Naphthalene, 2,6-dimethyl-

Other names: 2,6-Dimethylnaphthalene
Inchi: InChI=1S/C12H12/c1-9-3-5-12-8-10(2)4-6-11(12)7-9/h3-8H,1-2H3
InchiKey: YGYNBBAUIYTWBF-UHFFFAOYSA-N
Formula: C12H12
SMILES: Cc1ccc2cc(C)ccc2c1
Mol. weight [g/mol]: 156.22
CAS: 581-42-0

Physical Properties

Property code	Value	Unit	Source
af	0.4430		KDB
chs	-6431.40 ± 1.60	kJ/mol	NIST Webbook
ea	0.16 ± 0.07	eV	NIST Webbook
gf	249.96	kJ/mol	Joback Method
hf	113.65	kJ/mol	Joback Method
hfs	-5.70 ± 1.70	kJ/mol	NIST Webbook
hfus	25.30	kJ/mol	Solid-Liquid Equilibria of Binary Mixtures of Dimethylnaphthalene Isomers
hvap	47.55	kJ/mol	Joback Method
log10ws	-4.89		Estimated Solubility Method
log10ws	-4.89		Aqueous Solubility Prediction Method
logp	3.457		Crippen Method
mcvol	136.720	ml/mol	McGowan Method
pc	3010.00	kPa	KDB
rinpol	1400.00		NIST Webbook
rinpol	1380.40		NIST Webbook
rinpol	1400.00		NIST Webbook
rinpol	1408.80		NIST Webbook
rinpol	1401.00		NIST Webbook
rinpol	1408.00		NIST Webbook
rinpol	1403.00		NIST Webbook
rinpol	1402.00		NIST Webbook
rinpol	1387.00		NIST Webbook
rinpol	1399.00		NIST Webbook
rinpol	1395.60		NIST Webbook

rinpol	1408.80	NIST Webbook
rinpol	1388.00	NIST Webbook
rinpol	1372.00	NIST Webbook
rinpol	1403.00	NIST Webbook
rinpol	1377.00	NIST Webbook
rinpol	1400.90	NIST Webbook
rinpol	1400.00	NIST Webbook
rinpol	1390.60	NIST Webbook
rinpol	1400.90	NIST Webbook
rinpol	1407.30	NIST Webbook
rinpol	1390.60	NIST Webbook
rinpol	1400.90	NIST Webbook
rinpol	1407.30	NIST Webbook
rinpol	1400.90	NIST Webbook
rinpol	1400.00	NIST Webbook
rinpol	1381.69	NIST Webbook
rinpol	1381.93	NIST Webbook
rinpol	1382.00	NIST Webbook
rinpol	1409.00	NIST Webbook
rinpol	1377.00	NIST Webbook
rinpol	1416.00	NIST Webbook
rinpol	1400.20	NIST Webbook
rinpol	1394.00	NIST Webbook
rinpol	1396.00	NIST Webbook
rinpol	1388.00	NIST Webbook
rinpol	1388.00	NIST Webbook
rinpol	1389.00	NIST Webbook
rinpol	1372.00	NIST Webbook
rinpol	1380.00	NIST Webbook
rinpol	1372.00	NIST Webbook
rinpol	1400.00	NIST Webbook
rinpol	1382.00	NIST Webbook
rinpol	1409.00	NIST Webbook
rinpol	1408.00	NIST Webbook
rinpol	1416.00	NIST Webbook
rinpol	1384.00	NIST Webbook
rinpol	1388.30	NIST Webbook
rinpol	1410.00	NIST Webbook
rinpol	1411.00	NIST Webbook
rinpol	1388.00	NIST Webbook
rinpol	240.89	NIST Webbook
rinpol	237.58	NIST Webbook
rinpol	239.70	NIST Webbook
rinpol	240.42	NIST Webbook

rinpol	240.56		NIST Webbook
rinpol	239.97		NIST Webbook
rinpol	240.04		NIST Webbook
rinpol	241.00		NIST Webbook
rinpol	240.50		NIST Webbook
rinpol	237.23		NIST Webbook
rinpol	240.89		NIST Webbook
rinpol	233.90		NIST Webbook
rinpol	240.28		NIST Webbook
rinpol	237.58		NIST Webbook
rinpol	241.20		NIST Webbook
rinpol	240.30		NIST Webbook
rinpol	239.11		NIST Webbook
rinpol	237.60		NIST Webbook
rinpol	239.70		NIST Webbook
rinpol	239.70		NIST Webbook
rinpol	241.13		NIST Webbook
rinpol	237.58		NIST Webbook
rinpol	240.30		NIST Webbook
rinpol	240.50		NIST Webbook
rinpol	236.80		NIST Webbook
rinpol	237.58		NIST Webbook
rinpol	1396.00		NIST Webbook
rinpol	1380.00		NIST Webbook
rinpol	1400.90		NIST Webbook
rinpol	1390.60		NIST Webbook
rinpol	1381.69		NIST Webbook
rinpol	1388.30		NIST Webbook
rinpol	1403.00		NIST Webbook
rinpol	239.97		NIST Webbook
rinpol	240.68		NIST Webbook
rinpol	1380.40		NIST Webbook
rinpol	240.68		NIST Webbook
ripol	2038.00		NIST Webbook
ripol	2012.00		NIST Webbook
ripol	2038.00		NIST Webbook
ripol	2031.00		NIST Webbook
ripol	2012.00		NIST Webbook
ripol	2038.00		NIST Webbook
ss	227.86	J/mol×K	NIST Webbook
tb	535.20	K	KDB
tb	538.00 ± 4.00	K	NIST Webbook
tb	535.00 ± 1.50	K	NIST Webbook
tb	543.00 ± 4.00	K	NIST Webbook

