

1,1'-Binaphthalene, 3,3'-dimethyl-

Other names:	1,1'-Binaphthyl, 3,3'-dimethyl- 3,3'-Dimethyl-1,1'-binaphthyl
Inchi:	InChI=1S/C22H18/c1-15-11-17-7-3-5-9-19(17)21(13-15)22-14-16(2)12-18-8-4-6-10-20(1
InchiKey:	WSLHQYUWIBLCMQ-UHFFFAOYSA-N
Formula:	C22H18
SMILES:	Cc1cc(-c2cc(C)cc3ccccc23)c2ccccc2c1
Mol. weight [g/mol]:	282.38
CAS:	34042-82-5

Physical Properties

Property code	Value	Unit	Source
gf	533.96	kJ/mol	Joback Method
hf	311.91	kJ/mol	Joback Method
hfus	33.30	kJ/mol	Joback Method
hvap	75.05	kJ/mol	Joback Method
ie	8.20 ± 0.05	eV	NIST Webbook
ie	8.00	eV	NIST Webbook
log10ws	-8.63		Crippen Method
logp	6.277		Crippen Method
mvol	234.400	ml/mol	McGowan Method
pc	1996.55	kPa	Joback Method
tb	814.00	K	Joback Method
tc	1073.19	K	Joback Method
tf	506.02	K	Joback Method
vc	0.895	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	659.93	J/molxK	814.00	Joback Method
cpg	676.36	J/molxK	857.20	Joback Method
cpg	691.65	J/molxK	900.40	Joback Method
cpg	705.99	J/molxK	943.60	Joback Method
cpg	719.54	J/molxK	986.80	Joback Method

cpg	732.48	J/molxK	1029.99	Joback Method
cpg	745.00	J/molxK	1073.19	Joback Method
dvisc	0.0010419	Paxs	506.02	Joback Method
dvisc	0.0007718	Paxs	557.35	Joback Method
dvisc	0.0006014	Paxs	608.68	Joback Method
dvisc	0.0004872	Paxs	660.01	Joback Method
dvisc	0.0004068	Paxs	711.34	Joback Method
dvisc	0.0003481	Paxs	762.67	Joback Method
dvisc	0.0003037	Paxs	814.00	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C34042825&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

Legend

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
ie:	Ionization energy
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mccvol:	McGowan's characteristic volume
pc:	Critical Pressure
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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