# sulfaperine

**Inchi:** InChI=1S/C11H12N4O2S/c1-8-6-13-11(14-7-8)15-18(16,17)10-4-2-9(12)3-5-10/h2-7H,12
**InchiKey:** DZQVFHSCSRACSX-UHFFFAOYSA-N
**Formula:** C11H12N4O2S
**SMILES:** Cc1cnc(NS(=O)(=O)c2ccc(N)cc2)nc1
**Mol. weight [g/mol]:** 264.31

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| log10ws | -2.82 | | Aqueous Solubility Prediction Method |
| logp | 1.168 | | Crippen Method |
| mcvol | 186.340 | ml/mol | McGowan Method |
| tf | 535.65 | K | Aqueous Solubility Prediction Method |

## Sources

**McGowan Method:** http://link.springer.com/article/10.1007/BF02311772
**Crippen Method:** http://pubs.acs.org/doi/abs/10.1021/ci990307l
**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
**tf:** Normal melting (fusion) point

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