Naphthalene, 2-methyl-

Other names:	2-Methylnaphthalene
	2-Methylnapthalene
	2-methylnaphthalene
	BETA-METHYLNAPHTHALENE
	Methyl-2-naphthalene
	«beta»-Methylnaphthalene
	Â«betaÂ»-Methylnaphthalene
Inchi:	InChI=1S/C11H10/c1-9-6-7-10-4-2-3-5-11(10)8-9/h2-8H,1H3
InchiKey:	QIMMUPPBPVKWKM-UHFFFAOYSA-N
Formula:	C11H10
SMILES:	Cc1ccc2ccccc2c1
Mol. weight [g/mol]:	142.20
CAS:	91-57-6

Physical Properties

Property code	Value	Unit	Source
af	0.3820		KDB
affp	830.90	kJ/mol	NIST Webbook
affp	831.90	kJ/mol	NIST Webbook
basg	802.40	kJ/mol	NIST Webbook
basg	802.10	kJ/mol	NIST Webbook
chs	-5792.70 ± 2.20	kJ/mol	NIST Webbook
chs	-5802.70 ± 1.50	kJ/mol	NIST Webbook
dm	0.40	debye	KDB
ea	0.14 ± 0.07	eV	NIST Webbook
gf	216.30	kJ/mol	KDB
hf	106.20	kJ/mol	NIST Webbook
hf	116.20	kJ/mol	KDB
hf	116.10 ± 2.60	kJ/mol	NIST Webbook
hfs	35.00 ± 2.20	kJ/mol	NIST Webbook
hfs	44.90 ± 1.50	kJ/mol	NIST Webbook
hfus	14.92	kJ/mol	Joback Method
hsub	71.20	kJ/mol	NIST Webbook
hsub	71.30 ± 2.10	kJ/mol	NIST Webbook
hsub	65.69 ± 0.84	kJ/mol	NIST Webbook
hvap	45.31	kJ/mol	NIST Webbook
ie	7.91 ± 0.06	eV	NIST Webbook

ie	7.85	eV	NIST Webbook
ie	7.93	eV	NIST Webbook
ie	8.01 ± 0.03	eV	NIST Webbook
ie	7.96 ± 0.01	eV	NIST Webbook
ie	8.10 ± 0.03	eV	NIST Webbook
ie	8.45 ± 0.05	eV	NIST Webbook
ie	7.83	eV	NIST Webbook
ie	7.93	eV	NIST Webbook
ie	7.80	eV	NIST Webbook
ie	7.91 ± 0.02	eV	NIST Webbook
log10ws	-3.77		Aqueous Solubility Prediction Method
log10ws	-3.77		Estimated Solubility Method
logp	3.148		Crippen Method
mcvol	122.630	ml/mol	McGowan Method
pc	3293.06 ± 151.99	kPa	NIST Webbook
pc	3500.00	kPa	KDB
rinpol	221.20		NIST Webbook
rinpol	1262.00		NIST Webbook
rinpol	1307.00		NIST Webbook
rinpol	1259.00		NIST Webbook
rinpol	1279.00		NIST Webbook
rinpol	1304.00		NIST Webbook
rinpol	1282.60		NIST Webbook
rinpol	218.14		NIST Webbook
rinpol	218.21		NIST Webbook
rinpol	218.14		NIST Webbook
rinpol	220.50		NIST Webbook
rinpol	220.20		NIST Webbook
rinpol	220.40		NIST Webbook
rinpol	220.06		NIST Webbook
rinpol	218.14		NIST Webbook
rinpol	218.74		NIST Webbook
rinpol	216.32		NIST Webbook
rinpol	221.22		NIST Webbook
rinpol	220.10		NIST Webbook
rinpol	220.10		NIST Webbook
rinpol	218.10		NIST Webbook
rinpol	219.86		NIST Webbook
rinpol	1263.00		NIST Webbook
rinpol	1252.00		NIST Webbook
rinpol	1265.50		NIST Webbook
rinpol	1292.00		NIST Webbook
rinpol	1300.00		NIST Webbook

