

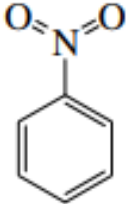
CHAPTER 4. CHEMICAL AND PHYSICAL INFORMATION

4.1 CHEMICAL IDENTITY

Nitrobenzene is a colorless to pale yellow oily liquid composed of a benzene ring with a single substituted nitro group. The compound is a synthetic chemical, and it does not occur naturally. It has an odor similar to bitter almonds or shoe polish. The chemical is primarily used in the synthesis of aniline and in producing the chemical intermediate to polyurethane. Nitrobenzene is also used as a solvent during petroleum refining and in the manufacture of cellulose ethers and acetates. It is a starting material for dinitrobenzenes, dichloroanilines, and other compounds including acetaminophen. Some of nitrobenzene's synonyms include mirbane oil and myrbane oil.

Table 4-1 lists common synonyms, trade names, and other pertinent identification information for nitrobenzene.

Table 4-1. Chemical Identity of Nitrobenzene

Characteristic	Information	Reference
Chemical name	Nitrobenzene	Pubchem 2021
Synonym(s) and Registered trade name(s)	Nitrobenzol; essence of mirbane, essence of myrbane; oil of mirbane; Mononitrobenzene; Nitrobenzol; Caswell No.600	Pubchem 2021
Chemical formula	C ₆ H ₅ NO ₂	Lide 2005
Chemical structure		Lide 2005
CAS registry number	98-95-3	Lei 2008; Lide 2005
UNII:	E57JCN6SSY	Pubchem 2021
EPA hazardous waste number	U169	Pubchem 2021
HSDB	104	Pubchem 2021

CAS = Chemical Abstracts Service; HSDB = Hazardous Substances Data Bank

4.2 PHYSICAL AND CHEMICAL PROPERTIES

Nitrobenzene is found in either crystal form or as an oily liquid. It is sparingly soluble in water and most organic solvents and it represents a fire hazard. It is completely miscible in diethyl ether, benzene, and alcohol. Nitrobenzene has a relatively high vapor pressure, which contributes to its flammability. Nitrobenzene has a relatively low K_{ow} value suggesting that it is unlikely to bioaccumulate.

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Nitrobenzene's low K_{oc} indicates its high to moderate mobility in soil. The Henry's Law constant for nitrobenzene suggests that it will volatilize from moist soil and water surfaces. The high vapor pressure of nitrobenzene indicates that if released into the air, it will exist solely as a vapor in the atmosphere. Table 4-2 lists important physical and chemical properties of nitrobenzene.

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Table 4-2. Physical and Chemical Properties of Nitrobenzene

Property	Information	Reference
Molecular weight	123.11 g/mol	Lei 2008; Lide 2005
Color	Colorless to greenish-yellow or yellow	Pubchem 2021
Physical state	Crystals or oily liquid	Haynes 2015
Melting point(s)	5.7 °C	Lide 2005
Boiling point(s)	210.8 °C	Lei 2008; Lide 2005
Critical temperature and pressure	720 K and 4.824 MN/M SQ	Pubchem 2021
Density	1.2037 g/cm ³ at 20 °C	Lide 2005
Viscosity	1.863 mPas at 25 °C	Lide 2005
Taste	Sweet (aqueous solutions)	Pubchem 2021
Odor	Volatile oil almond odor; pungent odor	Pubchem 2021
Odor threshold:		Pubchem 2021
Water	30-110 µg/L	
Air	4.7x10 ⁻³ ppm – 1.90 ppm	
Solubility:		Haynes 2015
Water	Slightly soluble in water; 2.1 g per kg H ₂ O at 25 °C	
Organic solvent(s) at 20 °C	Slightly soluble in carbon tetrachloride; very soluble in ethanol, diethyl ether, acetone, benzene	
Inorganic solvent(s)		
Partition coefficients:		
Log K _{ow}	1.85	Lei 2008; Lide 2005
Log K _{oc}	1.94	PubChem 2021
Relative Vapor Density	4.2 (air=1)	Pubchem 2021
Vapor pressure at 25 °C	0.245 mmHg	Pubchem 2021
Henry's law constant	2.3 at 25°C	Lei 2008
Degradation half-life in air via reaction with OH radicals	No data	
Dissociation constants:	pKa = 3.98 at 0°C	Lide 2005
Heat of combustion	-10,420 Btu/lb	Pubchem 2021
Heat of vaporization	55.01 kJ/mol at 25 °C	Haynes 2015
Autoignition temperature	900 °F	HSDB 2010
Flashpoint	88 °C	Haynes 2015
Flammability limits in air	1.8% by volume at 200°F	Lide 2005
Conversion factors:	4.05 mg/m ³ = 1 ppm	NIOSH 2018
Explosive limits	Moderate when exposed to heat or flame	Pubchem 2021
Incompatibilities and reactivity	Explosive reaction with solid or concentrated alkali and heat (e.g., sodium hydroxide or potassium hydroxide), aluminum chloride and phenol, aniline and glycerin, N ₂ O, AgClO ₄	Pubchem 2021

HSDB = Hazardous Substances Data Bank