

3,5-Dichlorophenol, tert-butyldimethylsilyl ether

Other names:	3,5-dichlorophenol, TBDMS 3,5-Dichlorophenol, tbdms derivative
Inchi:	InChI=1S/C12H18Cl2OSi/c1-12(2,3)16(4,5)15-11-7-9(13)6-10(14)8-11/h6-8H,1-5H3
InchiKey:	ZVYAFVOHYMRKHP-UHFFFAOYSA-N
Formula:	C12H18Cl2OSi
SMILES:	CC(C)(C)[Si](C)(C)Oc1cc(Cl)cc(Cl)c1
Mol. weight [g/mol]:	277.26

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.11		Crippen Method
logp	5.377		Crippen Method
rinpol	1591.30		NIST Webbook
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Sources

Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U333374&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307I

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/119-888-5/3-5-Dichlorophenol-tert-butyldimethylsilyl-ether.pdf>

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