1-aminoacridine

Inchi: InChI=1S/C13H10N2/c14-11-5-3-7-13-10(11)8-9-4-1-2-6-12(9)15-13/h1-8H,14H2
InchiKey: LOMMDWBTANPFEJ-UHFFFAOYSA-N
Formula: C13H10N2
SMILES: Nc1cccc2nc3ccccc3cc12
Mol. weight [g/mol]: 194.24

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.22		Aqueous Solubility Prediction Method
log10ws	-4.22		Estimated Solubility Method
logp	2.970		Crippen Method
mcvol	151.310	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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