2,3,4,6-Tetrachlorophenol, tert-butyldimethylsilyl ether

Other names: 2,3,4,6-tetrachlorophenol, TBDMS
2,3,4,6-Tetrachlorophenol, tbdms derivative

Inchi: InChI=1S/C12H16Cl4OSi/c1-12(2,3)18(4,5)17-11-8(14)6-7(13)9(15)10(11)16/h6H,1-5H3

InchiKey: MDKIRIDRLGYYBR-UHFFFAOYSA-N

Formula: C12H16Cl4OSi

SMILES: CC(C)(C)[Si](C)(C)Oc1c(Cl)cc(Cl)c(Cl)c1Cl

Mol. weight [g/mol]: 346.15

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.48		Crippen Method
logp	6.684		Crippen Method
rinpol	1991.40		NIST Webbook
rinpol	1991.40		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=U333388&Units=SI

Legend

log10ws: Log10 of Water solubility in mol/l

logp: Octanol/Water partition coefficient

rinpol: Non-polar retention indices