

4-hydroxy-5,6-dihydro-4H-thieno[5,4-b]thiopyran-2-sulfonamide

Inchi:	InChI=1S/C7H9NO3S3/c8-14(10,11)6-3-4-5(9)1-2-12-7(4)13-6/h3,5,9H,1-2H2,(H2,8,10,11)
InchiKey:	QUBSMEXIPLOOMC-UHFFFAOYSA-N
Formula:	C7H9NO3S3
SMILES:	NS(=O)(=O)c1cc2c(s1)SCCC2O
Mol. weight [g/mol]:	251.35

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.59		Aqueous Solubility Prediction Method
logp	0.925		Crippen Method
mcvol	155.810	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/AqueousDataset002.xlsx

Legend

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

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