2,4-Dichlorophenol, tert-butyldimethylsilyl ether

Other names: 2-4-dichlorophenol , TBDMS
Inchi: InChI=1S/C12H18Cl2OSi/c1-12(2,3)16(4,5)15-11-7-6-9(13)8-10(11)14/h6-8H,1-5H3
InchiKey: JYWHLWFKXXRKHZ-UHFFFAOYSA-N
Formula: C12H18Cl2OSi
SMILES: CC(C)(C)[Si](C)(C)Oc1ccc(Cl)cc1Cl
Mol. weight [g/mol]: 277.26

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.11		Crippen Method
logp	5.377		Crippen Method
rinpol	1631.90		NIST Webbook
rinpol	1631.90		NIST Webbook

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=U333365&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

Legend

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