RTI 12

Other names: 133627-12-0
Inchi: InChI=1S/C14H13ClN4O/c1-3-19-12-9(5-4-8-16-12)14(20)18(2)10-6-7-11(15)17-13(10)1
InchiKey: YSEMEGXOKULCML-UHFFFAOYSA-N
Formula: C14H13ClN4O
SMILES: CCN1c2ncccc2C(=O)N(C)c2ccc(Cl)nc21
Mol. weight [g/mol]: 288.74

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.11		Aqueous Solubility Prediction Method
log10ws	-4.11		Estimated Solubility Method
logp	2.878		Crippen Method
mcvol	203.470	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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