

### **3. CHEMICAL AND PHYSICAL INFORMATION**

#### **3.1 CHEMICAL IDENTITY**

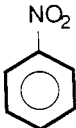
Table 3-1 lists common synonyms, trade names and other pertinent identification information for nitrobenzene.

#### **3.2 PHYSICAL AND CHEMICAL PROPERTIES**

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

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TABLE 3-1. Chemical Identity of Nitrobenzene

	Value	Reference
Chemical name	Nitrobenzene	NLM 1988
Synonyms	Nitrobenzol; Oil of Mirbane	MLM 1988
Trade name	Caswell No. 600	NLM 1988
Chemical formula	$C_6H_5NO_2$	NLM 1988
Chemical structure		
Identification numbers:		
CAS Registry	98-95-3	NLM 1988
NIOSH RTECS	DA6475000	HSDB 1988
EPA Hazardous Waste	U169, F004	NLM 1988, HSDB 1988
OHM/TADS	7216821	HSDB 1988
DOT/UN/NA/IMCO Shipping	UN 1662	NLM 1988
HSDB	104	NLM 1988
NCI	C60082	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 Nitrobenzene

Property	Value	Reference
Molecular weight	123.11	Weast 1985
Color	Yellow	Verschueren 1983
Physical state	Liquid	Verschueren 1983
Melting point	5.7°C	Weast 1985
Boiling point	210.8°C	Weast 1985
Density at 20°C	1.2037	Weast 1985
Odor	Bitter almonds, shoe polish	Verschueren 1983
Odor threshold:		
Water	0.11 mg/L	Amoore and Hautala 1983
Air	0.092 mg/m <sup>3</sup>	Amoore and Hautala 1983
Solubility:		
Water at 20°C	1900 mg/L	Mabey et al. 1982
Organic solvents	Soluble in alcohol, ether, acetone, benzene	Weast 1985
Partition coefficients:		
Log K <sub>ow</sub>	1.87	Mabey et al. 1982
Log K <sub>oc</sub>	1.56	Mabey et al. 1982
Vapor Pressure at 20°C	0.15 mmHg	Mabey et al. 1982
Henry's law constant	1.31 x 10 <sup>-5</sup> atm-m <sup>3</sup> /mol	Mabey et al. 1982
Autoignition temperature	482°C	Sax and Lewis 1987
Flashpoint	87.7°C	Sax and Lewis 1987
Flammability limits	No data	
Conversion factors	1 ppm = 5.12 mg/m <sup>3</sup>	Verschueren 1983
	1 mg/m <sup>3</sup> = 0.20 ppm	Verschueren 1983

