

6-HYDROXY-1,3-BENZOTHAZOLE-2-SULFONAMIDE

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/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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