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

Inchi: InChI=1S/C7H9NO5S3/c8-16(12,13)6-3-4-5(9)1-2-15(10,11)7(4)14-6/h3,5,9H,1-2H2,(H2
InchiKey: MAZCFXDIYXGRAD-UHFFFAOYSA-N
Formula: C7H9NO5S3
SMILES: NS(=O)(=O)c1cc2c(s1)S(=O)(=O)CCC2O
Mol. weight [g/mol]: 283.35

Physical Properties

Property code	Value	Unit	Source
log10ws	-1.65		Aqueous Solubility Prediction Method
logp	-0.394		Crippen Method
mcvol	167.550	ml/mol	McGowan Method
tf	440.65	K	Aqueous Solubility Prediction Method

Sources

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
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

Cheméo (https://www.chemeo.com) is the biggest free database of chemical and physical data for the process industry.