Naphthalene, 1,6-dimethyl-

Other names:	1,6-Dimethylnaphthalene
	Dimethylnaphthalene
Inchi:	InChI=1S/C12H12/c1-9-6-7-12-10(2)4-3-5-11(12)8-9/h3-8H,1-2H3
InchiKey:	CBMXCNPQDUJNHT-UHFFFAOYSA-N
Formula:	C12H12
SMILES:	Cc1ccc2c(C)cccc2c1
Mol. weight [g/mol]:	156.22
CAS:	575-43-9

Physical Properties

Property code	Value	Unit	Source
af	0.4430		KDB
gf	249.96	kJ/mol	Joback Method
hf	113.65	kJ/mol	Joback Method
hfus	8.50	kJ/mol	Solid-Liquid Equilibria of Binary Mixtures of Dimethylnaphthalene Isomers
hvap	47.55	kJ/mol	Joback Method
log10ws	-4.23		Crippen Method
logp	3.457		Crippen Method
mcvol	136.720	ml/mol	McGowan Method
pc	3010.00	kPa	KDB
rinpol	244.66		NIST Webbook
rinpol	243.30		NIST Webbook
rinpol	243.40		NIST Webbook
rinpol	243.30		NIST Webbook
rinpol	244.40		NIST Webbook
rinpol	244.29		NIST Webbook
rinpol	240.70		NIST Webbook
rinpol	243.80		NIST Webbook
rinpol	243.90		NIST Webbook
rinpol	240.72		NIST Webbook
rinpol	243.30		NIST Webbook
rinpol	244.06		NIST Webbook
rinpol	1427.00		NIST Webbook
rinpol	1387.00		NIST Webbook
rinpol	1431.00		NIST Webbook

rinpol	1431.00		NIST Webbook
rinpol	1431.00		NIST Webbook
rinpol	1443.00		NIST Webbook
rinpol	1402.00		NIST Webbook
rinpol	1387.00		NIST Webbook
rinpol	1419.00		NIST Webbook
rinpol	1408.40		NIST Webbook
rinpol	1419.60		NIST Webbook
rinpol	1427.30		NIST Webbook
rinpol	1442.60		NIST Webbook
rinpol	1408.40		NIST Webbook
rinpol	1419.60		NIST Webbook
rinpol	1427.30		NIST Webbook
rinpol	1383.86		NIST Webbook
rinpol	1428.00		NIST Webbook
rinpol	1418.70		NIST Webbook
rinpol	1387.00		NIST Webbook
rinpol	1414.00		NIST Webbook
rinpol	1427.00		NIST Webbook
rinpol	1471.00		NIST Webbook
rinpol	1397.00		NIST Webbook
rinpol	1402.20		NIST Webbook
rinpol	1425.00		NIST Webbook
rinpol	1426.00		NIST Webbook
rinpol	243.76		NIST Webbook
rinpol	240.72		NIST Webbook
rinpol	243.96		NIST Webbook
rinpol	246.56		NIST Webbook
rinpol	243.57		NIST Webbook
rinpol	242.97		NIST Webbook
rinpol	244.06		NIST Webbook
rinpol	243.50		NIST Webbook
rinpol	243.90		NIST Webbook
ripol	2006.00		NIST Webbook
ripol	2007.00		NIST Webbook
ripol	2006.00		NIST Webbook
tb	537.00 ± 5.00	K	NIST Webbook
tb	529.00 ± 6.00	K	NIST Webbook
tb	535.70 ± 2.00	K	NIST Webbook
tb	536.00 ± 4.00	K	NIST Webbook
tb	536.00 ± 3.00	K	NIST Webbook
tb	536.00 ± 4.00	K	NIST Webbook
tb	537.00 ± 4.00	K	NIST Webbook
tb	537.90 ± 2.00	K	NIST Webbook

tb	538.80 ± 1.50	K	NIST Webbook
tb	527.00 ± 10.00	K	NIST Webbook
tb	537.00 ± 0.60	K	NIST Webbook
tb	538.70	K	NIST Webbook
tb	536.20	K	KDB
tc	770.60	K	KDB
tf	259.00	K	KDB
vc	0.521	m3/kmol	KDB
zc	0.2449940		KDB

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	371.48	J/mol×K	761.14	Joback Method
cpg	296.31	J/mol×K	529.58	Joback Method
cpg	311.16	J/mol×K	568.17	Joback Method
cpg	325.00	J/mol×K	606.77	Joback Method
cpg	337.89	J/mol×K	645.36	Joback Method
cpg	349.89	J/mol×K	683.95	Joback Method
cpg	361.06	J/mol×K	722.55	Joback Method
dvisc	0.0002960	Pa×s	529.58	Joback Method
dvisc	0.0012561	Pa×s	309.16	Joback Method
dvisc	0.0008686	Pa×s	345.90	Joback Method
dvisc	0.0006448	Pa×s	382.63	Joback Method
dvisc	0.0005043	Pa×s	419.37	Joback Method
dvisc	0.0004103	Pa×s	456.11	Joback Method
dvisc	0.0003443	Pa×s	492.84	Joback Method
hfust	8.50	kJ/mol	257.00	NIST Webbook
hvapt	63.60	kJ/mol	398.00	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.49901e+01
Coeff. B	-4.99771e+03
Coeff. C	-5.41420e+01

Temperature range (K), min.	394.06
Temperature range (K), max.	570.51

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/T + C*ln(T) + D*T^2
Coeff. A	-1.16256e+01
Coeff. B	-4.99386e+03
Coeff. C	4.20934e+00
Coeff. D	-3.09034e-06
Temperature range (K), min.	421.15
Temperature range (K), max.	770.60

Sources

Solid-Liquid Equilibria of Binary Mixtures of Dimethylnaphthalene Isomers:	https://www.doi.org/10.1021/je700088n
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
KDB:	https://www.cheric.org/files/research/kdb/mol/mol774.mol
KDB Vapor Pressure Data:	https://www.cheric.org/research/kdb/hcprop/showprop.php?cmpid=774
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
The Yaws Handbook of Vapor Pressure:	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C575439&Units=SI

Legend

af:	Acentric Factor
cpg:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
gf:	Standard Gibbs free energy of formation
hf:	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
log10ws:	Log10 of Water solubility in mol/l

logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
pvap:	Vapor pressure
rinpol:	Non-polar retention indices
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume
zc:	Critical Compressibility