

3-Chlorophenol, trimethylsilyl ether

Other names:	Phenol, 3-chloro, TMS 3-Chlorophenol, tms derivative
Inchi:	InChI=1S/C9H13ClOSi/c1-12(2,3)11-9-6-4-5-8(10)7-9/h4-7H,1-3H3
InchiKey:	BFUAFRGEFKDQJD-UHFFFAOYSA-N
Formula:	C9H13ClOSi
SMILES:	C[Si](C)(C)Oc1cccc(Cl)c1
Mol. weight [g/mol]:	200.74

Physical Properties

Property code	Value	Unit	Source
log10ws	-1.16		Crippen Method
logp	3.554		Crippen Method
rinpol	1205.00		NIST Webbook
rinpol	1226.20		NIST Webbook

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U325592&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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/58-576-9/3-Chlorophenol-trimethylsilyl-ether.pdf>

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