

RTI 5

Other names: 11-ethyl-6-methylpyrido[3,2-c][1,5]benzodiazepin-5-one
Inchi: InChI=1S/C15H15N3O/c1-3-18-13-9-5-4-8-12(13)17(2)15(19)11-7-6-10-16-14(11)18/h4-
InchiKey: QIBWCUCLHZVYNL-UHFFFAOYSA-N
Formula: C15H15N3O
SMILES: CCN1c2ccccc2N(C)C(=O)c2cccnc21
Mol. weight [g/mol]: 253.31

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.32		Aqueous Solubility Prediction Method
log10ws	-3.32		Estimated Solubility Method
logp	2.830		Crippen Method
mcvol	195.340	ml/mol	McGowan Method

Sources

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>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>

Legend

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

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<https://www.chemeo.com/cid/104-532-5/RTI-5.pdf>

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