

famotidine

Inchi: InChI=1S/C21H27N5O4S/c1-15-13-24-19(14-23-15)20(27)22-12-11-16-7-9-18(10-8-16)3
InchiKey: XUFQPHANEPEMJ-UHFFFAOYSA-N
Formula: C21H27N5O4S
SMILES: Cc1cnc(C(=O)NCCc2ccc(S(=O)(=O)NC(=O)NC3CCCCC3)cc2)cn1
Mol. weight [g/mol]: 445.54

Physical Properties

| Property code | Value | Unit | Source |
|---------------|---------|--------|--------------------------------------|
| log10ws | -2.65 | | Aqueous Solubility Prediction Method |
| logp | 2.078 | | Crippen Method |
| mcvol | 329.500 | ml/mol | McGowan Method |
| tf | 481.65 | K | Aqueous Solubility Prediction Method |

Sources

Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>
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
tf: Normal melting (fusion) point

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