2,3,6-Trichlorophenol, trimethylsilyl ether

Other names: 2,3,6-Trichlorophenol, tms derivative
Inchi: InChI=1S/C9H11Cl3OSi/c1-14(2,3)13-9-7(11)5-4-6(10)8(9)12/h4-5H,1-3H3
InchiKey: BFMVRFQFQXIYTB-UHFFFAOYSA-N
Formula: C9H11Cl3OSi
SMILES: C[Si](C)(C)Oc1c(Cl)ccc(Cl)c1Cl
Mol. weight [g/mol]: 269.63

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.53		Crippen Method
logp	4.861		Crippen Method
rinpol	1537.90		NIST Webbook
rinpol	1537.90		NIST Webbook

Sources

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=U333409&Units=SI

Legend

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