2,3,6-Trichlorophenol, tert-butyldimethylsilyl ether

Other names: 2,3,6-trichlorophenol, TBDMS
2,3,6-Trichlorophenol, tbdms derivative
Inchi: InChI=1S/C12H17Cl3OSi/c1-12(2,3)17(4,5)16-11-9(14)7-6-8(13)10(11)15/h6-7H,1-5H3
InchiKey: NEGHPKXBLRQPHV-UHFFFAOYSA-N
Formula: C12H17Cl3OSi
SMILES: CC(C)(C)[Si](C)(C)Oc1c(Cl)ccc(Cl)c1Cl
Mol. weight [g/mol]: 311.71

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.79		Crippen Method
logp	6.031		Crippen Method
rinpol	1823.60		NIST Webbook
rinpol	1823.60		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=U333408&Units=SI

Legend

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