

1,2-Dichloro-3-trimethylsilyloxybenzene

Other names:	2,3-Dichlorophenol, trimethylsilyl ether Phenol, 2,3-dichloro, TMS 2,3-Dichlorophenol, tms derivative
Inchi:	InChI=1S/C9H12Cl2OSi/c1-13(2,3)12-8-6-4-5-7(10)9(8)11/h4-6H,1-3H3
InchiKey:	QAAZYQWMZYHYLZ-UHFFFAOYSA-N
Formula:	C9H12Cl2OSi
SMILES:	C[Si](C)(C)Oc1cccc(Cl)c1Cl
Mol. weight [g/mol]:	235.18
CAS:	67947-14-2

Physical Properties

Property code	Value	Unit	Source
log10ws	-1.85		Crippen Method
logp	4.207		Crippen Method
rinpol	1405.00		NIST Webbook
rinpol	1371.00		NIST Webbook
rinpol	1399.00		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=C67947142&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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