RTI 13

Other names: 11-ethyl-2-methyl-4-(trifluoromethyl)-5H-dipyrido[2,3-e:2',3'-f][1,4]diazepin-6-one
Inchi: InChI=1S/C15H13F3N4O/c1-3-22-12-9(5-4-6-19-12)14(23)21-11-10(15(16,17)18)7-8(2)2
InchiKey: KDDQDUIBYASSFC-UHFFFAOYSA-N
Formula: C15H13F3N4O
SMILES: CCN1c2ncccc2C(=O)Nc2c(C(F)(F)F)cc(C)nc21
Mol. weight [g/mol]: 322.29

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.21		Aqueous Solubility Prediction Method
log10ws	-4.21		Estimated Solubility Method
logp	3.528		Crippen Method
mcvol	210.630	ml/mol	McGowan Method

Sources

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

Latest version available from:
https://www.chemeo.com/cid/105-866-4/RTI-13.pdf