

3. CHEMICAL AND PHYSICAL INFORMATION

3.1 CHEMICAL IDENTITY

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

3.2 PHYSICAL AND CHEMICAL PROPERTIES

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

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TABLE 3-1. Chemical Identity of Chlorobenzene

Characteristic	Value	Reference
Chemical name	Chlorobenzene	NLM 1988 NLM 1988
Synonyms	Monochlorobenzene; benzene chloride; phenylchloride; MCB; chlorobenzol	NLM 1988
Trade name	Caswell no. 183A	NLM 1988
Chemical formula	C ₆ H ₅ Cl	NLM 1988
Chemical structure		
Identification numbers:		
CAS Registry	108-90-7	NLM 1988
NIOSH RTECS	CZ0175000	HSDB 1988
EPA Hazardous Waste	U037, F002	HSDB 1988
OHM/TADS	No data	
DOT/UN/NA/IMCO Shipping	UN 1134 IMCO 3.3	NLM 1988 HSDB 1988
HSDB	55	NLM 1988
NCI	C54886	NLM 1988

CAS = Chemical Abstracts Service; NIOSH = National Institute for Occupational Safety and Health; RTECS = Registry of Toxic Effects of Chemical Substances; EPA = Environmental Protection Agency; OHM/TADS = Oil and Hazardous Materials/Technical Assistance Data System; DOT/UN/NA/IMCO = Department of Transportation/United Nations/North America/International Maritime Dangerous Goods Code; HSDB = Hazardous Substances Data Bank; NCI = National Cancer Institute.

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TABLE 3-2. Physical and Chemical Properties of Chlorobenzene

Property	Value	Reference
Molecular weight	112.56	Weast 1985
Color	Colorless	Verschueren 1983
Physical state	Liquid	Verschueren 1983
Melting point	-45.6°C	Weast 1985
Boiling point	132°C	Weast 1985
Density at 20°C	1.1058	Weast 1985
Odor	Aromatic, almond-like	Sax and Lewis 1987
Odor threshold:		
Water	0.050 mg/L	Verschueren 1983
Air	1-8 mg/m ³	Verschueren 1983
Solubility:		
Water at 20°C	500 mg/L	Verschueren 1983
Organic solvents	Soluble in alcohol, ether, benzene	Weast 1985
Partition coefficients:		
Log octanol/water	2.84	Verschueren 1983
Log K _{oc}	2.52	Mabey et al. 1982
Vapor pressure at 20°C	8.8 mmHg	Verschueren 1983
Henry's law constant	3.58x10 ⁻³ atm-m ³ /mol	Mabey et al. 1982
Autoignition temperature	637°C	Sax and Lewis 1987
Flashpoint	29.4°C	Sax and Lewis 1987
Flammability limits	1.8%-9.6%	Sax and Lewis 1987
Conversion factors	1 ppm = 4.7 mg/m ³ 1 mg/m ³ = 0.22 ppm	Verschueren 1983

