Naphthalene, 1-methyl-

Other names:	.alpha.-methylnaphthalene
	1-Methylnaphthalene
	ALPHA-METHYLNAPHTHALENE
	Methyl-1-naphthalene
	«alpha»-Methylnaphthalene
	Â«alphaÂ»-Methylnaphthalene
Inchi:	InChI=1S/C11H10/c1-9-5-4-7-10-6-2-3-8-11(9)10/h2-8H,1H3
InchiKey:	QPUYECUOLPXSFR-UHFFFAOYSA-N
Formula:	C11H10
SMILES:	Cc1cccc2ccccc12
Mol. weight [g/mol]:	142.20
CAS:	90-12-0

Physical Properties

Property code	Value	Unit	Source
af	0.3100		KDB
affp	831.40	kJ/mol	NIST Webbook
affp	834.80	kJ/mol	NIST Webbook
basg	803.30	kJ/mol	NIST Webbook
basg	805.30	kJ/mol	NIST Webbook
chl	-5783.00 ± 5.80	kJ/mol	NIST Webbook
chl	-5814.00 ± 1.70	kJ/mol	NIST Webbook
chl	-5627.00	kJ/mol	NIST Webbook
dm	0.50	debye	KDB
ea	0.16 ± 0.12	eV	NIST Webbook
gf	217.80	kJ/mol	KDB
hf	116.90 ± 2.70	kJ/mol	NIST Webbook
hf	116.90	kJ/mol	KDB
hfl	56.20 ± 1.70	kJ/mol	NIST Webbook
hfus	14.92	kJ/mol	Joback Method
hvap	65.10 ± 1.10	kJ/mol	NIST Webbook
hvap	62.40	kJ/mol	NIST Webbook
hvap	60.70	kJ/mol	NIST Webbook
hvap	57.32 ± 0.42	kJ/mol	NIST Webbook
hvap	60.10 ± 0.80	kJ/mol	NIST Webbook
hvap	57.30 ± 0.40	kJ/mol	NIST Webbook
hvap	46.48	kJ/mol	NIST Webbook

hvap	60.70 ± 2.10	kJ/mol	NIST Webbook
ie	7.98	eV	NIST Webbook
ie	8.50 ± 0.05	eV	NIST Webbook
ie	7.90 ± 0.02	eV	NIST Webbook
ie	7.96 ± 0.03	eV	NIST Webbook
ie	7.80 ± 0.03	eV	NIST Webbook
ie	7.96 ± 0.01	eV	NIST Webbook
ie	8.01 ± 0.03	eV	NIST Webbook
ie	7.95	eV	NIST Webbook
ie	7.98	eV	NIST Webbook
log10ws	-3.70		Estimated Solubility Method
log10ws	-3.70		Aqueous Solubility Prediction Method
logp	3.148		Crippen Method
mcvol	122.630	ml/mol	McGowan Method
nfpaf	%!d(float64=2)		KDB
nfpah	%!d(float64=2)		KDB
pc	3600.00	kPa	KDB
pc	3600.00 ± 100.00	kPa	NIST Webbook
pc	3600.00 ± 100.00	kPa	NIST Webbook
pc	4356.98 ± 151.99	kPa	NIST Webbook
rinpol	1285.68		NIST Webbook
rinpol	224.80		NIST Webbook
rinpol	224.12		NIST Webbook
rinpol	223.42		NIST Webbook
rinpol	224.40		NIST Webbook
rinpol	219.93		NIST Webbook
rinpol	220.10		NIST Webbook
rinpol	221.00		NIST Webbook
rinpol	223.10		NIST Webbook
rinpol	223.10		NIST Webbook
rinpol	224.31		NIST Webbook
rinpol	221.04		NIST Webbook
rinpol	221.04		NIST Webbook
rinpol	223.06		NIST Webbook
rinpol	224.80		NIST Webbook
rinpol	223.00		NIST Webbook
rinpol	223.20		NIST Webbook
rinpol	221.04		NIST Webbook
rinpol	1263.00		NIST Webbook
rinpol	1298.00		NIST Webbook
rinpol	221.04		NIST Webbook
rinpol	223.01		NIST Webbook
rinpol	219.10		NIST Webbook

