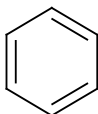


CHAPTER 4. CHEMICAL AND PHYSICAL INFORMATION

4.1 CHEMICAL IDENTITY

Information regarding the chemical identity of benzene is presented in Table 4-1. Although the term benzol is found in older literature and in Europe for the commercial product (Folkins 2012), benzene is the name presently used by the International Union of Pure and Applied Chemistry (IUPAC) and the American Society for Testing and Materials (ASTM) for the pure product (Fruscella 2002; NLM 2023).

Table 4-1. Chemical Identity of Benzene

Characteristic	Information	Reference
Chemical name	Benzene	NLM 2023
Synonym(s)	[6] Annulene, benzeen (Dutch), benzen (Polish), benzol, benzole; benzolo (Italian), coal naphtha, cyclohexatriene, fenzen (Czech), phene, phenyl hydride, pyrobenzol, pyrobenzole	NLM 2023
Registered trade name(s)	Polystream	IARC 1982
Chemical formula	C ₆ H ₆	NLM 2023
SMILES	C1=CC=CC=C1	NLM 2023
Chemical structure		NLM 2023
CAS Registry Number	71-43-2	NLM 2023

CAS = Chemical Abstracts Service; SMILES = simplified molecular-input line-entry system

4.2 PHYSICAL AND CHEMICAL PROPERTIES

Benzene is a flammable organic compound with a petroleum-like odor. It is formed from human activities and by natural processes. Benzene is slightly soluble in water and evaporates rapidly into air. Information regarding the physical and chemical properties of benzene is presented in Table 4-2. The major impurities found in commercial products are toluene, xylene, phenol, thiophene, carbon disulfide, acetonitrile, and pyridine (NIOSH 1974). Commercially refined benzene-535 is free of hydrogen sulfide and sulfur dioxide but contains a maximum of 1 ppm thiophene and a maximum of 0.15% nonaromatics (Fruscella 2002). Benzene is also commercially available as nitration-grade (99% pure), thiophene-free, 99 mole%, 99.94 mole%, and nanograde quality (NLM 2023).

4. CHEMICAL AND PHYSICAL INFORMATION

Table 4-2. Physical and Chemical Properties of Benzene

Property	Information	Reference
Molecular weight	78.11 g/mol	Budavari et al. 2001
Color	Clear, colorless liquid	Budavari et al. 2001
Physical state	Colorless to light yellow liquid	NLM 2023
Melting point	5.558°C	NLM 2023
Boiling point	80.08°C	NLM 2023
Density at 20°C, g/cm ³	0.8756	NLM 2023
Odor	Aromatic (petroleum-like)	NFPA 1994; NLM 2023
Odor threshold:		
Water	2.0 mg/L	NLM 2023
Air ^a	Detection range: 34–119 ppm (geometric mean: 61 ppm) Recognition: 97 ppm	AIHA 1989
Taste threshold	0.5–4.5 mg/L	NLM 2023
Solubility:		
Water at 25°C	w/w: 1,790 mg/L	NLM 2023
Organic solvent(s)	Alcohol, chloroform, ether, carbon disulfide, acetone, oils, carbon, tetrachloride, glacial acetic acid	Budavari et al. 2001
Partition coefficients:		NLM 2023; Karickhoff 1981; Kenaga 1980
Log K _{ow}	2.13	
Log K _{oc}	1.8–1.9	
Vapor pressure at 25°C	94.8 mm Hg	NLM 2023
Henry's law constant at 25°C	5.5x10 ⁻³ atm·m ³ /mol	Mackay and Leinonen 1975
Autoignition temperature	498°C	NFPA 1994
Flashpoint	-11°C (closed cup)	Budavari et al. 2001
NFPA hazard classification:		OSHA 2021
Health	2	
Flammability	3	
Reactivity	0	
Flammability limits in air	1.2% (lower limit); 7.8% (upper limit)	OSHA 2021
Conversion factors	1 ppm=3.26 mg/m ³ at 20°C and 1 atm pressure; 1 mg/m ³ =0.31 ppm	NLM 2023
Explosive limits	1.4% (lower limit); 8% (upper limit)	NLM 2023

^aOdor threshold values considered by AIHA (1989) to be acceptable based on review of peer-reviewed reports of odor thresholds for benzene (range 0.78–100 ppm).

NFPA = National Fire Protection Association. Level 3 flammability classification is highly flammable. A level 2 health classification means the material is hazardous.