2,2'-Biquinoline

Other names:	2,2'-Biquinolyl
	2,2'-Diquinolyl
	2,2'-Quinolyl
	2-quinolin-2-ylquinoline
	Cuproin
	Cuproine
	biquinoline
Inchi:	InChI=1S/C18H12N2/c1-3-7-15-13(5-1)9-11-17(19-15)18-12-10-14-6-2-4-8-16(14)20-18/
InchiKey:	WPTCSQBWLUUYDV-UHFFFAOYSA-N
Formula:	C18H12N2
SMILES:	c1ccc2nc(-c3ccc4ccccc4n3)ccc2c1
Mol. weight [g/mol]:	256.30
CAS:	119-91-5

Physical Properties

Property code	Value	Unit	Source
chs	-9049.40 ± 6.80	kJ/mol	NIST Webbook
hf	347.90 ± 7.90	kJ/mol	NIST Webbook
hfs	251.30 ± 7.00	kJ/mol	NIST Webbook
hsub	134.70 ± 1.30	kJ/mol	NIST Webbook
hsub	96.60	kJ/mol	NIST Webbook
log10ws	-5.40		Aqueous Solubility Prediction Method
log10ws	-5.40		Estimated Solubility Method
logp	4.450		Crippen Method
mcvol	198.000	ml/mol	McGowan Method
rinpol	422.56		NIST Webbook
rinpol	421.12		NIST Webbook
rinpol	422.56		NIST Webbook
tf	467.90	K	Aqueous Solubility Prediction Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
hsubt	129.50 ± 0.80	kJ/mol	402.00	NIST Webbook

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Aqueous Solubility Prediction Method:	http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa
Estimated Solubility Method:	http://pubs.acs.org/doi/suppl/10.1021/ci034243x/suppl_file/ci034243xsi20040112_053635.txt
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C119915&Units=SI

Legend

chs:	Standard solid enthalpy of combustion
hf:	Enthalpy of formation at standard conditions
hfs:	Solid phase enthalpy of formation at standard conditions
hsub:	Enthalpy of sublimation at standard conditions
hsubt:	Enthalpy of sublimation at a given temperature
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
rinpol:	Non-polar retention indices
tf:	Normal melting (fusion) point