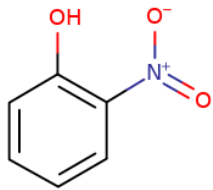


CHAPTER 4. CHEMICAL AND PHYSICAL INFORMATION

4.1 CHEMICAL IDENTITY

Nitrophenols (also referred to as 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-). All three of these nitrophenols are manmade. Table 4-1 lists common synonyms, trade names, and other pertinent identification information for 2-nitrophenol, Table 4-2 lists this information for 3-nitrophenol, and Table 4-3 lists this information for 4-nitrophenol.

Table 4-1. Chemical Identity of 2-Nitrophenol

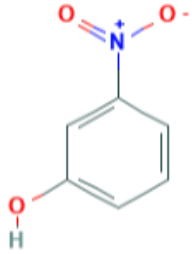
Characteristic	Information
Chemical Name	2-Nitrophenol
Synonym(s) and Registered trade name(s)	O-Hydroxynitrobenzene; 2-Hydroxynitrobenzene; o-Nitrophenol; Phenol, o-nitro-; Phenol, 2-nitro
Chemical formula	C ₆ H ₅ NO ₃
Chemical structure	
CAS registry number	88-75-5

CAS = Chemical Abstracts Service

Source: NLM 2022a

4. CHEMICAL AND PHYSICAL INFORMATION

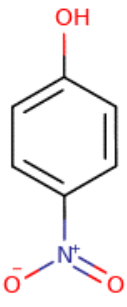
Table 4-2. Chemical Identity of 3-Nitrophenol

Characteristic	Information
Chemical Name	3-Nitrophenol
Synonym(s) and Registered trade name(s)	M-Hydroxynitrobenzene; 3-Hydroxynitrobenzene; m-Nitrophenol; Phenol, m-nitro-; Phenol, 3-nitro-;
Chemical formula	C ₆ H ₅ NO ₃
Chemical structure	
CAS registry number	554-84-7

CAS = Chemical Abstracts Service

Source: NLM 2022b

Table 4-3. Chemical Identity of 4-Nitrophenol

Characteristic	Information
Chemical Name	4-Nitrophenol
Synonym(s) and Registered trade name(s)	P-Hydroxynitrobenzene; 4-Hydroxynitrobenzene; Niphen; P-Nitrophenol; Paranitrophenol; Phenol, p-nitro-; Phenol, 4-nitro-; PNP
Chemical formula	C ₆ H ₅ NO ₃
Chemical structure	
CAS registry number	100-02-7

CAS = Chemical Abstracts Service

Source: NLM 2022c

4. CHEMICAL AND PHYSICAL INFORMATION

4.2 PHYSICAL AND CHEMICAL PROPERTIES

2-Nitrophenol is a light yellow, aromatic solid; 3- and 4-nitrophenol are colorless to pale yellow solids. The nitrophenols are expected to be highly soluble in water. They also have low vapor pressures, and therefore, low potential for long range atmospheric transport (Harrison et al. 2005). Tables 4-4, 4-5, and 4-6. List important physical and chemical properties of 2-, 3-, and 4-nitrophenol, respectively.

4. CHEMICAL AND PHYSICAL INFORMATION

Table 4-4. Physical and Chemical Properties of 2-Nitrophenol

Property	Information	Reference
Molecular weight	139.109	NLM 2022a
Color	Light yellow	O'Neil 2006
Physical state	Crystalline solid	NLM 2022a
Melting point	44–45°C	O'Neil 2006
Boiling point	216°C	Haynes et al. 2015
Density:	1.29 g/cm ³ at 40°C	Haynes et al. 2015
Odor	Aromatic	O'Neil 2006
Odor threshold:		
Water	10 mg/L	Verschueren1983
Air	8x10 ⁻¹¹ moles/m ³	Fazzalari 1978
Taste threshold	0.001 mg/L	Verschueren1983
Solubility:		
Water	2,100 mg/L at 20°C 2,500 mg/L at 25°C 10,800 mg/L at 100°C	Verschueren 1983 Yalkowsky et al. 2010 Verschueren 1983
Organic solvent(s)	Very soluble in ethanol, ether, acetone, benzene, pyridine, chlorine; freely soluble in carbon sulfide, alkali hydroxides	Budavari 1996; Haynes et al. 2015
Partition coefficients:		
Log K _{ow}	1.79	Hansch et al. 1995
Log K _{oc}	1.76–2.04	Gawlik et al. 1998; Tülp et al. 2009
Vapor pressure At 20°C	0.113 mm Hg at 25°C	NLM 2022a
Henry's law constant	1.3x10 ⁻⁵ at 20°C 1.63x10 ⁻⁵ at 25°C	Tremp et al. 1993 Harrison et al. 2002
Disassociation constant (pKa)	7.23	NLM 2022a
Autoignition temperature	550°C	NLM 2022a
Flashpoint	108°C	NLM 2022a
Flammability limits	No data	NLM 2022a
Conversion factors		
ppm (v/v) to mg/m ³ in air at 20°C	1 ppm=5.783 mg/m ³	NLM 2022a
mg/m ³ to ppm (v/v) in air at 20°C	1 mg/m ³ =0.173 ppm	
Explosive limits	No data	NLM 2022a

