

# 3«beta»-Hydroxy-7-oxo-5-cholestenoate, MeTMS

<b>Inchi:</b>	InChI=1S/C34H60O4Si2/c1-23(13-12-14-24(2)32(35)36-5)27-15-16-28-31-29(18-20-34(2
<b>InchiKey:</b>	UVNOUYZSBSWLFS-DTAJUKNISA-N
<b>Formula:</b>	C34H60O4Si2
<b>SMILES:</b>	COC(=O)C(C)CCCC(C)C1CCC2C3=C(O[Si](C)(C)C)C=C4CC(O[Si](C)(C)C)CCC4(C)C3
<b>Mol. weight [g/mol]:</b>	589.01

## Physical Properties

Property code	Value	Unit	Source
log10ws	-5.40		Crippen Method
logp	9.500		Crippen Method
rinpol	3680.00		NIST Webbook
rinpol	3680.00		NIST Webbook

## Sources

<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=R264443&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=R264443&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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