

# Cholanic acid, 3«alpha»,12«beta»-dihydroxy, Me-DMES

Inchi:	InChI=1S/C33H62O4Si2/c1-11-38(7,8)36-25-19-20-32(4)24(21-25)14-15-26-28-17-16-27
InchiKey:	LNGHMHTXKIMWLA-WUJMRCNGSA-N
Formula:	C33H62O4Si2
SMILES:	CC[Si](C)(C)OC1CCC2(C)C(CCC3C2CC(O[Si](C)(C)CC)C2(C)C(C(C)CCC(=O)OC)CCO
Mol. weight [g/mol]:	579.01

## Physical Properties

Property code	Value	Unit	Source
log10ws	-4.64		Crippen Method
logp	9.065		Crippen Method
rinpol	3386.00		NIST Webbook
ripol	3767.00		NIST Webbook
ripol	3767.00		NIST Webbook

## Sources

Crippen Method:	<a href="http://pubs.acs.org/doi/abs/10.1021/ci9903071">http://pubs.acs.org/doi/abs/10.1021/ci9903071</a>
Crippen Method:	<a href="https://www.cheméo.com/doc/models/crippen_log10ws">https://www.cheméo.com/doc/models/crippen_log10ws</a>
NIST Webbook:	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=R533883&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=R533883&amp;Units=SI</a>

## Legend

log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
rinpol:	Non-polar retention indices
ripol:	Polar retention indices

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