

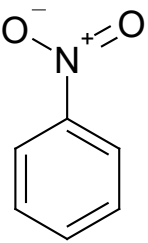
CHAPTER 4. CHEMICAL AND PHYSICAL INFORMATION

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	NLM 2021
Synonym(s) and registered trade name(s)	Nitrobenzol; essence of mirbane, essence of myrbane; oil of mirbane; mononitrobenzene; nitrobenzol; Caswell No.600	NLM 2021
Chemical formula	C ₆ H ₅ NO ₂	Lide 2005
Chemical structure		Lide 2005
CAS registry number	98-95-3	Lei et al. 2008; Lide 2005

CAS = Chemical Abstracts Service

4.2 PHYSICAL AND CHEMICAL PROPERTIES

Nitrobenzene is a liquid at room temperature. 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.

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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. 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.

Table 4-2. Physical and Chemical Properties of Nitrobenzene

Property	Information	Reference
Molecular weight	123.11 g/mol	Lei et al. 2008; Lide 2005
Color	Colorless to greenish-yellow or yellow	NLM 2021
Physical state	Crystals or oily liquid	Haynes 2015
Melting point(s)	5.7°C	Lide 2005
Boiling point(s)	210.8°C	Lei et al. 2008; Lide 2005
Critical temperature and pressure	720 K and 4.824 MN/M SQ	NLM 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)	NLM 2021
Odor	Volatile oil almond odor; pungent odor	NLM 2021
Odor threshold:		NLM 2021
Water	30–110 µg/L	
Air	4.7x10 ⁻³ –1.90 ppm	
Solubility:		Haynes 2015
Water	2.1 g/LH 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 et al. 2008; Lide 2005
Log K_{oc}	1.94	NLM 2021
Relative Vapor Density	4.2 (air=1)	NLM 2021
Vapor pressure at 25°C	0.245 mmHg	NLM 2021
Henry's law constant	2.3 x10 ⁻⁵ atm m ³ /mol at 25°C	Lei et al. 2008
Degradation half-life in air via reaction with OH radicals	44 days	EPA 2012
Heat of combustion	-10,420 Btu/pound	NLM 2021
Heat of vaporization	55.01 kJ/mol at 25°C	Haynes 2015
Autoignition temperature	900°F	NFPA 2002
Flashpoint	88°C	Haynes 2015

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Table 4-2. Physical and Chemical Properties of Nitrobenzene

Property	Information	Reference
Flammability limits in air	1.8% by volume at 200°F	Lide 2005
Conversion factors:	1 mg/m ³ =0.199 ppm ^a 1 ppm=5.04 mg/m ³	
Explosive limits	Moderate when exposed to heat or flame	NLM 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, and AgClO ₄	NLM 2021

^aConcentration (ppm) = 24.45 x concentration (mg/m³)/molecular weight at standard temperature and pressure.