

## 4. CHEMICAL AND PHYSICAL INFORMATION

### 4.1 CHEMICAL IDENTITY

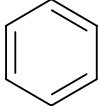
Information regarding the chemical identity of benzene is located in Table 4-1. Although the term benzol is found in older literature for the commercial product, benzene is the name presently approved by the International Union of Pure and Applied Chemistry (IUPAC), the Chemical Manufacturers Association (CMA), and the American Society for Testing and Materials (ASTM) for the pure product.

### 4.2 PHYSICAL AND CHEMICAL PROPERTIES

Information regarding the physical and chemical properties of benzene is located in Table 4-2. The major impurities found in commercial products are toluene, xylene, phenol, thiophene, carbon disulfide, acetylnitrile, and pyridine (NIOSH 1974). Commercial 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. Refined nitration-grade benzene is free of hydrogen sulfide and sulfur dioxide. Benzene is also commercially available as thiophene-free, 99 mole%, 99.94 mole%, and nanograde quality (HSDB 2007).

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**Table 4-1. Chemical Identity of Benzene**

Characteristic	Information	Reference
Chemical name	Benzene	HSDB 2007
Synonym(s)	Annulene, benzeen (Dutch), benzen (Polish), benzol, benzole; benzolo (Italian), coal naphtha, cyclohexatriene, fenzen (Czech), phene, phenyl hydride, pyrobenzol, pyrobenzole	HSDB 2007
Registered trade name(s)	Polystream	IARC 1982
Chemical formula	C <sub>6</sub> H <sub>6</sub>	Budavari et al. 2001
Chemical structure		Budavari et al. 2001
Identification numbers:		
CAS registry	71-43-2	HSDB 2007
NIOSH RTECS	CY-1400000	HSDB 2007
EPA hazardous waste	NA	
OHM/TADS	No Data	
DOT/UN/NA/IMCO shipping	UN1114; IMO3.2	HSDB 2007
HSDB	35	HSDB 2007
NCI	C55276	HSDB 2007
Merck	1066	Budavari et al. 2001

CAS = Chemical Abstracts Service; DOT/UN/NA/IMO=Department of Transportation/United Nations/North America/Intergovernmental 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

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**Table 4-2. Physical and Chemical Properties of Benzene**

Property	Information	Reference
Molecular weight	78.11	Budavari et al. 2001
Color	Clear, colorless liquid	Budavari et al. 2001
Physical state	colorless to light yellow liquid	HSDB 2007
Melting point	5.5 °C	Budavari et al. 2001
Boiling point	80.1 °C	Budavari et al. 2001
Density at 15 °C, g/cm <sup>3</sup>	0.8787	Budavari et al. 2001
Odor	Aromatic	NFPA 1994
Odor threshold:		
Water	2.0 mg/L	HSDB 2007
Air <sup>a</sup>	Detection range: 34–119 ppm (geometric mean: 61 ppm) Recognition: 97 ppm	AIHA 1989
Taste threshold:	0.5–4.5 mg/L	HSDB 2007
Solubility:		
Water at 25 °C	w/w: 0.188%	Budavari et al. 2001
Organic solvents	Alcohol, chloroform, ether, carbon disulfide, acetone, oils, carbon, tetrachloride, glacial acetic acid	Budavari et al. 2001
Partition coefficients:		HSDB 2007; Karickhoff 1981; Kenaga 1980
Log K <sub>ow</sub> <sup>b</sup>	2.13	
Log K <sub>oc</sub> <sup>c</sup>	1.8–1.9	
Vapor pressure at 20 °C	75 mm Hg	NFPA 1994
Henry's law constant at 25 °C	5.5x10 <sup>-3</sup> atm·m <sup>3</sup> /mol	Mackay and Leinonen 1975
Autoignition temperature	498 °C	NFPA 1994
Flashpoint	-11 °C (closed cup)	Budavari et al. 2001
NFPA hazard classification:		HSDB 2007
Health	2.2	
Flammability	3.3	
Reactivity	0.0	
Flammability limits in air	1.2% (lower limit); 7.8% (upper limit)	NFPA 1994
Conversion factors	1 ppm=3.26 mg/m <sup>3</sup> at 20 °C and 1 atm pressure; 1 mg/m <sup>3</sup> =0.31 ppm	HSDB 2007
Explosive limits	1.4% (lower limit); 8% (upper limit)	HSDB 2007

<sup>a</sup>Odor 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).

<sup>b</sup>K<sub>ow</sub> = octanol-water partitioning coefficient

<sup>c</sup>K<sub>oc</sub> = soil adsorption coefficient

NFPA = National Fire Protection Association