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

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,(H2,8,10,1
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/ci990307l
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