

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/ci9903071>

Legend

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

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