4,7-Dimethyl-1,10-phenanthroline

Other names:	1,10-Phenanthroline, 4,7-dimethyl- 4,7-Dimethyl-o-phenanthroline
Inchi:	InChI=1S/C14H12N2/c1-9-5-7-15-13-11(9)3-4-12-10(2)6-8-16-14(12)13/h3-8H,1-2H3
InchiKey:	JIVLDFFWTQYGSR-UHFFFAOYSA-N
Formula:	C14H12N2
SMILES:	Cc1ccnc2c1ccc1c(C)ccnc12
Mol. weight [g/mol]:	208.26
CAS:	3248-05-3

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.97		Aqueous Solubility Prediction Method
logp	3.400		Crippen Method
mcvol	165.400	ml/mol	McGowan Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C3248053&Units=SI
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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

Legend

log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume