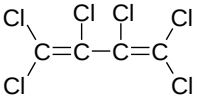
CHAPTER 4. CHEMICAL AND PHYSICAL INFORMATION

4.1 CHEMICAL IDENTITY

Information regarding the chemical identity of hexachlorobutadiene is located in Table 4-1.

Table 4-1. Chemical Identity of Hexachlorobutadiene

Characteristic	Information	Reference
Chemical name	Hexachlorobutadiene	Montgomery and Welkom 1990
Synonym(s) and registered trade name(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; NLM 2020
Chemical formula	C_4Cl_6	Montgomery and Welkom 1990
Chemical structure		Montgomery and Welkom 1990
CAS Registry Number	87-68-3	Montgomery and Welkom 1990

CAS = Chemical Abstracts Service

4.2 PHYSICAL AND CHEMICAL PROPERTIES

Information regarding the physical and chemical properties of hexachlorobutadiene is located in Table 4-2.

Table 4-2. Physical and Chemical Properties of Hexachlorobutadiene

Property	Information	Reference
Molecular weight	260.76	Montgomery and Welkom 1990
Color	Colorless	NLM 2020
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	NLM 2020
Odor	Mild to pungent	Montgomery and Welkom 1990
Odor threshold:		
Water	No data	
Air	12.0 mg/m^3	Ruth 1986

Table 4-2. Physical and Chemical Properties of Hexachlorobutadiene

Solubility:		
Water at 20°C	2–2.55 mg/L	Montgomery and Welkom 1990
Organic solvents	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	NLM 2020
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	
Explosive limits	No data	