

tubercidin

Inchi: InChI=1S/C11H14N4O4/c12-9-5-1-2-15(10(5)14-4-13-9)11-8(18)7(17)6(3-16)19-11/h1-2,4,6,8,10,12,14,16,18,20
InchiKey: HDZZVAMISRMYYHH-UHFFFAOYSA-N
Formula: C11H14N4O4
SMILES: Nc1ncnc2c1ccn2C1OC(CO)C(O)C1O
Mol. weight [g/mol]: 266.26

Physical Properties

Property code	Value	Unit	Source
log10ws	-1.95		Aqueous Solubility Prediction Method
log10ws	-1.95		Estimated Solubility Method
logp	-1.375		Crippen Method
mvol	179.470	ml/mol	McGowan Method

Sources

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/AqueousDataset002.xlsx>
Estimated Solubility Method: http://pubs.acs.org/doi/suppl/10.1021/ci034243x/suppl_file/ci034243xsi20040112_053635.txt

Legend

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

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