rinpol	218.90	NIST Webbook
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rinpol	223.50	NIST Webbook
rinpol	223.98	NIST Webbook
rinpol	223.83	NIST Webbook
rinpol	1330.12	NIST Webbook
rinpol	1293.70	NIST Webbook
rinpol	1318.00	NIST Webbook
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rinpol	1306.00	NIST Webbook
rinpol	1327.00	NIST Webbook
rinpol	1326.00	NIST Webbook
rinpol	1281.00	NIST Webbook
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rinpol	1318.00	NIST Webbook
rinpol	1268.00	NIST Webbook
rinpol	1264.70	NIST Webbook
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rinpol	1309.00	NIST Webbook
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rinpol	1263.00	NIST Webbook
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rinpol	1282.00	NIST Webbook
rinpol	1295.00	NIST Webbook
rinpol	1295.00	NIST Webbook
rinpol	1298.00	NIST Webbook
rinpol	1305.00	NIST Webbook
rinpol	1297.80	NIST Webbook
rinpol	1300.00	NIST Webbook

rinpol	1289.60	NIST Webbook
rinpol	1289.60	NIST Webbook
rinpol	1299.10	NIST Webbook
rinpol	1283.00	NIST Webbook
rinpol	1306.80	NIST Webbook
rinpol	1305.50	NIST Webbook
rinpol	1297.10	NIST Webbook
rinpol	1306.80	NIST Webbook
rinpol	1313.40	NIST Webbook
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ripol	1855.00		NIST Webbook
ripol	1884.00		NIST Webbook
ripol	1884.00		NIST Webbook
ripol	1880.00		NIST Webbook
ripol	1884.00		NIST Webbook
ripol	1860.00		NIST Webbook
ripol	1893.00		NIST Webbook
ripol	1875.00		NIST Webbook
sl	254.81	J/mol×K	NIST Webbook
tb	517.70	K	Critical properties of some alkylnaphthalenes
tb	517.89	K	KDB
tc	772.00 ± 1.50	K	NIST Webbook
tc	772.00 ± 1.00	K	NIST Webbook
tc	772.00 ± 1.00	K	NIST Webbook
tc	772.00	K	KDB
tc	784.00 ± 2.00	K	NIST Webbook

tc	273.15 ± 2.72	K	NIST Webbook
tf	242.67	K	KDB
tf	242.20	K	Solid-Liquid Equilibria of Binary Mixtures of Dimethylnaphthalene Isomers
tf	263.05	K	Aqueous Solubility Prediction Method
tt	242.66 ± 0.03	K	NIST Webbook
tt	242.66 ± 0.05	K	NIST Webbook
tt	242.70	K	KDB
tt	242.70 ± 0.03	K	NIST Webbook
tt	242.69 ± 0.02	K	NIST Webbook
vc	0.466	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	323.67	J/mol×K	736.41	Joback Method
cpg	313.94	J/mol×K	697.29	Joback Method
cpg	303.43	J/mol×K	658.18	Joback Method
cpg	292.07	J/mol×K	619.06	Joback Method
cpg	279.78	J/mol×K	579.95	Joback Method
cpg	266.51	J/mol×K	540.83	Joback Method
cpg	252.16	J/mol×K	501.72	Joback Method
cpl	224.39	J/mol×K	298.15	NIST Webbook
hfust	6.95	kJ/mol	242.70	NIST Webbook
hfust	6.95	kJ/mol	242.70	NIST Webbook
hfust	4.98	kJ/mol	240.70	NIST Webbook
hvapt	52.30	kJ/mol	470.50	NIST Webbook
hvapt	49.60	kJ/mol	480.00	NIST Webbook
hvapt	45.90	kJ/mol	480.00	NIST Webbook
hvapt	46.02	kJ/mol	517.80	KDB
hvapt	50.00	kJ/mol	540.00	NIST Webbook
hvapt	57.50	kJ/mol	295.50	NIST Webbook
hvapt	63.30	kJ/mol	323.50	NIST Webbook
rhol	1020.00	kg/m3	293.00	KDB
sfust	20.69	J/mol×K	240.70	NIST Webbook
sfust	28.62	J/mol×K	242.70	NIST Webbook
srf	0.04	N/m	298.20	KDB

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.49352e+01
Coeff. B	-4.73755e+03
Coeff. C	-5.57940e+01
Temperature range (K), min.	379.23
Temperature range (K), max.	548.07

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/T + C*ln(T) + D*T^2
Coeff. A	7.09337e+01
Coeff. B	-9.29434e+03
Coeff. C	-7.84021e+00
Coeff. D	2.38298e-06
Temperature range (K), min.	242.67
Temperature range (K), max.	772.04

Datasets

Viscosity, Pa*s

Temperature, K - Liquid	Pressure, kPa - Liquid	Viscosity, Pa*s - Liquid
298.15	100.00	0.0029130
298.15	20500.00	0.0036200
298.15	40100.00	0.0044300
298.15	80200.00	0.0067200
298.15	81400.00	0.0067800
298.15	100100.00	0.0083500
298.15	121300.00	0.0103000
298.15	140800.00	0.0127000
298.15	161500.00	0.0160000

