

# glybuthiazole

**Inchi:** InChI=1S/C12H16N4O2S2/c1-12(2,3)10-14-15-11(19-10)16-20(17,18)9-6-4-8(13)5-7-9/h  
**InchiKey:** DVQVBLBKEXITIK-UHFFFAOYSA-N  
**Formula:** C12H16N4O2S2  
**SMILES:** CC(C)(C)c1nnc(NS(=O))(=O)c2ccc(N)cc2)s1  
**Mol. weight [g/mol]:** 312.42

## Physical Properties

| Property code | Value   | Unit   | Source                               |
|---------------|---------|--------|--------------------------------------|
| log10ws       | -3.74   |        | Aqueous Solubility Prediction Method |
| logp          | 2.219   |        | Crippen Method                       |
| mcvol         | 221.080 | ml/mol | McGowan 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/AqueousDataset002.xlsx>  
**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

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