

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
rinpola	2092.00		NIST Webbook
rinpola	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/ci9903071

Legend

log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
rinpola:	Non-polar retention indices

Latest version available from:

<https://www.chemeo.com/cid/56-674-2/3-7-Dichloroquinoline-8-carboxylic-acid-trimethylsilyl-ester.pdf>

Generated by Cheméo on 2024-04-23 06:17:56.67450137 +0000 UTC m=+16142325.595078682.

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