

RTI 19

Other names:	11-ethyl-5-methylbenzo[b][1,4]benzodiazepin-6-one
Inchi:	InChI=1S/C16H16N2O/c1-3-18-13-9-5-4-8-12(13)16(19)17(2)14-10-6-7-11-15(14)18/h4-
InchiKey:	IUMRYNUBZSCOQG-UHFFFAOYSA-N
Formula:	C16H16N2O
SMILES:	CCN1c2ccccc2C(=O)N(C)c2ccccc21
Mol. weight [g/mol]:	252.32

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.75		Aqueous Solubility Prediction Method
log10ws	-4.75		Estimated Solubility Method
logp	3.435		Crippen Method
mcvol	199.450	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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