

# 5-hydroxy-7,7-dioxo-5,6-dihydro-4H-thieno[5,4-b]t

|                             |  |
|-----------------------------|--|
| <b>Inchi:</b>               | InChI=1S/C7H9NO5S3/c8-16(12,13)6-2-4-1-5(9)3-15(10,11)7(4)14-6/h2,5,9H,1,3H2,(H2 |
| <b>InchiKey:</b>            | APTGDJCKNMNFID-UHFFFAOYSA-N  |
| <b>Formula:</b>             | C7H9NO5S3  |
| <b>SMILES:</b>              | NS(=O)(=O)c1cc2c(s1)S(=O)(=O)CC(O)C2   |
| <b>Mol. weight [g/mol]:</b> | 283.35   |

## Physical Properties

| Property code | Value   | Unit   | Source                               |
|---------------|---------|--------|--------------------------------------|
| log10ws       | -1.54   |        | Aqueous Solubility Prediction Method |
| logp          | -0.914  |        | Crippen Method                       |
| mcvol         | 167.550 | 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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