N-(2-sulfamoyl-1,3-benzothiazol-6-yl)acetamide

Inchi: InChI=1S/C9H9N3O3S2/c1-5(13)11-6-2-3-7-8(4-6)16-9(12-7)17(10,14)15/h2-4H,1H3,(H,
InchiKey: RPVVBRXMFQZDHZ-UHFFFAOYSA-N
Formula: C9H9N3O3S2
SMILES: CC(=O)Nc1ccc2nc(S(N)(=O)=O)sc2c1
Mol. weight [g/mol]: 271.32

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.16		Aqueous Solubility Prediction Method
logp	0.902		Crippen Method
mcvol	174.700	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