

# Methyl (25RS)-3«beta»-hydroxy-5-cholesten-26-oate, trimethylsilyl ether

Other names: 3«beta»-hydroxy-5-cholestenoate, MeTMS  
Methyl 3-hydroxycholest-5-en-26-oate, tms derivative

<b>Inchi:</b>	InChI=1S/C31H54O3Si/c1-21(10-9-11-22(2)29(32)33-5)26-14-15-27-25-13-12-23-20-24(
<b>InchiKey:</b>	DNXGNXYNSBCWGX-QBUYVTDMSA-N
<b>Formula:</b>	C31H54O3Si
<b>SMILES:</b>	COC(=O)C(C)CCCC(C)C1CCC2C3CC=C4CC(O[Si](C)(C)C)CCC4(C)C3CCC12C
<b>Mol. weight [g/mol]:</b>	502.84

## Physical Properties

Property code	Value	Unit	Source
log10ws	-6.41		Crippen Method
logp	8.401		Crippen Method
rinpola	3425.00		NIST Webbook
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## 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.cheméo.com/doc/models/crippen_log10ws">https://www.cheméo.com/doc/models/crippen_log10ws</a>
<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=U99777&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U99777&amp;Units=SI</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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