3,7-Dichloroquinoline-8-carboxylic acid, ethyl ester

Inchi: InChI=1S/C12H9Cl2NO2/c1-2-17-12(16)10-9(14)4-3-7-5-8(13)6-15-11(7)10/h3-6H,2H2,1

InchiKey: VBMFMZCRPLYVHE-UHFFFAOYSA-N

Formula: C12H9Cl2NO2

SMILES: CCOC(=O)c1c(Cl)ccc2cc(Cl)cnc12

Mol. weight [g/mol]: 270.11

Physical Properties

Property code	Value	Unit	Source
log10ws	-5.07		Crippen Method
logp	3.718		Crippen Method
mcvol	178.620	ml/mol	McGowan Method
rinpol	2077.00		NIST Webbook
rinpol	2077.00		NIST Webbook

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=U373002&Units=SI

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

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.