

RTI 16

Inchi: InChI=1S/C14H14N4S/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: YNARWAUTTJJADX-UHFFFAOYSA-N
Formula: C14H14N4S
SMILES: CCN1c2ncccc2C(=S)N(C)c2cccnc21
Mol. weight [g/mol]: 270.36

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.63		Aqueous Solubility Prediction Method
log10ws	-4.63		Estimated Solubility Method
logp	2.760		Crippen Method
mcvol	201.710	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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