

Trimethyl(2,4,5-trichlorophenoxy)silane

Other names: Benzene, 1,2,4-trichloro-5-[(trimethylsilyl)oxy]-
Phenol, 2,4,5-trichloro, TMS

Inchi: InChI=1S/C9H11Cl3OSi/c1-14(2,3)13-9-5-7(11)6(10)4-8(9)12/h4-5H,1-3H3

InchiKey: FBOQWPLKFCNACJ-UHFFFAOYSA-N

Formula: C9H11Cl3OSi

SMILES: C[Si](C)(C)Oc1cc(Cl)c(Cl)cc1Cl

Mol. weight [g/mol]: 269.63

CAS: 1014-29-5

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.53		Crippen Method
logp	4.861		Crippen Method
rinpol	1495.00		NIST Webbook
rinpol	1521.10		NIST Webbook
rinpol	1495.00		NIST Webbook
rinpol	1521.10		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=C1014295&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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