

4. CHEMICAL AND PHYSICAL INFORMATION

4.1 CHEMICAL IDENTITY

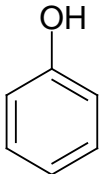
Information regarding the chemical identity of phenol is located in Table 4-1.

4.2 PHYSICAL AND CHEMICAL PROPERTIES

Information regarding the physical and chemical properties of phenol is located in Table 4-2.

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Table 4-1. Chemical Identity of Phenol

Characteristic	Information	Reference
Chemical name	Phenol	Lide 2005
Synonym(s)	Benzenol, hydroxylbenzene, monophenol, oxybenzene, phenyl alcohol, phenyl hydrate, phenyl hydroxide, phenylic acid, phenylic alcohol	Lewis 2000
Registered trade name(s)	Carbolic acid, phenic acid, phenic alcohol	Gardner et al. 1978
Chemical formula	C ₆ H ₆ O	Lide 2005
Chemical structure		Budavari et al. 1989
Identification numbers:		
CAS registry	108-95-2	HSDB 2008
NIOSH RTECS	SJ3325000	RTECS 2006
EPA hazardous waste	U188	EPA 1998; HSDB 2008
DOT/UN/NA/IMCO shipping	UN 1671 (solid) UN 2312 (molten) UN 2821 (solution) IMO 6.1 (solid, molten, solution)	HSDB 2008
HSDB	113	HSDB 2008
NCI	C50124	Lewis 2000

CAS = Chemical Abstracts Services; 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; RTECS=Registry of Toxic Effects of Chemical Substances

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Table 4-2. Physical and Chemical Properties of Phenol

Property	Information	Reference
Molecular weight	94.111	Lide 2005
Color	Colorless to light pink	HSDB 2008
Physical state	Crystalline solid liquid (w/ 8% H ₂ O)	
Melting point	40.89 °C	Lide 2005
Boiling point	181.87 °C	Lide 2005
Density at 20 °C/4 °C	1.0545 at 45 °C/4 °C	Lide 2005
Vapor density	3.24	Lewis 2000
Odor	Distinct aromatic, somewhat sickening, sweet and acrid odor	HSDB 2008
Odor threshold:		
Water	7.9 ppm (w/v) 1 ppm (w/v)	Amoore and Hautala 1983 Baker et al. 1978
Air	0.040 ppm (v/v)	Amoore and Hautala 1983
Solubility:		
Water at 25 °C	8.28x10 ⁴ mg/L	Southworth and Keller 1986
Organic solvent(s)	Soluble in water and ethanol, very soluble in ether, miscible with acetone and benzene	Lide 2005
Partition coefficients:		
Log K _{ow}	1.46	HSDB 2008
Log K _{oc}	1.21–1.96	Artiola-Fortuny and Fuller 1982; Boyd 1982; Briggs 1981; Sacan and Balcioglu 1996; Scott et al. 1983
Vapor pressure at 25 °C	0.35 mmHg	HSDB 2008
Henry's law constant	3.0x10 ⁷ atm m ³ -mol	Gaffney et al. 1987
Autoignition temperature	715 °C	Lewis 2000
Flashpoint, open cup	85 °C	HSDB 2008
Flashpoint, closed cup	79 °C	HSDB 2008
Flammability limits (in air, by % v)	1.7–8.6%	HSDB 2008
Conversion factors:		
ppm (v/v) to mg/m ³ in air (25 °C)	ppm (v/v)x3.92=mg/m ³	
mg/m ³ to ppm (v/v) in air (25 °C)	mg/m ³ x0.225=ppm (v/v)	

atm = atmosphere; v = volume; w = weight