

2,3,6-Trichlorophenol, tert-butyldimethylsilyl ether

Other names:	2,3,6-trichlorophenol, TBDMS 2,3,6-Trichlorophenol, tbdms derivative
Inchi:	InChI=1S/C12H17Cl3OSi/c1-12(2,3)17(4,5)16-11-9(14)7-6-8(13)10(11)15/h6-7H,1-5H3
InchiKey:	NEGHPKXBLRQPHV-UHFFFAOYSA-N
Formula:	C12H17Cl3OSi
SMILES:	CC(C)(C)[Si](C)(C)Oc1c(Cl)ccc(Cl)c1Cl
Mol. weight [g/mol]:	311.71

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.79		Crippen Method
logp	6.031		Crippen Method
rinpola	1823.60		NIST Webbook
rinpola	1823.60		NIST Webbook

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U333408&Units=SI

Legend

log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
rinpola:	Non-polar retention indices

Latest version available from:

<https://www.chemeo.com/cid/47-540-0/2-3-6-Trichlorophenol-tert-butyldimethylsilyl-ether.pdf>

Generated by Cheméo on 2024-04-19 20:32:25.821526749 +0000 UTC m=+15847994.742104095.

Cheméo (<https://www.chemeo.com>) is the biggest free database of chemical and physical data for the process industry.