

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/ci9903071
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

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