

Cholanoic acid, 1,3,4-trihydroxy, methyl ester, TMS

Inchi:	InChI=1S/C34H66O5Si3/c1-23(14-19-31(35)36-4)25-17-18-26-24-15-16-28-32(39-42(11,12)13)33-34
InchiKey:	KTNXXVNSEQTOOY-KTWMTLLBSA-N
Formula:	C34H66O5Si3
SMILES:	COC(=O)CCC(C)C1CCC2C3CCC4C(O[Si](C)(C)C)C(O[Si](C)(C)C)CC(O[Si](C)(C)C)C4
Mol. weight [g/mol]:	639.14

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.31		Crippen Method
logp	9.115		Crippen Method
rinpol	3464.00		NIST Webbook
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Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R394386&Units=SI

Legend

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

Latest version available from:

<https://www.chemeo.com/cid/43-392-9/Cholanoic-acid-1-3-4-trihydroxy-methyl-ester-TMS.pdf>

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