Naphthalene, 1,2-dimethyl-

Other names: 1,2-Dimethylnaphthalene
Inchi: InChI=1S/C12H12/c1-9-7-8-11-5-3-4-6-12(11)10(9)2/h3-8H,1-2H3
InchiKey: QNLZIZAQLLYXTC-UHFFFAOYSA-N
Formula: C12H12
SMILES: Cc1ccc2ccccc2c1C
Mol. weight [g/mol]: 156.22
CAS: 573-98-8

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	17.12	kJ/mol	Joback Method
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	1440.00		NIST Webbook
rinpol	1448.00		NIST Webbook
rinpol	1447.00		NIST Webbook
rinpol	1456.00		NIST Webbook
rinpol	1430.00		NIST Webbook
rinpol	1447.00		NIST Webbook
rinpol	1439.70		NIST Webbook
rinpol	1455.10		NIST Webbook
rinpol	1432.00		NIST Webbook
rinpol	1452.20		NIST Webbook
rinpol	1451.10		NIST Webbook
rinpol	1439.60		NIST Webbook
rinpol	1452.20		NIST Webbook
rinpol	1459.10		NIST Webbook
rinpol	1439.60		NIST Webbook
rinpol	1452.20		NIST Webbook
rinpol	1459.10		NIST Webbook
rinpol	1452.20		NIST Webbook

rinpol	1451.10		NIST Webbook
rinpol	1462.00		NIST Webbook
rinpol	1450.60		NIST Webbook
rinpol	1439.00		NIST Webbook
rinpol	1440.00		NIST Webbook
rinpol	1444.00		NIST Webbook
rinpol	1433.00		NIST Webbook
rinpol	1432.00		NIST Webbook
rinpol	1432.00		NIST Webbook
rinpol	248.92		NIST Webbook
rinpol	236.49		NIST Webbook
rinpol	249.53		NIST Webbook
rinpol	1420.20		NIST Webbook
rinpol	247.14		NIST Webbook
rinpol	249.02		NIST Webbook
rinpol	248.47		NIST Webbook
rinpol	248.24		NIST Webbook
rinpol	249.04		NIST Webbook
rinpol	248.70		NIST Webbook
rinpol	249.67		NIST Webbook
rinpol	248.50		NIST Webbook
rinpol	246.49		NIST Webbook
rinpol	247.30		NIST Webbook
rinpol	246.50		NIST Webbook
rinpol	249.70		NIST Webbook
rinpol	246.49		NIST Webbook
rinpol	248.60		NIST Webbook
rinpol	248.80		NIST Webbook
rinpol	248.80		NIST Webbook
rinpol	1432.00		NIST Webbook
rinpol	1433.00		NIST Webbook
rinpol	247.30		NIST Webbook
rinpol	248.80		NIST Webbook
rinpol	1420.20		NIST Webbook
rinpol	1430.00		NIST Webbook
rinpol	1447.00		NIST Webbook
rinpol	246.56		NIST Webbook
ripol	2073.00		NIST Webbook
ripol	2072.00		NIST Webbook
ripol	2072.00		NIST Webbook
ripol	2072.00		NIST Webbook
tb	539.70	K	NIST Webbook
tb	498.00 ± 30.00	K	NIST Webbook
tb	541.70 ± 2.00	K	NIST Webbook

tb	539.00 ± 6.00	K	NIST Webbook
tb	539.50	K	KDB
tc	775.30	K	KDB
tf	272.00	K	KDB
tf	270.15 ± 0.70	K	NIST Webbook
vc	0.521	m3/kmol	KDB
zc	0.2435090		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
hvapt	50.21	kJ/mol	539.50	KDB

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.43726e+01
Coeff. B	-4.33355e+03
Coeff. C	-9.54250e+01
Temperature range (K), min.	403.10
Temperature range (K), max.	573.69

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/T + C*ln(T) + D*T^2
Coeff. A	1.39506e+02
Coeff. B	-1.36972e+04
Coeff. C	-1.77204e+01
Coeff. D	6.76958e-06
Temperature range (K), min.	402.15
Temperature range (K), max.	775.34

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
KDB:	https://www.cheric.org/research/kdb/hcprop/showprop.php?cmpid=770
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C573988&Units=SI
The Yaws Handbook of Vapor Pressure:	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure
KDB Vapor Pressure Data:	https://www.cheric.org/research/kdb/hcprop/showprop.php?cmpid=770

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
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