

2,2'-Binaphthalene

Other names:

2,2'-Binaphthyl
«beta», «beta»'-Binaphthyl
2,2'-Dinaphthyl
2,2-Binaphthalene

Inchi:

InChI=1S/C20H14/c1-3-7-17-13-19(11-9-15(17)5-1)20-12-10-16-6-2-4-8-18(16)14-20/h1-

InchiKey:

MSBVBOUOMVTWKE-UHFFFAOYSA-N

Formula:

C20H14

SMILES:

c1ccc2cc(-c3ccc4ccccc4c3)ccc2c1

Mol. weight [g/mol]:

254.33

CAS:

612-78-2

Physical Properties

Property code	Value	Unit	Source
gf	536.38	kJ/mol	Joback Method
hf	376.13	kJ/mol	Joback Method
hfus	28.90	kJ/mol	Joback Method
hvap	69.27	kJ/mol	Joback Method
log10ws	-7.68		Crippen Method
logp	5.660		Crippen Method
mcvol	206.220	ml/mol	McGowan Method
pc	2460.47	kPa	Joback Method
rinpol	423.91		NIST Webbook
rinpol	421.55		NIST Webbook
rinpol	421.55		NIST Webbook
rinpol	421.30		NIST Webbook
rinpol	421.81		NIST Webbook
rinpol	422.40		NIST Webbook
rinpol	425.10		NIST Webbook
rinpol	426.40		NIST Webbook
rinpol	421.55		NIST Webbook
rinpol	425.10		NIST Webbook
rinpol	412.00		NIST Webbook
rinpol	426.90		NIST Webbook
rinpol	424.01		NIST Webbook
rinpol	424.40		NIST Webbook
rinpol	425.00		NIST Webbook
rinpol	423.91		NIST Webbook

tb	758.28	K	Joback Method
tc	1028.40	K	Joback Method
tf	461.20 ± 0.60	K	NIST Webbook
tf	461.90 ± 1.50	K	NIST Webbook
tf	460.80 ± 2.00	K	NIST Webbook
vc	0.783	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	622.13	J/mol×K	983.38	Joback Method
cpg	597.34	J/mol×K	893.34	Joback Method
cpg	583.72	J/mol×K	848.32	Joback Method
cpg	568.99	J/mol×K	803.30	Joback Method
cpg	552.94	J/mol×K	758.28	Joback Method
cpg	610.08	J/mol×K	938.36	Joback Method
cpg	633.72	J/mol×K	1028.40	Joback Method
dvisc	0.0013464	Paxs	458.44	Joback Method
dvisc	0.0003497	Paxs	758.28	Joback Method
dvisc	0.0004045	Paxs	708.31	Joback Method
dvisc	0.0004782	Paxs	658.33	Joback Method
dvisc	0.0005812	Paxs	608.36	Joback Method
dvisc	0.0007314	Paxs	558.39	Joback Method
dvisc	0.0009631	Paxs	508.41	Joback Method
hfust	38.90	kJ/mol	461.20	NIST Webbook
hfust	38.90	kJ/mol	461.20	NIST Webbook
sfust	84.40	J/mol×K	461.20	NIST Webbook

Sources

Crippen Method:

<http://pubs.acs.org/doi/abs/10.1021/ci990307I>

Crippen Method:

https://www.chemeo.com/doc/models/crippen_log10ws

Joback Method:

https://en.wikipedia.org/wiki/Joback_method

McGowan Method:

<http://link.springer.com/article/10.1007/BF02311772>

NIST Webbook:

<http://webbook.nist.gov/cgi/cbook.cgi?ID=C612782&Units=SI>

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
hfust:	Enthalpy of fusion at a given temperature
hvap:	Enthalpy of vaporization at standard conditions
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
rinpolar:	Non-polar retention indices
sfust:	Entropy of fusion at a given temperature
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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