RTI 23

Inchi: InChI=1S/C16H17N3O2/c1-4-19-13-9-11(21-3)8-10(2)14(13)18-16(20)12-6-5-7-17-15(12
InchiKey: PVVKNINYCJVIFZ-UHFFFAOYSA-N
Formula: C16H17N3O2
SMILES: CCN1c2cc(OC)cc(C)c2NC(=O)c2cccnc21
Mol. weight [g/mol]: 283.33

Physical Properties

Property code	Value	Unit	Source
log10ws	-5.15		Estimated Solubility Method
logp	3.122		Crippen Method
mcvol	215.300	ml/mol	McGowan Method

Sources

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
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