Pentachlorophenol, tert-butyldimethylsilyl ether

Other names: Pentachlorophenol, TBDMS
Pentachlorophenol, tbdms derivative

Inchi: InChI=1S/C12H15Cl5OSi/c1-12(2,3)19(4,5)18-11-9(16)7(14)6(13)8(15)10(11)17/h1-5H3

InchiKey: KDPIVORPBWXDGN-UHFFFAOYSA-N

Formula: C12H15Cl5OSi

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

Mol. weight [g/mol]: 380.60

Physical Properties

Property code	Value	Unit	Source
log10ws	-5.16		Crippen Method
logp	7.338		Crippen Method
rinpol	2192.70		NIST Webbook
rinpol	2192.70		NIST Webbook

Sources

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=U333392&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