

# 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	834.80	kJ/mol	NIST Webbook
affp	831.40	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	57.30 ± 0.40	kJ/mol	NIST Webbook
hvap	60.70 ± 2.10	kJ/mol	NIST Webbook
hvap	57.32 ± 0.42	kJ/mol	NIST Webbook
hvap	62.40	kJ/mol	NIST Webbook
hvap	65.10 ± 1.10	kJ/mol	NIST Webbook
hvap	60.10 ± 0.80	kJ/mol	NIST Webbook
hvap	46.48	kJ/mol	NIST Webbook

hvap	60.70	kJ/mol	NIST Webbook
ie	7.98	eV	NIST Webbook
ie	7.90 ± 0.02	eV	NIST Webbook
ie	7.98	eV	NIST Webbook
ie	7.96 ± 0.01	eV	NIST Webbook
ie	8.01 ± 0.03	eV	NIST Webbook
ie	7.80 ± 0.03	eV	NIST Webbook
ie	8.50 ± 0.05	eV	NIST Webbook
ie	7.96 ± 0.03	eV	NIST Webbook
ie	7.95	eV	NIST Webbook
log10ws	-3.70		Aqueous Solubility Prediction Method
log10ws	-3.70		Estimated Solubility Method
logp	3.148		Crippen Method
mcpvol	122.630	ml/mol	McGowan Method
nfpaf	%!d(float64=2)		KDB
nfpah	%!d(float64=2)		KDB
pc	3600.00 ± 100.00	kPa	NIST Webbook
pc	3600.00	kPa	KDB
pc	3600.00 ± 100.00	kPa	NIST Webbook
pc	4356.98 ± 151.99	kPa	NIST Webbook
rinpol	1289.00		NIST Webbook
rinpol	1306.80		NIST Webbook
rinpol	1313.40		NIST Webbook
rinpol	1288.10		NIST Webbook
rinpol	1297.10		NIST Webbook
rinpol	1306.80		NIST Webbook
rinpol	1313.40		NIST Webbook
rinpol	1306.80		NIST Webbook
rinpol	1305.50		NIST Webbook
rinpol	1296.00		NIST Webbook
rinpol	1285.68		NIST Webbook
rinpol	1286.53		NIST Webbook
rinpol	1287.00		NIST Webbook
rinpol	1316.00		NIST Webbook
rinpol	1272.66		NIST Webbook
rinpol	1283.05		NIST Webbook
rinpol	1289.57		NIST Webbook
rinpol	1307.25		NIST Webbook
rinpol	1319.04		NIST Webbook
rinpol	1326.55		NIST Webbook
rinpol	1282.00		NIST Webbook
rinpol	1325.00		NIST Webbook
rinpol	1307.00		NIST Webbook

rinpol	1330.00	NIST Webbook
rinpol	1293.00	NIST Webbook
rinpol	1301.00	NIST Webbook
rinpol	1286.00	NIST Webbook
rinpol	1321.00	NIST Webbook
rinpol	1323.00	NIST Webbook
rinpol	1323.00	NIST Webbook
rinpol	1326.00	NIST Webbook
rinpol	1326.00	NIST Webbook
rinpol	1309.00	NIST Webbook
rinpol	1284.00	NIST Webbook
rinpol	1294.00	NIST Webbook
rinpol	1294.00	NIST Webbook
rinpol	1294.00	NIST Webbook
rinpol	1312.00	NIST Webbook
rinpol	1299.00	NIST Webbook
rinpol	1301.00	NIST Webbook
rinpol	1289.00	NIST Webbook
rinpol	1314.00	NIST Webbook
rinpol	1315.00	NIST Webbook
rinpol	1317.00	NIST Webbook
rinpol	1317.00	NIST Webbook
rinpol	1315.00	NIST Webbook
rinpol	1325.00	NIST Webbook
rinpol	1286.00	NIST Webbook
rinpol	1312.40	NIST Webbook
rinpol	1288.00	NIST Webbook
rinpol	1328.00	NIST Webbook
rinpol	1282.00	NIST Webbook
rinpol	1290.00	NIST Webbook
rinpol	1276.00	NIST Webbook
rinpol	1276.00	NIST Webbook
rinpol	1277.00	NIST Webbook
rinpol	1272.00	NIST Webbook
rinpol	1278.00	NIST Webbook
rinpol	1284.00	NIST Webbook
rinpol	1297.10	NIST Webbook
rinpol	1269.00	NIST Webbook
rinpol	1282.00	NIST Webbook
rinpol	1308.00	NIST Webbook
rinpol	1310.00	NIST Webbook
rinpol	1306.00	NIST Webbook
rinpol	1293.00	NIST Webbook
rinpol	1321.00	NIST Webbook

