

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

<b>Inchi:</b>	InChI=1S/C7H9NO5S3/c8-16(12,13)7-2-6-5(14-7)1-4(9)3-15(6,10)11/h2,4,9H,1,3H2,(H2
<b>InchiKey:</b>	ZGRYQDHDZGJMNF-UHFFFAOYSA-N
<b>Formula:</b>	C7H9NO5S3
<b>SMILES:</b>	NS(=O)(=O)c1cc2c(s1)CC(O)CS2(=O)=O
<b>Mol. weight [g/mol]:</b>	283.35

## Physical Properties

Property code	Value	Unit	Source
log10ws	-1.59		Aqueous Solubility Prediction Method
logp	-0.914		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/ci9903071>

## Legend

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

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