

# Sparsomycin (3,8mg/ml)

**Inchi:** InChI=1S/C13H19N3O5S2/c1-8-10(12(19)16-13(20)14-8)3-4-11(18)15-9(5-17)6-23(21)7  
**InchiKey:** XKLZIVIOZDNKEQ-UHFFFAOYSA-N  
**Formula:** C13H19N3O5S2  
**SMILES:** CSCS(=O)CC(CO)NC(=O)C=Cc1c(C)[nH]c(=O)[nH]c1=O  
**Mol. weight [g/mol]:** 361.44

## Physical Properties

| Property code | Value   | Unit   | Source                               |
|---------------|---------|--------|--------------------------------------|
| log10ws       | -1.98   |        | Aqueous Solubility Prediction Method |
| log10ws       | -1.98   |        | Estimated Solubility Method          |
| logp          | -2.033  |        | Crippen Method                       |
| mcvol         | 253.660 | ml/mol | McGowan Method                       |

## Sources

**Estimated Solubility Method:** [http://pubs.acs.org/doi/suppl/10.1021/ci034243x/suppl\\_file/ci034243xsi20040112\\_053635.txt](http://pubs.acs.org/doi/suppl/10.1021/ci034243x/suppl_file/ci034243xsi20040112_053635.txt)  
**McGowan Method:** <http://link.springer.com/article/10.1007/BF02311772>  
**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>

## Legend

**log10ws:** Log10 of Water solubility in mol/l  
**logp:** Octanol/Water partition coefficient  
**mcvol:** McGowan's characteristic volume

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