rinpol	1281.00	NIST Webbook
rinpol	1301.70	NIST Webbook
rinpol	1273.00	NIST Webbook
rinpol	1316.00	NIST Webbook
rinpol	1317.00	NIST Webbook
rinpol	1271.00	NIST Webbook
rinpol	1282.00	NIST Webbook
rinpol	1268.00	NIST Webbook
rinpol	1288.00	NIST Webbook
rinpol	223.91	NIST Webbook
rinpol	224.60	NIST Webbook
rinpol	221.80	NIST Webbook
rinpol	221.04	NIST Webbook
rinpol	223.10	NIST Webbook
rinpol	223.01	NIST Webbook
rinpol	223.01	NIST Webbook
rinpol	1305.50	NIST Webbook
rinpol	224.16	NIST Webbook
rinpol	224.02	NIST Webbook
rinpol	223.78	NIST Webbook
rinpol	223.21	NIST Webbook
rinpol	222.08	NIST Webbook
rinpol	223.83	NIST Webbook
rinpol	223.98	NIST Webbook
rinpol	223.50	NIST Webbook
rinpol	224.13	NIST Webbook
rinpol	220.05	NIST Webbook
rinpol	223.42	NIST Webbook
rinpol	224.53	NIST Webbook
rinpol	219.83	NIST Webbook
rinpol	218.90	NIST Webbook
rinpol	219.10	NIST Webbook
rinpol	223.01	NIST Webbook
rinpol	221.04	NIST Webbook
rinpol	224.80	NIST Webbook
rinpol	224.12	NIST Webbook
rinpol	223.42	NIST Webbook
rinpol	224.12	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	1269.00	NIST Webbook
rinpol	1293.00	NIST Webbook
rinpol	1316.00	NIST Webbook
rinpol	1288.00	NIST Webbook
rinpol	1306.80	NIST Webbook
rinpol	1283.00	NIST Webbook
rinpol	1299.10	NIST Webbook
rinpol	1289.60	NIST Webbook
rinpol	1289.60	NIST Webbook
rinpol	1300.00	NIST Webbook
rinpol	1297.80	NIST Webbook
rinpol	1305.00	NIST Webbook
rinpol	1298.00	NIST Webbook
rinpol	1295.00	NIST Webbook
rinpol	1282.00	NIST Webbook
rinpol	1268.00	NIST Webbook
rinpol	1263.00	NIST Webbook
rinpol	1267.90	NIST Webbook
rinpol	1294.00	NIST Webbook
rinpol	1279.00	NIST Webbook
rinpol	1302.00	NIST Webbook
rinpol	1309.00	NIST Webbook
rinpol	1267.90	NIST Webbook
rinpol	1264.70	NIST Webbook
rinpol	1268.00	NIST Webbook
rinpol	1318.00	NIST Webbook
rinpol	1303.00	NIST Webbook
rinpol	1281.00	NIST Webbook
rinpol	1326.00	NIST Webbook
rinpol	1327.00	NIST Webbook
rinpol	1306.00	NIST Webbook
rinpol	1278.00	NIST Webbook
rinpol	1277.00	NIST Webbook
rinpol	1326.00	NIST Webbook

