Reverse Transcriptase inhibitor 1

Other names: 132312-85-7
Inchi: InChI=1S/C14H14N4O/c1-3-18-12-10(6-4-8-15-12)14(19)17(2)11-7-5-9-16-13(11)18/h4-9
InchiKey: SVFKQHLOBRUZGV-UHFFFAOYSA-N
Formula: C14H14N4O
SMILES: CCN1c2ncccc2C(=O)N(C)c2cccnc21
Mol. weight [g/mol]: 254.29

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.62		Aqueous Solubility Prediction Method
log10ws	-2.62		Estimated Solubility Method
logp	2.225		Crippen Method
mcvol	191.230	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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