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

Other names: 8-Quinolinecarboxylic acid, 3,7-dichloro-, trimethylsilyl ester
Quinclorac TMS ester

Inchi: InChI=1S/C13H13Cl2NO2Si/c1-19(2,3)18-13(17)11-10(15)5-4-8-6-9(14)7-16-12(8)11/h4-

InchiKey: JDVKVDVHSOTTPW-UHFFFAOYSA-N

Formula: C13H13Cl2NO2Si

SMILES: C[Si](C)(C)OC(=O)c1c(Cl)ccc2cc(Cl)cnc12

Mol. weight [g/mol]: 314.24

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.54		Crippen Method
logp	4.533		Crippen Method
rinpol	2092.00		NIST Webbook
rinpol	2092.00		NIST Webbook

Sources

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=U373123&Units=SI

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

log10ws: Log10 of Water solubility in mol/l

logp: Octanol/Water partition coefficient

rinpol: Non-polar retention indices