tb	534.35 ± 0.60	K	NIST Webbook
tb	535.20	K	NIST Webbook
tb	535.00 ± 4.00	K	NIST Webbook
tb	534.00 ± 4.00	K	NIST Webbook
tc	769.20	K	KDB
tf	384.15 ± 0.50	K	NIST Webbook
tf	336.00 ± 4.00	K	NIST Webbook
tf	385.00	K	KDB
tf	385.00	K	Solid-Liquid Phase Equilibria of Binary and Ternary Mixtures for 2,6-Dimethylnaphthalene and 2,7-Dimethylnaphthalene with Ethanol or Methanol
tf	387.40 ± 2.00	K	NIST Webbook
tf	383.27 ± 0.10	K	NIST Webbook
tf	383.90 ± 0.20	K	NIST Webbook
tt	383.31 ± 0.02	K	NIST Webbook
tt	383.31 ± 0.03	K	NIST Webbook
tt	384.41	K	Solubilities of 2,6-Dimethylnaphthalene in Six Pure Solvents and Two Binary Solvent Systems
vc	0.521	m3/kmol	KDB
zc	0.2454400		KDB

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	325.00	J/mol×K	606.77	Joback Method
cpg	296.31	J/mol×K	529.58	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
cpg	371.48	J/mol×K	761.14	Joback Method
cpg	311.16	J/mol×K	568.17	Joback Method
cps	203.55	J/mol×K	298.15	NIST Webbook
cps	202.50	J/mol×K	298.15	NIST Webbook
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
dvisc	0.0002960	Pa×s	529.58	Joback Method
hfust	25.06	kJ/mol	383.32	NIST Webbook
hfust	25.30	kJ/mol	385.20	NIST Webbook
hfust	25.06	kJ/mol	383.30	NIST Webbook
hfust	25.06	kJ/mol	383.30	NIST Webbook
hsubt	84.40 ± 1.90	kJ/mol	366.50	NIST Webbook
hsubt	84.10	kJ/mol	291.50	NIST Webbook
hsubt	82.50	kJ/mol	383.00	NIST Webbook
hsubt	84.00 ± 0.40	kJ/mol	379.20	NIST Webbook
hvapt	57.30	kJ/mol	401.00	NIST Webbook
hvapt	57.40	kJ/mol	401.00	NIST Webbook
hvapt	56.60	kJ/mol	401.00	NIST Webbook
hvapt	55.70	kJ/mol	401.00	NIST Webbook
sfust	65.37	J/mol×K	383.32	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.46482e+01
Coeff. B	-4.69173e+03
Coeff. C	-6.82240e+01
Temperature range (K), min.	384.55
Temperature range (K), max.	570.73

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/T + C*ln(T) + D*T^2
Coeff. A	8.33648e+01
Coeff. B	-1.04756e+04
Coeff. C	-9.52974e+00
Coeff. D	2.60426e-06
Temperature range (K), min.	383.32
Temperature range (K), max.	777.00

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Solid-Liquid Phase Equilibria of Binary and Ternary Mixtures for 2,6-Dimethylnaphthalene and 2,7-Dimethylnaphthalene with Ethanol or Methanol:	https://www.doi.org/10.1021/je049607b
KDB:	https://www.cheric.org/files/research/kdb/mol/mol777.mol
Solubilities of 2,6-Dimethylnaphthalene in Six Pure Solvents and Two Binary Solvent Systems:	https://www.doi.org/10.1021/acs.jced.8b01209
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C581420&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Solid-Liquid Equilibria of Binary Mixtures of Dimethylnaphthalene Isomers:	https://www.doi.org/10.1021/je700088n
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
Solubility and Density of 2,6-Dimethylnaphthalene in C1-C7 1-Alkanols:	https://www.doi.org/10.1021/je049967z
Aqueous Solubility Prediction Method:	http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa
KDB Vapor Pressure Data:	https://www.cheric.org/research/kdb/hcprop/showprop.php?cmpid=777
Estimated Solubility Method:	http://pubs.acs.org/doi/suppl/10.1021/ci034243x/suppl_file/ci034243xsi20040112_053635.txt

Legend

af:	Acentric Factor
chs:	Standard solid enthalpy of combustion
cpg:	Ideal gas heat capacity
cps:	Solid phase heat capacity
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
hsubt:	Enthalpy of sublimation 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

sfust:	Entropy of fusion at a given temperature
ss:	Solid phase molar entropy at standard conditions
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
tt:	Triple Point Temperature
vc:	Critical Volume
zc:	Critical Compressibility