

# Cholanic acid, 3«beta»,7«beta»-dihydroxy, Me-DMES

<b>Inchi:</b>	InChI=1S/C33H62O4Si2/c1-11-38(7,8)36-25-17-19-32(4)24(21-25)22-29(37-39(9,10)12-
<b>InchiKey:</b>	HBVFSTTUJXVCFB-JAIZZOPSSA-N
<b>Formula:</b>	C33H62O4Si2
<b>SMILES:</b>	CC[Si](C)(C)OC1CCC2(C)C(C1)CC(O[Si](C)(C)CC)C1C2CCC2(C)C(C(C)CCC(=O)OC)C
<b>Mol. weight [g/mol]:</b>	579.01

## Physical Properties

Property code	Value	Unit	Source
log10ws	-4.64		Crippen Method
logp	9.065		Crippen Method
rinpol	3487.00		NIST Webbook
ripol	3884.00		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=R534222&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=R534222&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
<b>ripol:</b>	Polar retention indices

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