

2,3,6-Trichlorophenol, trimethylsilyl ether

Other names:	2,3,6-Trichlorophenol, tms derivative
Inchi:	InChI=1S/C9H11Cl3OSi/c1-14(2,3)13-9-7(11)5-4-6(10)8(9)12/h4-5H,1-3H3
InchiKey:	BFMVRFQFQXIYTB-UHFFFAOYSA-N
Formula:	C9H11Cl3OSi
SMILES:	C[Si](C)(C)Oc1c(Cl)ccc(Cl)c1Cl
Mol. weight [g/mol]:	269.63

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.53		Crippen Method
logp	4.861		Crippen Method
rinpol	1537.90		NIST Webbook
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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=U333409&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/40-925-0/2-3-6-Trichlorophenol-trimethylsilyl-ether.pdf>

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