glybuthiazole

Inchi: InChI=1S/C12H16N4O2S2/c1-12(2,3)10-14-15-11(19-10)16-20(17,18)9-6-4-8(13)5-7-9/h
InchiKey: DVQVBLBKEXITIK-UHFFFAOYSA-N
Formula: C12H16N4O2S2
SMILES: CC(C)(C)c1nnc(NS(=O)(=O)c2ccc(N)cc2)s1
Mol. weight [g/mol]: 312.42

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.74		Aqueous Solubility Prediction Method
logp	2.219		Crippen Method
mcvol	221.080	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
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