

fluconazole

Other names: 2-(2,4-difluorophenyl)-1,3-bis(1,2,4-triazol-1-yl)propan-2-ol
Inchi: InChI=1S/C13H12F2N6O/c14-10-1-2-11(12(15)3-10)13(22,4-20-8-16-6-18-20)5-21-9-17-13
InchiKey: RFHAOTPXVQNOHP-UHFFFAOYSA-N
Formula: C13H12F2N6O
SMILES: OC(Cn1cncn1)(Cn1cncn1)c1ccc(F)cc1F
Mol. weight [g/mol]: 306.28

Physical Properties

Property code	Value	Unit	Source
log10ws	-1.80		Aqueous Solubility Prediction Method
log10ws	-1.80		Estimated Solubility Method
logp	0.736		Crippen Method
mcvol	200.640	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/AqueousDataset002.xlsx>
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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