sulfamethomidine

Inchi: InChI=1S/C12H14N4O3S/c1-8-14-11(7-12(15-8)19-2)16-20(17,18)10-5-3-9(13)4-6-10/h3
InchiKey: QKLSCPPJEVXONT-UHFFFAOYSA-N
Formula: C12H14N4O3S
SMILES: COc1cc(NS(=O)(=O)c2ccc(N)cc2)nc(C)n1
Mol. weight [g/mol]: 294.34

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.54		Aqueous Solubility Prediction Method
logp	1.177		Crippen Method
mcvol	206.300	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/AqueousDa

Legend

log10ws: Log10 of Water solubility in mol/l
logp: Octanol/Water partition coefficient
mcvol: McGowan's characteristic volume