Phenol, 2,4-dichloro, TMS

Other names: 2,4-Dichlorophenol, trimethylsilyl ether
Inchi: InChI=1S/C9H12Cl2OSi/c1-13(2,3)12-9-5-4-7(10)6-8(9)11/h4-6H,1-3H3
InchiKey: VHDCHSYJMDMWMW-UHFFFAOYSA-N
Formula: C9H12Cl2OSi
SMILES: C[Si](C)(C)Oc1ccc(Cl)cc1Cl
Mol. weight [g/mol]: 235.18

Physical Properties

Property code	Value	Unit	Source
log10ws	-1.85		Crippen Method
logp	4.207		Crippen Method
rinpol	1377.00		NIST Webbook
rinpol	1345.00		NIST Webbook
rinpol	1371.60		NIST Webbook
rinpol	1371.60		NIST Webbook
rinpol	1345.00		NIST Webbook
rinpol	1377.00		NIST Webbook

Sources

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=U333366&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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