

2,6-Dichlorophenol, trimethylsilyl ether

Other names:	Phenol, 2,6-dichloro, TMS 2,6-Dichlorophenol, tms derivative
Inchi:	InChI=1S/C9H12Cl2OSi/c1-13(2,3)12-9-7(10)5-4-6-8(9)11/h4-6H,1-3H3
InchiKey:	OCWVIRQSLAUUCY-UHFFFAOYSA-N
Formula:	C9H12Cl2OSi
SMILES:	C[Si](C)(C)Oc1c(Cl)cccc1Cl
Mol. weight [g/mol]:	235.18

Physical Properties

Property code	Value	Unit	Source
log10ws	-1.85		Crippen Method
logp	4.207		Crippen Method
rinpol	1359.40		NIST Webbook
rinpol	1366.00		NIST Webbook
rinpol	1326.00		NIST Webbook
rinpol	1359.40		NIST Webbook
rinpol	1366.00		NIST Webbook
rinpol	1326.00		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=U333358&Units=SI

Legend

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

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