

3. CHEMICAL AND PHYSICAL INFORMATION

3.1 CHEMICAL IDENTITY

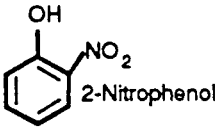
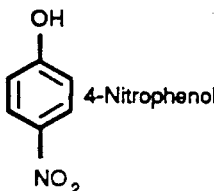
Mononitrophenols exist in three isomeric forms: 2-nitrophenol (or ortho- or o-), 3-nitrophenol (or meta- or m-), and 4-nitrophenol (or para- or p-). In this document, the two high-production-volume chemicals, 2-nitrophenol and 4-nitrophenol will be discussed. Data pertaining to the chemical identities of these two nitrophenols are listed in Table 3-1.

3.2 PHYSICAL AND CHEMICAL PROPERTIES

The physical and chemical properties of the two nitrophenols are presented in Table 3-2. Both the nitrophenols are weak acids compared to carboxylic acids, but the nitro substitution makes them both stronger acids than phenol. 2-Nitrophenol is volatile in steam, but 4-nitrophenol is not. The nitrophenols can be converted to their water-soluble salts by alkaline hydroxides. The OH-group in these compounds is susceptible to substitution reactions with the formation of ethers and esters. The nitro group can be reduced to the amino group under strong reducing conditions. The nitrophenols may also undergo ring substitution reactions (EPA 1985; Morrison and Boyd 1969).

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TABLE 3-1. Chemical Identities of 2-Nitrophenol and 4-Nitrophenol

Characteristic	2-Nitrophenol	4-Nitrophenol	Reference
Chemical name	2-Nitrophenol	4-Nitrophenol	
Synonyms	2-Hydroxynitro- benzene o-nitrophenol	4-Hydroxynitro- benzene p-nitrophenol, PNP	HSDB 1989
Trade names	Atonik	No data	OHM/TADS 1989
Chemical formula	$C_6H_5NO_3$	$C_6H_5NO_3$	HSDB 1989
Chemical structure	 2-Nitrophenol	 4-Nitrophenol	Windholz 1983
Identification numbers:			HSDB 1989
CAS registry	88-75-5	100-02-7	
NIOSH RTECS	21000	22750	
EPA hazardous waste	No data	U170	
OHM/TADS	7800021	7800022	
DOT/UN/NA/IMCO shipping	UN1663;IMO6.1	UN1663;IMO6.1	
HSDB	1133	1157	
NCI	No data	C55992	

CAS = Chemical Abstracts Service

DOT/UN/NA/IMCO = Department of Transportation/United Nations/North America/International 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 3-2. Physical and Chemical Properties of 2-Nitrophenol and 4-Nitrophenol

Property	2-Nitrophenol	4-Nitrophenol	Reference
Molecular weight	139.11	139.11	
Color	Light yellow	Colorless to light yellow	HSDB 1989
Physical state	Crystalline solid	Crystalline solid	HSDB 1989
Melting point	44-45°C	113-114°C	HSDB 1989
Boiling point	216°C	297°C	HSDB 1989
Density	1.495 g/cc at 14°C	1.270 g/cc at 20°C	HSDB 1989
Dissociation constant (pKa)	7.21-7.23	7.08-7.18	Pearce and Simkins 1968; Polster et al. 1986; Schwarzenbach et al. 1988
Odor	Peculiar aromatic	Slight odor	HSDB 1989; Verschuieren 1963
Odor threshold:			
Water	no data	2.5 mg/L	Verschuieren 1963
Air	0.0012 mg/m ³	2.3 mg/m ³	Verschuieren 1983
Solubility:			
Distilled water	1400 mg/L at 25°C; 2100 mg/L at 25°C	16,000 mg/L at 25°C	Leuenberger et al. 1985; Verschuieren 1983
Sea water	1160 mg/L at 20°C	10,795 mg/L at 20°C	Hashimoto et al. 1984
Organic solvents	Soluble in benzene, CS ₂ , alkali hydroxides, ethanol, ethyl ether, and acetone	Soluble in toluene, ethanol, chloroform, ethyl ether, and alkali hydroxides	HSDB 1989
Partition coefficients:			
Log octanol/water	1.79	1.91	Hansch and Leo 1985
Log K _{oc}	2.06	2.18-2.42	Boyd 1982; Hodson and Williams 1938
Vapor pressure (mmHg)	0.12; 0.11 at 25°C	0.0003 at 30°C	Leuenberger et al. 1985; McCrady et al. 1985; Scala and Banerjee 1982
Henry's law constant	1.6x10 ⁻⁵ atm-m ³ /mol at 25°C	3.5x10 ⁻⁹ atm-m ³ /mol at 25-30°C	Leuenberger et al. 1985; McCrady et al. 1985
Autoignition temperature	No data	No data	HSDB 1989
Flashpoint	73.5°C	No data	OHM/TADS 1989
Flammability limits	No data	No data	HSDB 1985
Conversion factors:			
ppm (v/v) to mg/m ³ in air at 20°C	1 ppm = 5.783 mg/m ³	1 ppm = 5.783 mg/m ³	
mg/m ³ to ppm (v/v) in air at 20°C	1 mg/m ³ = 0.173 ppm	1 mg/m ³ = 0.173 ppm	
Explosive limits	no data	no data	

