

2,3,4,6-Tetrachlorophenol, trimethylsilyl ether

Other names:	Phenol, 2,3,4,6-tetrachloro, TMS 2,3,4,6-Tetrachlorophenol, tms derivative
Inchi:	InChI=1S/C9H10Cl4OSi/c1-15(2,3)14-9-6(11)4-5(10)7(12)8(9)13/h4H,1-3H3
InchiKey:	UJHOMCKIMOTJHO-UHFFFAOYSA-N
Formula:	C9H10Cl4OSi
SMILES:	C[Si](C)(C)Oc1c(Cl)cc(Cl)c(Cl)c1Cl
Mol. weight [g/mol]:	304.07

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.22		Crippen Method
logp	5.514		Crippen Method
rinpol	1656.00		NIST Webbook
rinpol	1697.60		NIST Webbook

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U333389&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/53-818-5/2-3-4-6-Tetrachlorophenol-trimethylsilyl-ether.pdf>

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