7-Chloro-3-methyl-quinoline-8-carboxylic acid, ethyl ester

Other names: 8-Quinolinecarboxylic acid, 7-chloro-3-methyl-, ethyl ester
Inchi: InChI=1S/C13H12ClNO2/c1-3-17-13(16)11-10(14)5-4-9-6-8(2)7-15-12(9)11/h4-7H,3H2,1
InchiKey: CCLHMJNBSPIFMT-UHFFFAOYSA-N
Formula: C13H12ClNO2
SMILES: CCOC(=O)c1c(Cl)ccc2cc(C)cnc12
Mol. weight [g/mol]: 249.69

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.86		Crippen Method
logp	3.373		Crippen Method
mcvol	180.470	ml/mol	McGowan Method
rinpol	2068.00		NIST Webbook

Sources

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=U373121&Units=SI

Legend

log10ws: Log10 of Water solubility in mol/l
logp: Octanol/Water partition coefficient
mcvol: McGowan's characteristic volume
rinpol: Non-polar retention indices

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