4-oxo-5,6-dihydrothieno[5,4-b]thiopyran-2-sulfona

Inchi: InChI=1S/C7H7NO3S3/c8-14(10,11)6-3-4-5(9)1-2-12-7(4)13-6/h3H,1-2H2,(H2,8,10,11)
InchiKey: WKLCYOHFTPREOW-UHFFFAOYSA-N
Formula: C7H7NO3S3
SMILES: NS(=O)(=O)c1cc2c(s1)SCCC2=O
Mol. weight [g/mol]: 249.34

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.55		Aqueous Solubility Prediction Method
logp	1.074		Crippen Method
mcvol	151.510	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