rinpol	1318.00		NIST Webbook
rinpol	1318.00		NIST Webbook
rinpol	1318.00		NIST Webbook
rinpol	1293.70		NIST Webbook
rinpol	1330.12		NIST Webbook
rinpol	1264.70		NIST Webbook
rinpol	224.42		NIST Webbook
rinpol	1295.00		NIST Webbook
ripol	1884.00		NIST Webbook
ripol	1875.00		NIST Webbook
ripol	1878.00		NIST Webbook
ripol	1903.00		NIST Webbook
ripol	1905.00		NIST Webbook
ripol	1898.00		NIST Webbook
ripol	1908.00		NIST Webbook
ripol	1844.00		NIST Webbook
ripol	1878.00		NIST Webbook
ripol	1878.00		NIST Webbook
ripol	1893.00		NIST Webbook
ripol	1860.00		NIST Webbook
ripol	1884.00		NIST Webbook
ripol	1880.00		NIST Webbook
ripol	1895.00		NIST Webbook
ripol	1884.00		NIST Webbook
ripol	1855.00		NIST Webbook
ripol	1855.00		NIST Webbook
ripol	1850.00		NIST Webbook
ripol	1908.00		NIST Webbook
ripol	1860.00		NIST Webbook
ripol	1855.00		NIST Webbook
ripol	1894.00		NIST Webbook
ripol	1875.00		NIST Webbook
ripol	1915.00		NIST Webbook
ripol	1894.00		NIST Webbook
ripol	1891.00		NIST Webbook
ripol	1896.00		NIST Webbook
sl	254.81	J/mol×K	NIST Webbook
tb	517.89	K	KDB
tb	517.70	K	Critical properties of some alkylnaphthalenes
tc	772.00 ± 1.50	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	772.00 ± 1.00	K	NIST Webbook

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

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	323.67	J/molxK	736.41	Joback Method
cpg	303.43	J/molxK	658.18	Joback Method
cpg	292.07	J/molxK	619.06	Joback Method
cpg	279.78	J/molxK	579.95	Joback Method
cpg	266.51	J/molxK	540.83	Joback Method
cpg	252.16	J/molxK	501.72	Joback Method
cpg	313.94	J/molxK	697.29	Joback Method
cpl	224.39	J/molxK	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	45.90	kJ/mol	480.00	NIST Webbook
hvapt	49.60	kJ/mol	480.00	NIST Webbook
hvapt	52.30	kJ/mol	470.50	NIST Webbook
hvapt	57.50	kJ/mol	295.50	NIST Webbook
hvapt	63.30	kJ/mol	323.50	NIST Webbook
hvapt	50.00	kJ/mol	540.00	NIST Webbook
hvapt	46.02	kJ/mol	517.80	KDB
rho1	1020.00	kg/m3	293.00	KDB
sfust	20.69	J/molxK	240.70	NIST Webbook
sfust	28.62	J/molxK	242.70	NIST Webbook
srf	0.04	N/m	298.20	KDB

# Correlations

Information	Value
Property code	pvap
Equation	$\ln(P_{vp}) = A + B/(T + C)$
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	$\ln(P_{vp}) = A + B/T + C*\ln(T) + D*T^2$
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

