

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/ci9903071>

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

Latest version available from:

<https://www.cheméo.com/cid/100-814-6/Quinoline-8-carboxylic-acid.pdf>

Generated by Cheméo on 2024-05-02 13:33:13.311695343 +0000 UTC m=+16946042.232272659.

Cheméo (<https://www.cheméo.com>) is the biggest free database of chemical and physical data for the process industry.