

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

|                             |  |
|-----------------------------|--|
| <b>Inchi:</b>               | InChI=1S/C7H9NO4S3/c8-15(11,12)6-4-5-2-1-3-14(9,10)7(5)13-6/h4H,1-3H2,(H2,8,11,1 |
| <b>InchiKey:</b>            | VVSSGCCPNDSLPL-UHFFFAOYSA-N  |
| <b>Formula:</b>             | C7H9NO4S3  |
| <b>SMILES:</b>              | NS(=O)(=O)c1cc2c(s1)S(=O)(=O)CCC2  |
| <b>Mol. weight [g/mol]:</b> | 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

|  |   |
|--|---|
| <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> |
| <b>McGowan Method:</b>                       | <a href="http://link.springer.com/article/10.1007/BF02311772">http://link.springer.com/article/10.1007/BF02311772</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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