RTI 15

Other names: 11-Ethyl-2,4-dimethyl-5,11-dihydro-6H-dipyrido[2,3-e:3',2'-b][1,4]diazepin-6-one
Inchi: InChI=1S/C15H16N4O/c1-4-19-13-11(6-5-7-16-13)15(20)18-12-9(2)8-10(3)17-14(12)19/h
InchiKey: UDDMNBYVRLYNKY-UHFFFAOYSA-N
Formula: C15H16N4O
SMILES: CCN1c2ncccc2C(=O)Nc2c(C)cc(C)nc21
Mol. weight [g/mol]: 268.32

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.55		Aqueous Solubility Prediction Method
log10ws	-4.55		Estimated Solubility Method
logp	2.817		Crippen Method
mcvol	205.320	ml/mol	McGowan Method

Sources

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

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/109-983-0/RTI-15.pdf