Neocuproine

Other names:	1,10-Phenanthroline, 2,9-dimethyl- 2,9-Dimethyl-o-phenanthroline 2,9-Dimethylphenanthroline 2,9-dimethyl-1,10-phenanthroline Neo-Cuproin
Inchi:	InChI=1S/C14H12N2/c1-9-3-5-11-7-8-12-6-4-10(2)16-14(12)13(11)15-9/h3-8H,1-2H3
InchiKey:	IYRGXJIJGHOCFS-UHFFFAOYSA-N
Formula:	C14H12N2
SMILES:	Cc1ccc2ccc3ccc(C)nc3c2n1
Mol. weight [g/mol]:	208.26
CAS:	484-11-7

Physical Properties

Property code	Value	Unit	Source
hfus	17.60	kJ/mol	Heat capacities and molar enthalpies and entropies of fusion for anhydrous 1,10-phenanthroline and 2,9-dimethyl-1,10-phenanthroline
log10ws	-5.56		Crippen Method
logp	3.400		Crippen Method
mcvol	165.400	ml/mol	McGowan Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
hfust	17.60	kJ/mol	435.90	NIST Webbook

Sources

Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Heat capacities and molar enthalpies and entropies of fusion for anhydrous 1,10-phenanthroline and 2,9-dimethyl-1,10-phenanthroline:	https://www.doi.org/10.1016/j.tca.2007.10.001

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C484117&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

hfus:	Enthalpy of fusion at standard conditions
hfust:	Enthalpy of fusion at a given temperature
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume