Benznidazole

Inchi: InChI=1S/C12H12N4O3/c17-11(14-8-10-4-2-1-3-5-10)9-15-7-6-13-12(15)16(18)19/h1-7H
InchiKey: CULUWZNBISUWAS-UHFFFAOYSA-N
Formula: C12H12N4O3
SMILES: O=C(Cn1ccnc1[N+](=O)[O-])NCc1ccccc1
Mol. weight [g/mol]: 260.25

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.81		Aqueous Solubility Prediction Method
log10ws	-2.81		Estimated Solubility Method
logp	1.108		Crippen Method
mcvol	185.650	ml/mol	McGowan Method

Sources

Aqueous Solubility Prediction Method: http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa
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/ci990307l

Legend

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

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