

RTI 9

Other names: 5-ethylbenzo[b][1,4]benzoxazepin-6-one
Inchi: InChI=1S/C15H13NO2/c1-2-16-12-8-4-6-10-14(12)18-13-9-5-3-7-11(13)15(16)17/h3-10H
InchiKey: MRBRHCRUXKHKKI-UHFFFAOYSA-N
Formula: C15H13NO2
SMILES: CCN1C(=O)c2ccccc2Oc2ccccc21
Mol. weight [g/mol]: 239.27

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.68		Aqueous Solubility Prediction Method
log10ws	-3.68		Estimated Solubility Method
logp	3.459		Crippen Method
mcvol	181.250	ml/mol	McGowan Method

Sources

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

Legend

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

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