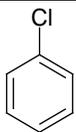


CHAPTER 4. CHEMICAL AND PHYSICAL INFORMATION

4.1 CHEMICAL IDENTITY

Data pertaining to the chemical identity of chlorobenzene are listed in Table 4-1.

Table 4-1. Chemical Identity of Chlorobenzene

Characteristic	Information	Reference
Chemical name	Chlorobenzene	NLM 2020
Synonym(s) and registered trade name(s)	Monochlorobenzene; Benzene chloride; Phenylchloride; MCB; Chlorobenzol; Caswell no. 183A	NLM 2020
Chemical formula	C ₆ H ₅ Cl	NLM 2020
Chemical structure		NLM 2020
CAS Registry Number	108-90-7	NLM 2020

CAS = Chemical Abstracts Service

4.2 PHYSICAL AND CHEMICAL PROPERTIES

The odor threshold for chlorobenzene in humans has been reported to be as low as 0.21 ppm or 0.97 mg/m³ (Leonardos et al. 1969). However, others have reported its “almond-like odor” to be “barely perceptible” at 60 ppm (Von Burg 1981; Willhite and Book 1990). The physical and chemical properties of chlorobenzene are presented in Table 4-2.

Table 4-2. Physical and Chemical Properties of Chlorobenzene

Property	Information	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

4. CHEMICAL AND PHYSICAL INFORMATION

Table 4-2. Physical and Chemical Properties of Chlorobenzene

Property	Information	Reference
Odor threshold:	Conflicting data	Leonardos et al. 1969
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 K _{ow}	2.84	Verschueren 1983
Log K _{oc}	2.52	EPA 1982
Vapor pressure at 20°C	8.8 mmHg	Verschueren 1983
Henry's law constant at 25°C	3.58x10 ⁻³ atm-m ³ /mol	EPA 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
Explosive limits	1.3-11 vol% in air)	NIOSH 2015