Naphthalene, 2,3-dimethyl-

Other names: 2,3-Dimethylnaphthalene
GUAJEN
Inchi: InChI=1S/C12H12/c1-9-7-11-5-3-4-6-12(11)8-10(9)2/h3-8H,1-2H3
InchiKey: WWGUMAYGTYQSGA-UHFFFAOYSA-N
Formula: C12H12
SMILES: Cc1cc2ccccc2cc1C
Mol. weight [g/mol]: 156.22
CAS: 581-40-8

Physical Properties

Property code	Value	Unit	Source
af	0.4430		KDB
chs	-6434.78 ± 0.88	kJ/mol	NIST Webbook
chs	-6431.00 ± 1.10	kJ/mol	NIST Webbook
ea	0.17 ± 0.13	eV	NIST Webbook
gf	249.96	kJ/mol	Joback Method
hf	79.90	kJ/mol	NIST Webbook
hf	76.10 ± 2.00	kJ/mol	NIST Webbook
hfs	-2.30 ± 1.10	kJ/mol	NIST Webbook
hfs	-6.10 ± 1.90	kJ/mol	NIST Webbook
hfus	23.97	kJ/mol	Solid-Liquid Equilibria of Binary Mixtures of Dimethylnaphthalene Isomers
hsub	82.20	kJ/mol	NIST Webbook
hsub	82.20 ± 0.40	kJ/mol	NIST Webbook
hvap	47.55	kJ/mol	Joback Method
ie	8.11	eV	NIST Webbook
ie	8.20 ± 0.05	eV	NIST Webbook
ie	7.89 ± 0.03	eV	NIST Webbook
log10ws	-4.72		Aqueous Solubility Prediction Method
log10ws	-4.72		Estimated Solubility Method
logp	3.457		Crippen Method
mcvol	136.720	ml/mol	McGowan Method
pc	3010.00	kPa	KDB
rinpol	1410.00		NIST Webbook
rinpol	244.50		NIST Webbook

rinpol	1420.00	NIST Webbook
rinpol	242.64	NIST Webbook
rinpol	246.51	NIST Webbook
rinpol	246.73	NIST Webbook
rinpol	246.03	NIST Webbook
rinpol	1427.00	NIST Webbook
rinpol	1444.00	NIST Webbook
rinpol	1435.00	NIST Webbook
rinpol	1410.00	NIST Webbook
rinpol	1408.20	NIST Webbook
rinpol	243.55	NIST Webbook
rinpol	242.64	NIST Webbook
rinpol	246.30	NIST Webbook
rinpol	247.02	NIST Webbook
rinpol	1408.20	NIST Webbook
rinpol	1433.00	NIST Webbook
rinpol	1433.00	NIST Webbook
rinpol	1434.00	NIST Webbook
rinpol	1442.30	NIST Webbook
rinpol	1395.00	NIST Webbook
rinpol	1419.00	NIST Webbook
rinpol	1433.00	NIST Webbook
rinpol	1427.30	NIST Webbook
rinpol	1441.70	NIST Webbook
rinpol	1420.00	NIST Webbook
rinpol	1399.00	NIST Webbook
rinpol	1438.00	NIST Webbook
rinpol	1442.00	NIST Webbook
rinpol	1446.00	NIST Webbook
rinpol	1410.00	NIST Webbook
rinpol	1435.00	NIST Webbook
rinpol	1438.00	NIST Webbook
rinpol	1427.00	NIST Webbook
rinpol	1400.00	NIST Webbook
rinpol	1408.00	NIST Webbook
rinpol	1400.00	NIST Webbook
rinpol	1430.00	NIST Webbook
rinpol	1444.00	NIST Webbook
rinpol	1443.00	NIST Webbook
rinpol	1418.00	NIST Webbook
rinpol	1442.00	NIST Webbook
rinpol	1419.60	NIST Webbook
rinpol	1446.00	NIST Webbook
rinpol	1447.00	NIST Webbook