rinpol	1294.80	NIST Webbook
rinpol	1273.00	NIST Webbook
rinpol	217.29	NIST Webbook
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rinpol	221.50	NIST Webbook
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rinpol	220.22	NIST Webbook
rinpol	216.60	NIST Webbook
rinpol	216.19	NIST Webbook
rinpol	217.00	NIST Webbook
rinpol	221.57	NIST Webbook
rinpol	220.47	NIST Webbook
rinpol	217.33	NIST Webbook
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rinpol	220.50	NIST Webbook
rinpol	221.10	NIST Webbook
rinpol	221.27	NIST Webbook
rinpol	1259.00	NIST Webbook
rinpol	1278.70	NIST Webbook
rinpol	1300.00	NIST Webbook
rinpol	1300.00	NIST Webbook
rinpol	1301.00	NIST Webbook
rinpol	1307.00	NIST Webbook
rinpol	1264.00	NIST Webbook
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rinpol	1271.10	NIST Webbook
rinpol	1293.90	NIST Webbook
rinpol	1287.00	NIST Webbook
rinpol	1265.50	NIST Webbook
rinpol	1271.10	NIST Webbook
rinpol	1304.00	NIST Webbook
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rinpol	1270.79	NIST Webbook
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rinpol	1299.00	NIST Webbook
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rinpol	220.98		NIST Webbook
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rinpol	220.89		NIST Webbook
rinpol	220.11		NIST Webbook
rinpol	1284.00		NIST Webbook
rinpol	220.93		NIST Webbook
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ripol	1868.00		NIST Webbook
ripol	1872.00		NIST Webbook
ripol	1856.00		NIST Webbook
ripol	1809.00		NIST Webbook
ripol	1856.00		NIST Webbook
ripol	1845.00		NIST Webbook
ripol	1852.00		NIST Webbook
ripol	1852.00		NIST Webbook
ripol	1856.00		NIST Webbook
sl	203.80	J/mol×K	NIST Webbook
sl	219.99	J/mol×K	NIST Webbook
tb	514.20	K	NIST Webbook
tb	517.25 ± 0.50	K	NIST Webbook
tb	514.00 ± 3.00	K	NIST Webbook

tb	514.20 ± 0.08	K	NIST Webbook
tb	513.00 ± 5.00	K	NIST Webbook
tb	514.00 ± 3.00	K	NIST Webbook
tb	514.30 ± 0.60	K	NIST Webbook
tb	514.20	K	Critical properties of some alkylnaphthalenes
tb	514.00 ± 2.00	K	NIST Webbook
tb	514.00 ± 3.00	K	NIST Webbook
tb	514.00 ± 3.00	K	NIST Webbook
tb	514.30 ± 0.50	K	NIST Webbook
tb	514.29 ± 0.20	K	NIST Webbook
tb	514.29 ± 0.20	K	NIST Webbook
tb	515.00 ± 1.00	K	NIST Webbook
tb	514.00 ± 2.77	K	NIST Webbook
tb	516.00 ± 5.00	K	NIST Webbook
tb	514.26	K	KDB
tc	761.00	K	KDB
tc	764.55 ± 2.00	K	NIST Webbook
tc	761.00 ± 1.00	K	NIST Webbook
tc	761.15 ± 1.50	K	NIST Webbook
tf	307.85	K	Solid-Liquid Equilibria of Binary Mixtures of Dimethylnaphthalene Isomers
tf	306.85	K	Aqueous Solubility Prediction Method
tf	307.50	K	KDB
tt	307.20 ± 0.25	K	NIST Webbook
tt	307.72 ± 0.05	K	NIST Webbook
tt	307.72 ± 0.08	K	NIST Webbook
vc	0.462	m3/kmol	KDB
zc	0.2555580		KDB

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	279.78	J/mol×K	579.95	Joback Method
cpg	252.16	J/mol×K	501.72	Joback Method
cpg	313.94	J/mol×K	697.29	Joback Method
cpg	323.67	J/mol×K	736.41	Joback Method
cpg	292.07	J/mol×K	619.06	Joback Method
cpg	303.43	J/mol×K	658.18	Joback Method
cpg	266.51	J/mol×K	540.83	Joback Method

cpl	195.98	J/mol×K	298.15	NIST Webbook
cpl	228.00	J/mol×K	310.40	NIST Webbook
dvisc	0.0007043	Pa×s	357.49	Joback Method
dvisc	0.0005408	Pa×s	393.55	Joback Method
dvisc	0.0014596	Pa×s	285.37	Joback Method
dvisc	0.0003605	Pa×s	465.66	Joback Method
dvisc	0.0003074	Pa×s	501.72	Joback Method
dvisc	0.0009733	Pa×s	321.43	Joback Method
dvisc	0.0004341	Pa×s	429.60	Joback Method
hfust	12.13	kJ/mol	307.70	NIST Webbook
hfust	12.13	kJ/mol	307.70	NIST Webbook
hfust	5.61	kJ/mol	288.50	NIST Webbook
hfust	11.97	kJ/mol	307.20	NIST Webbook
hsubt	61.71 ± 0.84	kJ/mol	283.00	NIST Webbook
hvapt	51.20	kJ/mol	469.00	NIST Webbook
hvapt	48.40	kJ/mol	479.50	NIST Webbook
hvapt	46.40	kJ/mol	479.50	NIST Webbook
hvapt	46.02	kJ/mol	514.20	KDB
rhol	995.60	kg/m3	308.15	Liquid-liquid phase equilibrium for ternary mixtures of formamide (or ethylene glycol, or monoethanolamine) + indole + 2-methylnaphthalene at 308.15 K
rhol	990.00	kg/m3	313.00	KDB
sfust	39.43	J/mol×K	307.70	NIST Webbook
sfust	19.43	J/mol×K	288.50	NIST Webbook
sfust	39.00	J/mol×K	307.20	NIST Webbook
srf	0.03	N/m	353.20	KDB

