

4. CHEMICAL AND PHYSICAL INFORMATION

4.1 CHEMICAL IDENTITY

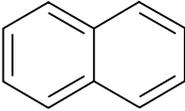
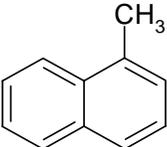
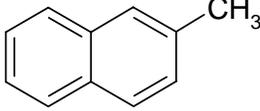
Information regarding the chemical identity of naphthalene, 1-methylnaphthalene, and 2-methylnaphthalene is located in Table 4-1.

4.2 PHYSICAL AND CHEMICAL PROPERTIES

Information regarding the physical and chemical properties of naphthalene, 1-methylnaphthalene, and 2-methylnaphthalene is located in Table 4-2.

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Table 4-1. Chemical Identity of Naphthalene, 1-Methylnaphthalene, and 2-Methylnaphthalene

Characteristic	Naphthalene	1-Methylnaphthalene	2-Methylnaphthalene	Reference
Synonyms	Tar camphor; albicarbon; naphthene; mothballs; moth- flakes; white tar; and others	Alpha-methyl- naphthalene; naphthalene, 1-methyl; naphthalene, alpha- methyl	Beta-methyl- naphthalene; naphthalene, 2-methyl; naphthalene, beta- methyl	HSDB 2004
Trade name	Caswell No. 5877®	No data	No data	HSDB 2004
Chemical formula	C ₁₀ H ₈	C ₁₁ H ₁₀	C ₁₁ H ₁₀	HSDB 2004
Chemical structure				HSDB 2004
Identification numbers:				
CAS registry	91-20-3	90-12-0	91-57-6	HSDB 2004
NIOSH RTECS	QJ0525000	QJ9630000	QJ9635000	NIOSH 1987
EPA hazardous waste	U165	No data	No data	HSDB 2004
OHM/TADS	7216808	No data	No data	Agency for Toxic Substances and Disease Registry 1995
DOT/UN/NA/IMCO shipping	UN1334, UN2304, IMCO 4.1	No data	No data	HSDB 2004
HSDB	184	5268	5274	HSDB 2004
NCI	C52904	No data	No data	HSDB 2004

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 4-2. Physical and Chemical Properties of Naphthalene, 1-Methylnaphthalene, and 2-Methylnaphthalene

Property	Naphthalene	1-Methyl-naphthalene	2-Methyl-naphthalene	Reference
Molecular weight	128.19	142.20	142.20	Weast et al. 1985
Color	White	Colorless	No data	Verschuieren 1983
Physical state	Solid	Liquid	Solid	Verschuieren 1983
Melting point	80.5 °C	-22 °C	34.6 °C	Weast et al. 1985
Boiling point	218 °C	244.6 °C	241 °C	Sax and Lewis 1989; Weast et al. 1985
Density at 20 °C	1.145 g/mL	1.0202 g/mL	1.0058 g/mL	Weast et al. 1985
Odor	Strong (tar or mothballs)	No data	No data	HSDB 2004
Odor threshold:				
Water	0.021 mg/L	0.0075 mg/L	0.01 mg/L	Amoore and Hautala 1983; HSDB 2004; Verschuieren 1983
Air	0.44 mg/m ³	No data	0.0581–0.2905 mg/m ³	Amoore and Hautala 1983; Ruth 1986
Solubility:				
Water at 25 °C	31.7 mg/L	25.8 mg/L	24.6 mg/L	EPA 1982e; HSDB 2004
Organic solvents	Soluble in benzene, alcohol, ether, acetone	Soluble in alcohol, ether, benzene	Soluble in alcohol, ether, benzene	Sax and Lewis 1989; Weast et al. 1985
Partition coefficients:				
Log K _{ow}	3.29	3.87	3.86	EPA 1982e; HSDB 1995
Log K _{oc}	2.97	No data	3.39	EPA 1982e; GDCH 1992; Kenaga 1980
Vapor pressure	0.087 mmHg	0.054 mmHg	0.068 mmHg	EPA 1982e; HSDB 1995
Henry's law constant	4.6x10 ⁻⁴ atm-m ³ /mol	3.6x10 ⁻⁴ atm-m ³ /mol	4.99x10 ⁻⁴ atm-m ³ /mol	EPA 1982e; Yaws et al. 1991
Autoignition temperature	567 °C	529 °C	No data	Sax and Lewis 1989
Flashpoint	79 °C (open cup)	No data	No data	Sax and Lewis 1989
Flammability limits	0.9–5.9%	No data	No data	HSDB 2004
Conversion factors	1 ppm=5.24 mg/m ³ 1 mg/m ³ =0.191 ppm	1 ppm=5.91 mg/m ³ 1 mg/m ³ =0.17 ppm	1 ppm=5.91 mg/m ³ 1 mg/m ³ =0.17 ppm	Verschuieren 1983
Explosive limits	No data	No data	No data	