

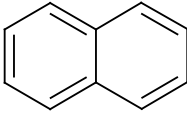
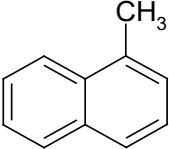
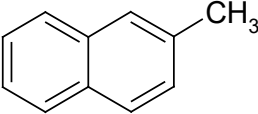
CHAPTER 4. CHEMICAL AND PHYSICAL INFORMATION

4.1 CHEMICAL IDENTITY

Naphthalene is a two-ringed aromatic hydrocarbon with a molecular formula of $C_{10}H_8$; it is the smallest PAH with two fused benzene rings. Both 1- and 2-methylnaphthalene contain a single methyl substituent in their structure, connected one (alpha) or two (beta) carbon atoms away from the joined rings.

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

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

Characteristic	Naphthalene	1-Methylnaphthalene	2-Methylnaphthalene	Reference
Synonyms and registered trade name(s)	Tar camphor; albocarbon; naphthene; mothballs; moth-flakes; white tar; and others; Caswell No. 587®	Alpha-methylnaphthalene; naphthalene, 1-methyl; naphthalene, alpha-methyl	Beta-methylnaphthalene; naphthalene, 2-methyl; naphthalene, beta-methyl	NLM 2023a, 2023b, 2023c
Chemical formula	$C_{10}H_8$	$C_{11}H_{10}$	$C_{11}H_{10}$	NLM 2023a, 2023b, 2023c
SMILES	<chem>C1=CC=C2C=CC=CC2=C1</chem>	<chem>CC1=CC=CC2=CC=CC=C12</chem>	<chem>CC1=CC2=CC=CC=C2C=C1</chem>	NLM 2023a, 2023b, 2023c
Chemical structure				NLM 2023a, 2023b, 2023c
CAS Registry Number	91-20-3	90-12-0	91-57-6	NLM 2023a, 2023b, 2023c

CAS = Chemical Abstracts Service; SMILES = simplified molecular-input line-entry system

4.2 PHYSICAL AND CHEMICAL PROPERTIES

Naphthalene is a white solid with a strong characteristic odor. Naphthalene has relatively low vapor pressure; it sublimates slowly at room temperature and appreciably above its melting point. It has low solubility in water but is very soluble in several organic solvents such as benzene, ethanol, and ether.

4. CHEMICAL AND PHYSICAL INFORMATION

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

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	128.17	142.20	142.20	NLM 2023a, 2023b, 2023c
Color	White	Colorless	No data	NLM 2023a, 2023b, 2023c
Physical state	Solid	Liquid	Solid	NLM 2023a, 2023b, 2023c
Melting point	80.2°C	-22°C	34.6°C	NLM 2023a, 2023b, 2023c
Boiling point	217.9°C	244°C	241.1°C	NLM 2023a, 2023b, 2023c
Density at 20°C	1.162 g/mL	1.0202 g/mL	1.0058 g/mL	NLM 2023a, 2023b, 2023c
Vapor density (air = 1)	4.42	4.91	No data	NLM 2023a, 2023b, 2023c
Odor	Strong (tar or mothballs)	No data	No data	NLM 2023a, 2023b, 2023c
Odor threshold:				
Water	0.021 mg/L; 6.80 mg/L	0.0075 mg/L	0.01 mg/L	Amoore and Hautala 1983; NLM 2023a; Verschueren 1983
Air	0.44 mg/m ³	0.12 mg/m ³	0.0581– 0.2905 mg/m ³	NLM 2023a, 2023b, 2023c
Solubility:				
Water at 25°C	31 mg/L	25.8 mg/L	24.6 mg/L	NLM 2023a, 2023b, 2023c
Organic solvents	Soluble in benzene, alcohol, ether, acetone	Soluble in alcohol, ether, benzene	Soluble in alcohol, ether, benzene	NLM 2023a, 2023b, 2023c
Partition coefficients:				
Log K _{ow}	3.30	3.87	3.86	NLM 2023a, 2023b, 2023c
Log K _{oc}	2.05–3.97	3.36; 3.64	3.00–5.96	NLM 2023a, 2023b, 2023c
Vapor pressure at 25°C	0.085 mmHg (sublimes)	0.067 mmHg	0.055 mmHg	NLM 2023a, 2023b, 2023c

4. CHEMICAL AND PHYSICAL INFORMATION

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

Henry's law constant at 25°C	4.4x10 ⁻⁴ atm-m ³ /mol	5.14x10 ⁻⁴ atm-m ³ /mol	5.18x10 ⁻⁴ atm-m ³ /mol	NLM 2023a, 2023b, 2023c
Autoignition temperature	526°C	529°C	No data	NLM 2023a, 2023b, 2023c
Flashpoint (closed cup)	79°C	82°C	98°C	NLM 2023a, 2023b, 2023c
Vapor pressure at 25°C	0.085 mmHg	0.067 mmHg	0.055 mmHg	NLM 2023a, 2023b, 2023c
Henry's law constant at 25°C	4.4x10 ⁻⁴ atm-m ³ /mol	5.14x10 ⁻⁴ atm-m ³ /mol	5.18x10 ⁻⁴ atm-m ³ /mol	NLM 2023a, 2023b, 2023c
Autoignition temperature	526°C	529°C	No data	NLM 2023a, 2023b, 2023c
Flashpoint (closed cup)	79°C	82°C	98°C	NLM 2023a, 2023b, 2023c
Flammability limits	0.9–5.9%	No data	No data	NLM 2023a, 2023b, 2023c
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	Verschueren 1983
Explosive limits	No data	No data	No data	