<b>KDB:</b>	<a href="https://www.thermo.com/files/research/kdb/mol/mol760.mol">https://www.thermo.com/files/research/kdb/mol/mol760.mol</a>
<b>McGowan Method:</b>	<a href="http://link.springer.com/article/10.1007/BF02311772">http://link.springer.com/article/10.1007/BF02311772</a>
<b>KDB Pure (Korean Thermophysical Properties Databank):</b>	<a href="https://www.thermo.com/research/kdb/hcprop/showprop.php?cmpid=760">https://www.thermo.com/research/kdb/hcprop/showprop.php?cmpid=760</a>
<b>KDB Vapor Pressure Data:</b>	<a href="https://www.thermo.com/research/kdb/hcprop/showprop.php?cmpid=760">https://www.thermo.com/research/kdb/hcprop/showprop.php?cmpid=760</a>
<b>Joback Method:</b>	<a href="https://en.wikipedia.org/wiki/Joback_method">https://en.wikipedia.org/wiki/Joback_method</a>
<b>Viscosity of Liquid Di-isodecyl Phthalate at Temperatures Between 274 and 300 K and Pressures up to 20 MPa:</b>	<a href="https://www.doi.org/10.1021/je101256z">https://www.doi.org/10.1021/je101256z</a>
<b>Critical Properties of some Alkyl naphthalenes:</b>	<a href="https://www.doi.org/10.1016/j.fluid.2013.08.041">https://www.doi.org/10.1016/j.fluid.2013.08.041</a>
<b>Crippen Method:</b>	<a href="http://pubs.acs.org/doi/abs/10.1021/ci990307l">http://pubs.acs.org/doi/abs/10.1021/ci990307l</a>
<b>Experimental solubility data of various n-alkane waxes: effects of alkane chain length, nature of the solvent, and carbon constants. Using Internal Standards and Debye-Huckel Values:</b>	<a href="https://www.doi.org/10.1016/j.fluid.2004.10.021">https://www.doi.org/10.1016/j.fluid.2004.10.021</a>
<b>Aqueous Solubility Prediction Method:</b>	<a href="https://www.doi.org/10.1021/je3010535">https://www.doi.org/10.1021/je3010535</a>
<b>Viscosity and Density of Five Hydrocarbon Liquids at Pressures up to 20 MPa and Temperatures up to 473 K:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=C90120&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C90120&amp;Units=SI</a>
<b>Estimation of Solubility Method:</b>	<a href="http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDataset002.xlsx">http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDataset002.xlsx</a>
<b>Phase equilibria for the [(water + 1-methylnaphthalene + p-xylene)] system at T = (573, 623 and 653) K:</b>	<a href="https://www.doi.org/10.1021/je800417q">https://www.doi.org/10.1021/je800417q</a>
	<a href="http://pubs.acs.org/doi/suppl/10.1021/ci034243x/suppl_file/ci034243xsi20040112_053635.txt">http://pubs.acs.org/doi/suppl/10.1021/ci034243x/suppl_file/ci034243xsi20040112_053635.txt</a>
	<a href="https://www.doi.org/10.1016/j.jct.2013.01.029">https://www.doi.org/10.1016/j.jct.2013.01.029</a>

## Legend

<b>af:</b>	Acentric Factor
<b>affp:</b>	Proton affinity
<b>basg:</b>	Gas basicity
<b>chl:</b>	Standard liquid enthalpy of combustion
<b>cpg:</b>	Ideal gas heat capacity
<b>cpl:</b>	Liquid phase heat capacity
<b>dm:</b>	Dipole Moment
<b>dvisc:</b>	Dynamic viscosity
<b>ea:</b>	Electron affinity
<b>gf:</b>	Standard Gibbs free energy of formation
<b>hf:</b>	Enthalpy of formation at standard conditions
<b>hfl:</b>	Liquid phase enthalpy of formation at standard conditions
<b>hfus:</b>	Enthalpy of fusion at standard conditions
<b>hfust:</b>	Enthalpy of fusion at a given temperature
<b>hvap:</b>	Enthalpy of vaporization at standard conditions
<b>hvapt:</b>	Enthalpy of vaporization at a given temperature
<b>ie:</b>	Ionization energy
<b>log10ws:</b>	Log10 of Water solubility in mol/l
<b>logp:</b>	Octanol/Water partition coefficient
<b>mcvol:</b>	McGowan's characteristic volume
<b>nfpaf:</b>	NFPA Fire Rating
<b>nfpah:</b>	NFPA Health Rating
<b>pc:</b>	Critical Pressure
<b>pvap:</b>	Vapor pressure
<b>rho:</b>	Liquid Density
<b>rinpol:</b>	Non-polar retention indices
<b>ripol:</b>	Polar retention indices
<b>sfust:</b>	Entropy of fusion at a given temperature
<b>sl:</b>	Liquid phase molar entropy at standard conditions
<b>srf:</b>	Surface Tension
<b>tb:</b>	Normal Boiling Point Temperature
<b>tc:</b>	Critical Temperature
<b>tf:</b>	Normal melting (fusion) point
<b>tt:</b>	Triple Point Temperature
<b>vc:</b>	Critical Volume

Latest version available from:

<https://www.chemeo.com/cid/18-114-5/Naphthalene-1-methyl.pdf>

Generated by Cheméo on 2024-04-25 15:47:15.672552061 +0000 UTC m=+16349284.593129376.

Cheméo (<https://www.chemeo.com>) is the biggest free database of chemical and physical data for the process industry.