

# Cholanic acid, 3«beta»,7«alpha»,12«alpha»-trihydroxy, Me-TMS

Other names:	3«beta»,7«alpha»,12«alpha»-Trihydroxy-5«beta»-cholanic acid, methyl ester, TMS
Inchi:	InChI=1S/C34H66O5Si3/c1-23(14-17-31(35)36-4)26-15-16-27-32-28(22-30(34(26,27)3)33-29)32
InchiKey:	DQKFOBXAKZGIPX-PKXBEQHYS A-N
Formula:	C34H66O5Si3
SMILES:	COC(=O)CCC(C)C1CCC2C3C(O[Si](C)(C)C)CC4CC(O[Si](C)(C)C)CCC4(C)C3CC(O[Si](C)(C)C)C
Mol. weight [g/mol]:	639.14

## Physical Properties

Property code	Value	Unit	Source
log10ws	-2.31		Crippen Method
logp	9.115		Crippen Method
rinp	3198.00		NIST Webbook
rinp	3198.00		NIST Webbook
rip	3378.00		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=R534133&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=R534133&amp;Units=SI</a>

## Legend

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

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