

kebuzone

Inchi: InChI=1S/C19H18N2O3/c1-14(22)12-13-17-18(23)20(15-8-4-2-5-9-15)21(19(17)24)16-10
InchiKey: LGYTZKPVOAIUKX-UHFFFAOYSA-N
Formula: C19H18N2O3
SMILES: CC(=O)CCC1C(=O)N(c2ccccc2)N(c2ccccc2)C1=O
Mol. weight [g/mol]: 322.36

Physical Properties

| Property code | Value | Unit | Source |
|---------------|---------|--------|--------------------------------------|
| log10ws | -3.27 | | Aqueous Solubility Prediction Method |
| log10ws | -3.27 | | Estimated Solubility Method |
| logp | 2.967 | | Crippen Method |
| mcvol | 244.860 | ml/mol | McGowan Method |

Sources

Estimated Solubility Method: 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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