

# Cholecalciferol, trimethylsilyl ether

<b>Other names:</b>	(3S,5Z,7E)-3-Methoxy-9,10-secocholesta-5,7,10-triene Cholecalciferol, tms derivative
<b>Inchi:</b>	InChI=1S/C30H52OSi/c1-22(2)11-9-12-24(4)28-18-19-29-25(13-10-20-30(28,29)5)15-16
<b>InchiKey:</b>	GWVMYANKBNXDQN-RYQLWAFASA-N
<b>Formula:</b>	C30H52OSi
<b>SMILES:</b>	C=C1CCC(O[Si](C)(C)C)CC1=CC=C1CCCC2(C)C1CCC2C(C)CCCC(C)C
<b>Mol. weight [g/mol]:</b>	456.82

## Physical Properties

Property code	Value	Unit	Source
log10ws	-7.67		Crippen Method
logp	9.478		Crippen Method
rinpol	3104.10		NIST Webbook

## Sources

<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=U332996&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U332996&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>
<b>Crippen Method:</b>	<a href="https://www.chemeo.com/doc/models/crippen_log10ws">https://www.chemeo.com/doc/models/crippen_log10ws</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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<https://www.chemeo.com/cid/46-715-7/Cholecalciferol-trimethylsilyl-ether.pdf>

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