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

Inchi: InChI=1S/C7H7NO3S3/c8-14(10,11)6-3-5-7(13-6)4(9)1-2-12-5/h3H,1-2H2,(H2,8,10,11)
InchiKey: AIVXUNRQBRKFJO-UHFFFAOYSA-N
Formula: C7H7NO3S3
SMILES: NS(=O)(=O)c1cc2c(s1)C(=O)CCS2
Mol. weight [g/mol]: 249.34

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.49		Aqueous Solubility Prediction Method
logp	1.074		Crippen Method
mcvol	151.510	ml/mol	McGowan Method
tf	486.65	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.