RTI 3

Other names: 3-amino-6,9-dimethylpyrido[2,3-b][1,5]benzoxazepin-5-one
Inchi: InChI=1S/C14H13N3O2/c1-8-3-4-11-12(5-8)19-13-10(14(18)17(11)2)6-9(15)7-16-13/h3-
InchiKey: MUKSMBAVCDPKRC-UHFFFAOYSA-N
Formula: C14H13N3O2
SMILES: Cc1ccc2c(c1)Oc1ncc(N)cc1C(=O)N2C
Mol. weight [g/mol]: 255.28

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.04		Aqueous Solubility Prediction Method
log10ws	-3.04		Estimated Solubility Method
logp	2.355		Crippen Method
mcvol	187.120	ml/mol	McGowan Method

Sources

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/ci990307l
Aqueous Solubility Prediction Method: http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa

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/110-716-4/RTI-3.pdf