Information	Reference
Chemical name	Hexachlorobutadiene	Montgomery and Welkom 1990
Synonym(s)	Perchlorobutadiene; HCBd; 1,1,2,3,4,4-Hexachloro- 1,3-butadiene; 1,3-Hexachlorobutadiene; Dolen-Pur; GP-40-66:120	Montgomery and Welkom 1990 HSDB 1993
Registered trade name(s)	No data	
Chemical formula	C ₄ Cl ₆	Montgomery and Welkom 1990
Chemical structure		Montgomery and Welkom 1990
Identification numbers:		
CAS registry	87-68-3	Montgomery and Welkom 1990
NIOSH RTECS	EJ0700000	HSDB 1993
EPA hazardous waste	U128	HSDB 1993
OHM/TADS	OHM 8100011	HSDB 1993
DOT/UN/NA/IMCO shipping	UN 2279	HSDB 1993
	IMCO 6.1	HSDB 1993
HSDB	2870	HSDB 1993
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 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

3. CHEMICAL AND PHYSICAL INFORMATION

TABLE 3-2. Physical and Chemical Properties of Hexachlorobutadiene

Property	Information	Reference
Molecular weight	260.76	Montgomery and Welkom 1990
Color	Colorless	HSDB 1993
Physical state	Liquid	Montgomery and Welkom 1990
Melting point	-21°C	Montgomery and Welkom 1990
Boiling point	215°C	Montgomery and Welkom 1990
Density: at 20°C	1.55 g/cm ³	HSDB 1993
Odor	Mild to pungent	Montgomery and Welkom 1990
Odor threshold: Water	No data	
Air	12.0 mg/m ³	Ruth 1986
Solubility: Water at 20°C	2-2.55 mg/L	Montgomery and Welkom 1990
Organic solvent(s)	Soluble in ethanol and ether	Montgomery and Welkom 1990
Partition coefficients: Log K _{ow}	4.78	Montgomery and Welkom 1990
Log K _{oc}	3.67	Montgomery and Welkom 1990
Vapor pressure at 25°C	0.15 mmHg	Montgomery and Welkom 1990
Henry's law constant:	0.001-0.026 atm-m ³ /mol	Montgomery and Welkom 1990
Autoignition temperature	610°C	Sax and Lewis 1989
Flashpoint	Noncombustible	Montgomery and Welkom 1990
Flammability limits	Noncombustible	Montgomery and Welkom 1990
Conversion factors	1 ppm = 10.5 mg/m ³ 1 mg/m ³ = 0.095 ppm	ACGIH 1991
Explosive limits	No data	

