

# Clofoctol, tert-butyldimethylsilyl ether

<b>Other names:</b>	Clofoctol, tbdms derivative
<b>Inchi:</b>	InChI=1S/C27H40Cl2OSi/c1-25(2,3)18-27(7,8)21-12-14-24(30-31(9,10)26(4,5)6)20(16-2
<b>InchiKey:</b>	TWKXUBZYVZFJTK-UHFFFAOYSA-N
<b>Formula:</b>	C27H40Cl2OSi
<b>SMILES:</b>	CC(C)(C)CC(C)(C)c1ccc(O[Si](C)(C)C(C)(C)C)c(Cc2ccc(Cl)cc2Cl)c1
<b>Mol. weight [g/mol]:</b>	479.60

## Physical Properties

Property code	Value	Unit	Source
log10ws	-7.95		Crippen Method
logp	9.682		Crippen Method
rinpol	2740.90		NIST Webbook

## Sources

<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>
<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=U333471&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U333471&amp;Units=SI</a>

## Legend

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

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