

2,4,6-Trichlorophenol, trimethylsilyl ether

Other names:	2,4,6-Trichlorophenol, trimethylsilyl ether
Inchi:	InChI=1S/C9H11Cl3OSi/c1-14(2,3)13-9-7(11)4-6(10)5-8(9)12/h4-5H,1-3H3
InchiKey:	RIYJZVOGDQXZPS-UHFFFAOYSA-N
Formula:	C9H11Cl3OSi
SMILES:	C[Si](C)(C)Oc1c(Cl)cc(Cl)cc1Cl
Mol. weight [g/mol]:	269.63

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.42		Cheméo Relay (1.0)
logp	4.861		Crippen Method
rinpol	1466.00		NIST Webbook
rinpol	1498.40		NIST Webbook
rinpol	1498.40		NIST Webbook
rinpol	1466.00		NIST Webbook
tf	335.09	K	Cheméo Relay (1.0)

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U333453&Units=SI

Legend

log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
rinpol:	Non-polar retention indices
tf:	Normal melting (fusion) point

Latest version available from:

<https://www.chemeo.com/cid/67-783-9/2-4-6-Trichlorophenol-trimethylsilyl-ether.pdf>

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