

RTI 10

Other names:	6-methylpyrido[2,3-b][1,5]benzoxazepin-5-one
Inchi:	InChI=1S/C13H10N2O2/c1-15-10-6-2-3-7-11(10)17-12-9(13(15)16)5-4-8-14-12/h2-8H,1H
InchiKey:	BBMMISOHGVCAMY-UHFFFAOYSA-N
Formula:	C13H10N2O2
SMILES:	CN1C(=O)c2cccnc2Oc2ccccc21
Mol. weight [g/mol]:	226.24

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.67		Aqueous Solubility Prediction Method
log10ws	-3.67		Estimated Solubility Method
logp	2.464		Crippen Method
mcvol	163.050	ml/mol	McGowan Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
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

Legend

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

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