

# 7«alpha»,26-dihydroxy-4-cholesten-3-one, TMS

<b>Inchi:</b>	InChI=1S/C36H68O3Si3/c1-26(25-37-40(5,6)7)15-14-16-27(2)30-17-18-31-34-32(20-22-
<b>InchiKey:</b>	LVBALRWAXSVALG-BLLMLTCESA-N
<b>Formula:</b>	C36H68O3Si3
<b>SMILES:</b>	CC(CCCC(C)C1CCC2C3C(O[Si](C)(C)C)CC4=CC(O[Si](C)(C)C)=CCC4(C)C3CCC12C)
<b>Mol. weight [g/mol]:</b>	633.18

## Physical Properties

Property code	Value	Unit	Source
log10ws	-4.27		Crippen Method
logp	11.035		Crippen Method
rinpol	3555.00		NIST Webbook
rinpol	3555.00		NIST Webbook

## Sources

<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=R493993&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=R493993&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.cheméo.com/doc/models/crippen_log10ws">https://www.cheméo.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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