

2-Quinolinecarboxylic acid, 4-hydroxy-8-methoxy-, ethyl ester

Inchi:	InChI=1S/C13H13NO4/c1-3-18-13(16)9-7-10(15)8-5-4-6-11(17-2)12(8)14-9/h4-7H,3H2,1
InchiKey:	CXMNCVQZLHTTBT-UHFFFAOYSA-N
Formula:	C13H13NO4
SMILES:	CCOC(=O)c1cc(O)c2cccc(OC)c2n1
Mol. weight [g/mol]:	247.25
CAS:	55895-59-5

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.37		Crippen Method
logp	2.126		Crippen Method
mcvol	179.970	ml/mol	McGowan Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C55895595&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

Legend

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

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