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:	https://www.chemeo.com/doc/models/crippen_log10ws
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U333388&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

Latest version available from:
https://www.chemeo.com/cid/75-386-1/2-3-4-6-Tetrachlorophenol-tert-butyldimethylsilyl-ether.pdf
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