2-Quinolinecarboxylic acid

Other names:	Quinaldic acid
	Quinaldinic acid
	Quinoline-2-carboxylic acid
Inchi:	InChI=1S/C10H7NO2/c12-10(13)9-6-5-7-3-1-2-4-8(7)11-9/h1-6H,(H,12,13)
InchiKey:	LOAUVZALPPNFOQ-UHFFFAOYSA-N
Formula:	C10H7NO2
SMILES:	O=C(O)c1ccc2ccccc2n1
Mol. weight [g/mol]:	173.17
CAS:	93-10-7

Physical Properties

Property code	Value	Unit	Source
log10ws	-1.09		Aqueous Solubility Prediction Method
logp	1.933		Crippen Method
mcvol	125.960	ml/mol	McGowan Method
tf	429.82	K	Aqueous Solubility Prediction Method

Sources

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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C93107&Units=SI

Legend

log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
tf:	Normal melting (fusion) point