

# 4,4,7-trioxo-5,6-dihydrothieno[4,5-b]thiopyran-2-s

<b>Inchi:</b>	InChI=1S/C7H7NO5S3/c8-16(12,13)6-3-5-7(14-6)4(9)1-2-15(5,10)11/h3H,1-2H2,(H2,8,1
<b>InchiKey:</b>	HYVMOJOTZLNZPF-UHFFFAOYSA-N
<b>Formula:</b>	C7H7NO5S3
<b>SMILES:</b>	NS(=O)(=O)c1cc2c(s1)C(=O)CCS2(=O)=O
<b>Mol. weight [g/mol]:</b>	281.34

## Physical Properties

Property code	Value	Unit	Source
log10ws	-3.67		Aqueous Solubility Prediction Method
logp	-0.244		Crippen Method
mcvol	163.250	ml/mol	McGowan Method

## Sources

<b>McGowan Method:</b>	<a href="http://link.springer.com/article/10.1007/BF02311772">http://link.springer.com/article/10.1007/BF02311772</a>
<b>Crippen Method:</b>	<a href="http://pubs.acs.org/doi/abs/10.1021/ci9903071">http://pubs.acs.org/doi/abs/10.1021/ci9903071</a>
<b>Aqueous Solubility Prediction Method:</b>	<a href="http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa">http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa</a>

## 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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