6-HYDROXY-1,3-BENZOTHIAZOLE-2-SULFONAMI

Inchi: InChI=1S/C7H6N2O3S2/c8-14(11,12)7-9-5-2-1-4(10)3-6(5)13-7/h1-3,10H,(H2,8,11,12)
InchiKey: NOOBQTYVTDBXTL-UHFFFAOYSA-N
Formula: C7H6N2O3S2
SMILES: NS(=O)(=O)c1nc2ccc(O)cc2s1
Mol. weight [g/mol]: 230.27

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.50		Aqueous Solubility Prediction Method
logp	0.649		Crippen Method
mcvol	140.840	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