7,7-dioxo-5,6-dihydro-4H-thieno[5,4-b]thiopyran-2

Inchi: InChI=1S/C7H9NO4S3/c8-15(11,12)6-4-5-2-1-3-14(9,10)7(5)13-6/h4H,1-3H2,(H2,8,11,12

InchiKey: VVSSGCCPNDSLPL-UHFFFAOYSA-N

Formula: C7H9NO4S3

SMILES: NS(=O)(=O)c1cc2c(s1)S(=O)(=O)CCC2

Mol. weight [g/mol]: 267.35

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.68		Aqueous Solubility Prediction Method
logp	0.115		Crippen Method
mcvol	161.680	ml/mol	McGowan 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