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.42077e+01
Coeff. B	-4.16371e+03
Coeff. C	-7.98020e+01
Temperature range (K), min.	378.92
Temperature range (K), max.	547.83

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/T + C*ln(T) + D*T^2
Coeff. A	1.20141e+02
Coeff. B	-1.17450e+04
Coeff. C	-1.51199e+01
Coeff. D	6.43805e-06
Temperature range (K), min.	307.73
Temperature range (K), max.	761.00

Datasets

Specific volume, m3/kg

Temperature, K - Liquid	Pressure, kPa - Liquid	Specific volume, m3/kg - Liquid
303.15	100.00	0.0010
313.15	100.00	0.0010
323.15	100.00	0.0010
333.14	100.00	0.0010
333.15	100.00	0.0010
333.15	10000.00	0.0010
333.15	20000.00	0.0010
333.15	30000.00	0.0010
333.15	40000.00	0.0010
333.15	50000.00	0.0010
333.15	60000.00	0.0010
333.15	70000.00	0.0010
333.15	80000.00	0.0010
333.15	90000.00	0.0010
333.15	100000.00	0.0010
343.15	100.00	0.0010
343.15	10000.00	0.0010
343.15	20000.00	0.0010
343.15	30000.00	0.0010
343.15	40000.00	0.0010
343.15	50000.00	0.0010
343.15	60000.00	0.0010

343.15	70000.00	0.0010
343.15	80000.00	0.0010
343.15	90000.00	0.0010
343.15	100000.00	0.0010
343.15	110000.00	0.0010
343.15	120000.00	0.0010
343.15	130000.00	0.0010
343.15	140000.00	0.0010
353.15	100.00	0.0010

Reference *https://www.doi.org/10.1007/s10765-009-0625-z*

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Critical properties of some alkylnaphthalenes:	https://www.doi.org/10.1016/j.fluid.2013.08.041
PVT Relationships of Binary Mixtures of Indole with 2-Methylnaphthalene and Biphenyl at 333.15 K and Pressures up to 270 MPa:	https://www.doi.org/10.1007/s10765-009-0625-z
KDB:	https://www.cheric.org/files/research/kdb/mol/mol761.mol
Estimated Solubility Method:	http://pubs.acs.org/doi/suppl/10.1021/ci034243x/suppl_file/ci034243xsi20040112_053635.txt
KDB Vapor Pressure Data:	https://www.cheric.org/research/kdb/hcprop/showprop.php?cmpid=761
Determination of Henry's Law Constants Using Internal Standards with Benchmark Values:	https://www.doi.org/10.1021/je3010535
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C91576&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Aqueous Solubility Prediction Method:	http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa
Solid-Liquid Equilibria of Binary Mixtures of Dimethylnaphthalene Isomers:	https://www.doi.org/10.1021/je700088n
Liquid-liquid phase equilibrium for ternary mixtures of formamide (or ethyleneglycol, or monoethanolamine) + indole + 2-methylnaphthalene at 308.15 K:	https://www.doi.org/10.1016/j.fluid.2015.04.001
Solubility Determination and Thermodynamic Models for 2,6-Dimethylnaphthalene in Different Solvents from T = (278.15 to 303.15) K:	https://www.doi.org/10.1021/je5010627
The Yaws Handbook of Vapor Pressure:	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure

Legend

af:	Acentric Factor
affp:	Proton affinity
basg:	Gas basicity
chs:	Standard solid enthalpy of combustion
cpg:	Ideal gas heat capacity
cpl:	Liquid phase heat capacity
dm:	Dipole Moment

dvisc:	Dynamic viscosity
ea:	Electron affinity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfs:	Solid phase enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hfust:	Enthalpy of fusion at a given temperature
hsub:	Enthalpy of sublimation at standard conditions
hsubt:	Enthalpy of sublimation at a given temperature
hvap:	Enthalpy of vaporization at standard conditions
hvapt:	Enthalpy of vaporization at a given temperature
ie:	Ionization energy
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
pvap:	Vapor pressure
rhol:	Liquid Density
rinpol:	Non-polar retention indices
ripol:	Polar retention indices
sfust:	Entropy of fusion at a given temperature
sl:	Liquid phase molar entropy at standard conditions
srf:	Surface Tension
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
tt:	Triple Point Temperature
vc:	Critical Volume
vols:	Specific Volume
zc:	Critical Compressibility