

2,4,5-Trichlorophenol, tert-butyldimethylsilyl ether

Other names:	2,4,5-trichlorophenol, TBDMS 2,4,5-Trichlorophenol, tbdms derivative
Inchi:	InChI=1S/C12H17Cl3OSi/c1-12(2,3)17(4,5)16-11-7-9(14)8(13)6-10(11)15/h6-7H,1-5H3
InchiKey:	COHILCNIYMTIIO-UHFFFAOYSA-N
Formula:	C12H17Cl3OSi
SMILES:	CC(C)(C)[Si](C)(C)Oc1cc(Cl)c(Cl)cc1Cl
Mol. weight [g/mol]:	311.71

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.79		Crippen Method
logp	6.031		Crippen Method
rinpol	1783.10		NIST Webbook
rinpol	1783.10		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=U333396&Units=SI

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/36-552-9/2-4-5-Trichlorophenol-tert-butyldimethylsilyl-ether.pdf>

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