7-hydroxy-4,4-dioxo-6,7-dihydro-5H-thieno[4,5-b]t

Inchi: InChI=1S/C7H9NO5S3/c8-16(12,13)6-3-5-7(14-6)4(9)1-2-15(5,10)11/h3-4,9H,1-2H2,(H2
InchiKey: LNVGTRNKWNAINT-UHFFFAOYSA-N
Formula: C7H9NO5S3
SMILES: NS(=O)(=O)c1cc2c(s1)C(O)CCS2(=O)=O
Mol. weight [g/mol]: 283.35

Physical Properties

Property code	Value	Unit	Source
log10ws	-1.28		Aqueous Solubility Prediction Method
logp	-0.394		Crippen Method
mcvol	167.550	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/ci990307l

Legend

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