

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

<b>Inchi:</b>	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)
<b>InchiKey:</b>	WKLCYOHFTPREOW-UHFFFAOYSA-N
<b>Formula:</b>	C7H7NO3S3
<b>SMILES:</b>	NS(=O)(=O)c1cc2c(s1)SCCC2=O
<b>Mol. weight [g/mol]:</b>	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/ci9903071>

**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

<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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