

RTI 6

Inchi: InChI=1S/C16H19N5O2/c1-3-21-14-11(5-4-8-17-14)16(23)18-12-6-7-13(19-15(12)21)20
InchiKey: RSPPUQXSQYBMEE-UHFFFAOYSA-N
Formula: C16H19N5O2
SMILES: CCN1c2nc(N(C)CCO)ccc2NC(=O)c2cccnc21
Mol. weight [g/mol]: 313.36

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.36		Estimated Solubility Method
logp	1.629		Crippen Method
mcvol	235.260	ml/mol	McGowan Method

Sources

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