4. CHEMICAL AND PHYSICAL INFORMATION

Table 4-5. Physical and Chemical Properties of 3-Nitrophenol

Property	Information	Reference
Molecular weight	139.11 g/mol	NLM 2022b
Color	Colorless to pale yellow	NLM 2022b
Physical state	Crystalline solid	NLM 2022b
Melting point	96.8°C	NLM 2022b
Boiling point	194°C	NLM 2022b
Density: At 20°C/4°C	1.485	O'Neil 2006
Odor	Aromatic to sweetish	Sittig 1981
Odor threshold: Water Air	0.6 m/L 3.0 mg/m ³	Verschueren 1983
Taste threshold	No data	
Solubility: Water Organic solvent(s)	13,550 mg/L at 25°C 133,000 mg/L at 90°C Very soluble in acetone, ether, ethanol, benzene	Yalkowsky et al. 2010 Verschueren 1983 Haynes et al. 2015
Partition coefficients: Log K _{ow} Log K _{oc}	2.00 1.68	Hansch et al. 1995 Borisover and Graber 1997
Vapor pressure	5.85x10 ⁻⁵ mm Hg at 25°C	Bannan et al. 2017
Henry's law constant	2.00x10 ⁻⁹ atm-m ³ /mole at 25°C	NLM 2022b
Dissociation constant	8.36	NLM 2022b
Autoignition temperature	400°C	NLM 2022b
Flashpoint	>100°C	NLM 2022b
Flammability limits	No data	NLM 2022b
Conversion factors ppm (v/v) to mg/m ³ in air at 20°C mg/m ³ to ppm (v/v) in air at 20°C	1 mg/m ³ =0.18 ppm 1 ppm=5.69 mg/m ³	NLM 2022b
Explosive limits	No data	NLM 2022b

4. CHEMICAL AND PHYSICAL INFORMATION

Table 4-6. Physical and Chemical Properties of 4-Nitrophenol

Property	Information	Reference
Molecular weight	139.11	O'Neil 2006
Color	Colorless to slightly yellow	O'Neil 2006
Physical state	Solid	NLM 2022c
Melting point	113–114°C	O'Neil 2006
Boiling point	279°C	Lewis 2007
Density: At 20°C	1.479 g/cm ³	Lewis 2007
Odor	Odorless	O'Neil 2006
Odor threshold:		
Water	2.5 mg/L	Verschueren1983
Air	2.3 mg/m ³	
Taste threshold	43.4 mg/L	NLM 2022c
Solubility:		
Water	10,000 mg/L at 15°C 15,600 mg/L at 25°C	Verschueren1983 Yalkowsky et al. 2010
Organic solvent(s)	Very soluble in ethanol, ether, and acetone; freely soluble in alcohol, chloroform; soluble in solution of fixed alkali hydroxides and carbonates	Haynes et al. 2015; O'Neil 2006
Partition coefficients:		
Log K _{ow}	1.91	Hansch et al. 1995
Log K _{oc}	2.37	Schüürmann et al. 2006
Vapor pressure	1.2x10 ⁻⁵ mm Hg at 25°C	Bannan et al. 2017
Henry's law constant	1.28x10 ⁻⁸ atm-m ³ /mol at 20°C	Tremp et al. 1993
Dissociation constant	7.15	NLM 2022c
Autoignition temperature	490°C	NLM 2022c
Flashpoint	169°C	NLM 2022c
Flammability limits	No data	NLM 2022c
Conversion factors		
ppm (v/v) to mg/m ³ in air at 20°C	1 mg/m ³ =0.173 ppm	NLM 2022c
mg/m ³ to ppm (v/v) in air at 20°C	1 ppm=5.783 mg/m ³	
Explosive limits	No data	NLM 2022c