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/ci990307l

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