

# Pentachlorophenol, tert-butyldimethylsilyl ether

<b>Other names:</b>	Pentachlorophenol, TBDMS Pentachlorophenol, tbdms derivative
<b>Inchi:</b>	InChI=1S/C12H15Cl5OSi/c1-12(2,3)19(4,5)18-11-9(16)7(14)6(13)8(15)10(11)17/h1-5H3
<b>InchiKey:</b>	KDPVORPBWXdGN-UHFFFAOYSA-N
<b>Formula:</b>	C12H15Cl5OSi
<b>SMILES:</b>	CC(C)(C)[Si](C)(C)Oc1c(Cl)c(Cl)c(Cl)c(Cl)c1Cl
<b>Mol. weight [g/mol]:</b>	380.60

## Physical Properties

Property code	Value	Unit	Source
log10ws	-5.16		Crippen Method
logp	7.338		Crippen Method
rinpola	2192.70		NIST Webbook
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## Sources

<b>Crippen Method:</b>	<a href="https://www.chemeo.com/doc/models/crippen_log10ws">https://www.chemeo.com/doc/models/crippen_log10ws</a>
<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=U333392&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U333392&amp;Units=SI</a>
<b>Crippen Method:</b>	<a href="http://pubs.acs.org/doi/abs/10.1021/ci9903071">http://pubs.acs.org/doi/abs/10.1021/ci9903071</a>

## Legend

<b>log10ws:</b>	Log10 of Water solubility in mol/l
<b>logp:</b>	Octanol/Water partition coefficient
<b>rinpola:</b>	Non-polar retention indices

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