

7-hydroxy-6,7-dihydro-5H-thieno[4,5-b]thiopyran-2-sulfonamide

Inchi:	InChI=1S/C7H9NO3S3/c8-14(10,11)6-3-5-7(13-6)4(9)1-2-12-5/h3-4,9H,1-2H2,(H2,8,10,11)1H
InchiKey:	UGQVTTBSGZLNIL-UHFFFAOYSA-N
Formula:	C7H9NO3S3
SMILES:	NS(=O)(=O)c1cc2c(s1)C(O)CCS2
Mol. weight [g/mol]:	251.35

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.25		Aqueous Solubility Prediction Method
logp	0.925		Crippen Method
mcvol	155.810	ml/mol	McGowan Method
tf	430.65	K	Aqueous Solubility Prediction Method

Sources

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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

Legend

log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
tf:	Normal melting (fusion) point

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