

3-«alpha»,7-«alpha»-Dihydroxy-5-«beta»-cholesta acid, methyl ester, TMS

InChI: InChI=1S/C34H64O4Si2/c1-23(13-12-14-24(2)32(35)36-5)27-15-16-28-31-29(18-20-34(2)33)/2-4,25-26,27,28,29,30,31,32,33,34,35,36,37,38,39,40,41,42,43,44,45,46,47,48,49,50,51,52,53,54,55,56,57,58,59,60,61,62,63,64,65,66,67,68,69,70,71,72,73,74,75,76,77,78,79,80,81,82,83,84,85,86,87,88,89,90,91,92,93,94,95,96,97,98,99,100/s1-2,3-4,5-6,7-8,9-10,11-12,13-14,15-16,17-18,19-20,21-22,23-24,25-26,27-28,29-30,31-32,33-34,35-36,37-38,39-40,41-42,43-44,45-46,47-48,49-50,51-52,53-54,55-56,57-58,59-60,61-62,63-64,65-66,67-68,69-70,71-72,73-74,75-76,77-78,79-80,81-82,83-84,85-86,87-88,89-90,91-92,93-94,95-96,97-98,99-100

InChIKey: TVTGQRYURIZRAM-VAKMOCNYSAN

Formula: C₃₄H₆₄O₄Si₂

SMILES: COC(=O)C(C)CCCC(C)C1CCC2C3C(O[Si](C)(C)C)CC4CC(O[Si](C)(C)C)CCC4(C)C3C

Mol. weight [g/mol]: 593.04

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.82		Crippen Method
logp	9.311		Crippen Method
rinpol	3427.00		NIST Webbook

Sources

Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>

Crippen Method: https://www.cheméo.com/doc/models/crippen_log10ws

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=R390042&Units=SI>

Legend

log10ws: Log10 of Water solubility in mol/l

logp: Octanol/Water partition coefficient

rinpol: Non-polar retention indices

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