1,3-benzothiazole-2-sulfonamide

Inchi: InChI=1S/C7H6N2O2S2/c8-13(10,11)7-9-5-3-1-2-4-6(5)12-7/h1-4H,(H2,8,10,11)
InchiKey: SDYMYAFSQACTQP-UHFFFAOYSA-N
Formula: C7H6N2O2S2
SMILES: NS(=O)(=O)c1nc2ccccc2s1
Mol. weight [g/mol]: 214.27

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.63		Aqueous Solubility Prediction Method
logp	0.944		Crippen Method
mcvol	134.970	ml/mol	McGowan Method

Sources

Aqueous Solubility Prediction Method: http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa
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