

4. CHEMICAL AND PHYSICAL INFORMATION

4.1 CHEMICAL IDENTITY

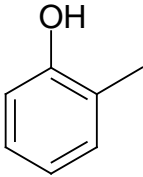
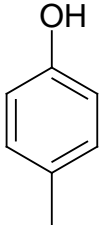
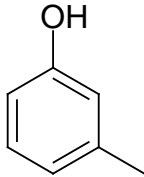
Data pertaining to the chemical identity of cresols are listed in Table 4-1.

4.2 PHYSICAL AND CHEMICAL PROPERTIES

The physical and chemical properties of cresols are presented in Table 4-2.

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Table 4-1. Chemical Identity of Cresols

Characteristics	<i>o</i> -Cresol	<i>p</i> -Cresol	<i>m</i> -Cresol	<i>o</i> -, <i>m</i> -, <i>p</i> -Cresol	References
Chemical name	<i>o</i> -Cresol	<i>p</i> -Cresol	<i>m</i> -Cresol	(<i>o</i> , <i>m</i> , <i>p</i>)-Cresol	ChemID 2008
Synonyms	2-Methylphenol; 2-hydroxy- toluene; <i>o</i> -cresylic acid	4-Methylphenol; 4-hydroxy- toluene; <i>p</i> -cresylic acid	3-Methylphenol 3-hydroxy- toluene; <i>m</i> -cresylic acid	Methylphenol; hydroxytoluene; cresylic acid	ChemID 2008; HSDB 2008; SANSS 1989
Trade names	No data	No data	No data	No data	
Chemical formula	C ₇ H ₈ O	C ₇ H ₈ O	C ₇ H ₈ O	C ₇ H ₈ O	ChemID 2008
Chemical structure				Mixture of three previous isomers	
Identification numbers:					
CAS registry	95-48-7	106-44-5	108-39-4	1319-77-3	ChemID 2008
NIOSH RTECS	GO6300000	GO6475000	GO61250000	GO5950000	SANSS 1989
EPA hazardous waste	F004; U052	F004; U052	F004; U052	F004; U052	HSDB 2008
DOT/UN/NA/IMCO shipping	UN 2022; UN 3455; UN 2076; IMO 6.1	UN 2022; UN 3455; UN 2076; IMO 6.1	UN 2022; UN 3455; UN 2076; IMO 6.1	UN 2022; UN 3455; UN 2076; IMO 6.1	HSDB 2008
HSDB	1813	1814	1815	250	HSDB 2008
NCI	No data	No data	No data	No data	

CAS = Chemical Abstracts Service; DOT/UN/NA/IMCO = Department of Transportation/United Nations/North America/Intergovernmental Maritime Consultative Organization; EPA = Environmental Protection Agency; HSDB = Hazardous Substance 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 Cresols

Property	<i>o</i> -Cresol	<i>m</i> -Cresol	<i>p</i> -Cresol	Mixture of <i>o</i> -, <i>p</i> -, and <i>m</i> -cresol	References
Molecular weight	108.14	108.14	108.14	108.14	O'Neil et al. 2001
Color	White crystals darken with age	Colorless to yellowish	No data	Colorless, yellowish, brownish-yellow, or pinkish	O'Neil et al. 2001
Physical state	Solid	Liquid	Solid	Liquid	O'Neil et al. 2001
Melting point	30.944 °C	12.22 °C	34.739 °C	11–35 °C	Lewis 2001; Riddick et al. 1986
Boiling point					
1 atm	191.004 °C	202.32 °C	201.94 °C	191–203 °C	Riddick et al. 1986
10 mmHg	74.9 °C	86 °C	85.7 °C	No data	Lewis 2001; Lide 2005
Density (20 °C)	1.047 g/mL	1.034 g/mL	1.0341 g/mL	1.030–1.038 g/mL	O'Neil et al. 2001
Odor	Phenol-like	Phenol-like	Phenol-like	Phenol-like	O'Neil et al. 2001
Odor threshold					
Water	No data	0.037 ppm	No data	No data	Amoore and Hautala 1983
Air	No data	0.00028 ppm	No data	No data	Amoore and Hautala 1983
Solubility					
Water at 25 °C	25,950 ppm	22,700 ppm	21,520 ppm	No data	Yalkowsky et al. 1987
Organic solvents	Alcohol, ether, acetone, benzene, chloroform, alkali hydroxides (aqueous)	Alcohol, ether, acetone, benzene, chloroform, alkali hydroxides (aqueous)	Alcohol, ether, acetone, benzene, chloroform, alkali hydroxides (aqueous)	Alcohol, glycol, base	Lewis 2001; Lide 2005; O'Neil et al. 2001
Partition coefficients					
Log octanol/water	1.95	1.96	1.94	No data	Hansch and Leo 1985
Log K _{oc}	1.03	1.54	1.69	No data	Artiola-Fortuny and Fuller 1982; Boyd 1982
Vapor pressure					
25 °C	0.299 mmHg	0.138 mmHg	0.11 mmHg	No data	AIChE 1989,2000, Chao et al. 1983

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Henry's law constant atm/m ³ -molecule at 25 °C	1.2x10 ⁻⁶	8.65x10 ⁻⁷ (calculated from vapor pressure and water solubility)	7.92x10 ⁻⁷	No data	Gaffney et al. 1987; Hine and Mookerjee 1975
Flashpoint (closed cup)	81 °C	85 °C	86 °C	82 °C	Lewis 2001
Flammability limits	1.4% (lower)	1.1% (lower)	1.1% (lower)		HSDB 2008
Conversion factors					
ppm (v/v) to mg/m ³ in air (20 °C)	4.50	4.50	4.50	4.50	Verschueren 1983
mg/m ³ to ppm (v/v) in air (20 °C)	0.22	0.22	0.22	0.22	Verschueren 1983
Bioconcentration factor					
Log BCF	1.25 (calculated from K _{ow})	1.30	1.24 (calculated from K _{ow})	No data	Freitag et al. 1985; Thomas 1982
Explosive limits	No data	No data	No data	No data	