rinpol	1420.00		NIST Webbook
rinpol	246.51		NIST Webbook
rinpol	243.55		NIST Webbook
rinpol	247.04		NIST Webbook
rinpol	246.42		NIST Webbook
rinpol	245.70		NIST Webbook
rinpol	246.73		NIST Webbook
rinpol	246.20		NIST Webbook
rinpol	246.29		NIST Webbook
rinpol	247.04		NIST Webbook
rinpol	239.00		NIST Webbook
rinpol	246.03		NIST Webbook
rinpol	243.55		NIST Webbook
rinpol	244.50		NIST Webbook
rinpol	246.50		NIST Webbook
rinpol	243.60		NIST Webbook
rinpol	1395.00		NIST Webbook
ripol	2008.00		NIST Webbook
ripol	2009.00		NIST Webbook
ripol	2008.00		NIST Webbook
ripol	2008.00		NIST Webbook
ss	225.85	J/mol×K	NIST Webbook
tb	541.15 ± 0.60	K	NIST Webbook
tb	542.40 ± 1.50	K	NIST Webbook
tb	541.20	K	KDB
tb	541.00 ± 5.00	K	NIST Webbook
tc	777.80	K	KDB
tf	376.15 ± 0.60	K	NIST Webbook
tf	378.40 ± 0.30	K	NIST Webbook
tf	378.00 ± 2.00	K	NIST Webbook
tf	378.00	K	KDB
tt	377.49 ± 0.01	K	NIST Webbook
vc	0.521	m3/kmol	KDB
zc	0.2427260		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	361.06	J/mol×K	722.55	Joback Method

cpg	349.89	J/mol×K	683.95	Joback Method
cpg	337.89	J/mol×K	645.36	Joback Method
cpg	325.00	J/mol×K	606.77	Joback Method
cpg	311.16	J/mol×K	568.17	Joback Method
cps	216.47	J/mol×K	298.15	NIST Webbook
cps	215.00	J/mol×K	298.00	NIST Webbook
dvisc	0.0003443	Pa×s	492.84	Joback Method
dvisc	0.0004103	Pa×s	456.11	Joback Method
dvisc	0.0008686	Pa×s	345.90	Joback Method
dvisc	0.0002960	Pa×s	529.58	Joback Method
dvisc	0.0006448	Pa×s	382.63	Joback Method
dvisc	0.0005043	Pa×s	419.37	Joback Method
dvisc	0.0012561	Pa×s	309.16	Joback Method
hfust	15.90	kJ/mol	378.00	NIST Webbook
hfust	15.90	kJ/mol	378.00	NIST Webbook
hfust	23.97	kJ/mol	377.20	NIST Webbook
hsubt	82.80	kJ/mol	353.00	NIST Webbook
hsubt	79.90 ± 0.40	kJ/mol	289.50	NIST Webbook
hsubt	79.90 ± 0.30	kJ/mol	378.30	NIST Webbook
hsubt	82.20 ± 0.40	kJ/mol	293.50	NIST Webbook
hsubt	61.10 ± 0.10	kJ/mol	377.70	NIST Webbook
hvapt	60.00	kJ/mol	393.00	NIST Webbook
hvapt	60.90 ± 0.70	kJ/mol	380.00	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.46295e+01
Coeff. B	-4.62605e+03
Coeff. C	-7.90620e+01
Temperature range (K), min.	378.16
Temperature range (K), max.	575.52

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/T + C*ln(T) + D*T^2
Coeff. A	8.45876e+01
Coeff. B	-1.05543e+04

Coeff. C	-9.75616e+00
Coeff. D	3.18558e-06
Temperature range (K), min.	378.15
Temperature range (K), max.	777.78

Sources

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
KDB:	https://www.cheric.org/files/research/kdb/mol/mol776.mol
Aqueous Solubility Prediction Method:	http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C581408&Units=SI
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
KDB Vapor Pressure Data:	https://www.cheric.org/research/kdb/hcprop/showprop.php?cmpid=776
Solid-Liquid Equilibria of Binary Mixtures of Dimethylnaphthalene Isomers:	https://www.doi.org/10.1021/je700088n
Estimated Solubility Method:	http://pubs.acs.org/doi/suppl/10.1021/ci034243x/suppl_file/ci034243xsi20040112_053635.txt
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

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
hsub:	Enthalpy of sublimation at standard conditions
hsubt:	Enthalpy of sublimation 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
pc:	Critical Pressure
pvap:	Vapor pressure
rinpol:	Non-polar retention indices
ripol:	Polar retention indices
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