

Phenol, 2,4,6-trichloro, TMS

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	-2.53		Crippen Method
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

Sources

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=U333453&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci990307l>
Crippen Method: https://www.cheméo.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.cheméo.com/cid/67-783-9/Phenol-2-4-6-trichloro-TMS.pdf>

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