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

Inchi: InChI=1S/C7H9NO5S3/c8-16(12,13)6-2-4-1-5(9)3-15(10,11)7(4)14-6/h2,5,9H,1,3H2,(H2,

InchiKey: APTGDJCKNMNFID-UHFFFAOYSA-N

Formula: C7H9NO5S3

SMILES: NS(=O)(=O)c1cc2c(s1)S(=O)(=O)CC(O)C2

Mol. weight [g/mol]: 283.35

Physical Properties

Property code	Value	Unit	Source
log10ws	-1.54		Aqueous Solubility Prediction Method
logp	-0.914		Crippen Method
mcvol	167.550	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