

3,4-Dichlorophenol, tert-butyldimethylsilyl ether

Other names:	3,4-dichlorophenol, TBDMS 3,4-Dichloro-1-dimethyl(tert-butyl)silyloxybenzene
Inchi:	InChI=1S/C12H18Cl2OSi/c1-12(2,3)16(4,5)15-9-6-7-10(13)11(14)8-9/h6-8H,1-5H3
InchiKey:	OUAAHASYLQJLQV-UHFFFAOYSA-N
Formula:	C12H18Cl2OSi
SMILES:	CC(C)(C)[Si](C)(C)Oc1ccc(Cl)c(Cl)c1
Mol. weight [g/mol]:	277.26
CAS:	188645-81-0

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.11		Crippen Method
logp	5.377		Crippen Method
rinpol	1653.80		NIST Webbook
rinpol	1622.00		NIST Webbook

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C188645810&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

Latest version available from:

<https://www.chemeo.com/cid/48-494-1/3-4-Dichlorophenol-tert-butyldimethylsilyl-ether.pdf>

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