298.15	100.00	0.0029200
298.15	121300.00	0.0103000
323.15	100.00	0.0017400
323.15	39600.00	0.0024900
323.15	79600.00	0.0035100
323.15	80400.00	0.0035400
323.15	120800.00	0.0049600
323.15	123300.00	0.0051200
323.15	160500.00	0.0070200
323.15	193000.00	0.0091800
323.15	100.00	0.0017300
348.15	100.00	0.0011900
348.15	40800.00	0.0016600
348.15	78900.00	0.0022200
348.15	79300.00	0.0022400
348.15	121400.00	0.0030300
348.15	121900.00	0.0030500
348.15	162200.00	0.0040500
348.15	189900.00	0.0049300
348.15	100.00	0.0011900
373.15	100.00	0.0008690
373.15	41500.00	0.0012000
373.15	79800.00	0.0015700
373.15	80100.00	0.0015800
373.15	120300.00	0.0020600
373.15	121700.00	0.0020700
373.15	159700.00	0.0026300
373.15	189500.00	0.0031400
373.15	100.00	0.0008690
398.15	100.00	0.0006640
398.15	40500.00	0.0009050
398.15	79700.00	0.0011800
398.15	82700.00	0.0012000
398.15	120500.00	0.0015100
398.15	160500.00	0.0019000
398.15	162900.00	0.0019200
398.15	202400.00	0.0023900
398.15	100.00	0.0006650
423.15	100.00	0.0005300
423.15	40500.00	0.0007220
423.15	81000.00	0.0009370
423.15	81900.00	0.0009410
423.15	120500.00	0.0011700
423.15	160000.00	0.0014500

423.15	161000.00	0.0014600
423.15	199700.00	0.0017800
423.15	100.00	0.0005300
448.15	100.00	0.0004350
448.15	40200.00	0.0005920
448.15	80100.00	0.0007620
448.15	81800.00	0.0007690
448.15	120700.00	0.0009570
448.15	160100.00	0.0011600
448.15	160800.00	0.0011700
448.15	200800.00	0.0014100
448.15	100.00	0.0004350
473.15	100.00	0.0003640
473.15	40600.00	0.0005010
473.15	81000.00	0.0006450
473.15	81500.00	0.0006460
473.15	121600.00	0.0008020
473.15	160800.00	0.0009720
473.15	160900.00	0.0009700
473.15	200200.00	0.0011600
473.15	100.00	0.0003640

Reference *https://www.doi.org/10.1021/je800417q*

Sources

KDB Pure (Korean Thermophysical Properties Databank):	https://www.cheric.org/research/kdb/hcprop/showprop.php?cmpid=760
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C90120&Units=SI
Solid-Liquid Equilibria of Binary Mixtures of Dimethylnaphthalene Isomers:	https://www.doi.org/10.1021/je700088n
KDB:	https://www.cheric.org/files/research/kdb/mol/mol760.mol
Phase equilibria for the [{water + 1-methylnaphthalene + p-xylene}] system at T = (573, 623 and 653) K:	https://www.doi.org/10.1016/j.jct.2013.01.029
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
Estimated Solubility Method:	http://pubs.acs.org/doi/suppl/10.1021/ci034243x/suppl_file/ci034243xsi20040112_053635.txt
Experimental solubility data of various n-alkane waxes: effects of alkane chain length, alkane odd versus even carbon number structures, and solvent chemistry on solubility:	https://www.doi.org/10.1016/j.fluid.2004.10.021
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Aqueous Solubility Prediction Method:	http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa
Critical properties of some alkylnaphthalenes:	https://www.doi.org/10.1016/j.fluid.2013.08.041
The Yaws Handbook of Vapor Pressure:	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure
Viscosity and Density of Five Hydrocarbon Liquids at Pressures up to 200 MPa and Temperatures up to 473 K:	https://www.doi.org/10.1021/je800417q

KDB Vapor Pressure Data:	https://www.cheric.org/research/kdb/hcprop/showprop.php?cmpid=760
Viscosity of Liquid Di-isodecyl Phthalate at Temperatures Between (274 and 373) K and at Pressures up to 140 MPa:	https://www.doi.org/10.1021/je101256z

Legend

af:	Acentric Factor
affp:	Proton affinity
basg:	Gas basicity
chl:	Standard liquid 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
hfl:	Liquid phase enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hfust:	Enthalpy of fusion 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
nfpaf:	NFPA Fire Rating
nfpah:	NFPA Health Rating
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

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