

RTI 11

Inchi: InChI=1S/C15H14N2O2/c1-9-3-5-13-11(7-9)15(18)17(2)12-8-10(16)4-6-14(12)19-13/h3-8
InchiKey: COGWTYZJZRNZQG-UHFFFAOYSA-N
Formula: C15H14N2O2
SMILES: Cc1ccc2c(c1)C(=O)N(C)c1cc(N)ccc1O2
Mol. weight [g/mol]: 254.29

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.93		Estimated Solubility Method
logp	2.960		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/ci9903071>

Legend

log10ws: Log10 of Water solubility in mol/l
logp: Octanol/Water partition coefficient
mcvol: McGowan's characteristic volume

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