Quinoline-8-carboxylic acid

Inchi: InChI=1S/C10H7NO2/c12-10(13)8-5-1-3-7-4-2-6-11-9(7)8/h1-6H,(H,12,13)
InchiKey: QRDZFPUVLYEQTA-UHFFFAOYSA-N
Formula: C10H7NO2
SMILES: O=C(O)c1cccc2cccnc12
Mol. weight [g/mol]: 173.17

Physical Properties

Property code	Value	Unit	Source
log10ws	-1.74		Aqueous Solubility Prediction Method
logp	1.933		Crippen Method
mcvol	125.960	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/ci990307l
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