RTI 2

Other names: 5,11-diethyldipyrido[2,3-b:3',2'-e][1,4]diazepin-6-one
Inchi: InChI=1S/C15H16N4O/c1-3-18-12-8-6-10-17-14(12)19(4-2)13-11(15(18)20)7-5-9-16-13/h
InchiKey: ISMYLNZMKJLINI-UHFFFAOYSA-N
Formula: C15H16N4O
SMILES: CCN1C(=O)c2cccnc2N(CC)c2ncccc21
Mol. weight [g/mol]: 268.32

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.86		Aqueous Solubility Prediction Method
log10ws	-2.86		Estimated Solubility Method
logp	2.615		Crippen Method
mcvol	205.320	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