Benzoic acid, 3,6-dichloro-2-hydroxy, TMS

Inchi: InChI=1S/C13H20Cl2O3Si2/c1-19(2,3)17-12-10(15)8-7-9(14)11(12)13(16)18-20(4,5)6/h7
InchiKey: KUISTZYDIDGLCU-UHFFFAOYSA-N
Formula: C13H20Cl2O3Si2
SMILES: C[Si](C)(C)OC(=O)c1c(Cl)ccc(Cl)c1O[Si](C)(C)C
Mol. weight [g/mol]: 351.37

Physical Properties

Property code	Value	Unit	Source
log10ws	-0.98		Crippen Method
logp	5.199		Crippen Method
rinpol	1781.00		NIST Webbook
rinpol	1781.00		NIST Webbook

Sources

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R44188&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