

metiazinic acid

Inchi: InChI=1S/C15H13NO2S/c1-16-11-4-2-3-5-13(11)19-14-7-6-10(8-12(14)16)9-15(17)18/h2
InchiKey: LMINNBXUMGNKMM-UHFFFAOYSA-N
Formula: C15H13NO2S
SMILES: CN1c2ccccc2Sc2ccc(CC(=O)O)cc21
Mol. weight [g/mol]: 271.34

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.94		Aqueous Solubility Prediction Method
logp	3.546		Crippen Method
mcvol	197.600	ml/mol	McGowan 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

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