

Cholanoic acid, 3,6-dihydroxy, methyl ester, TMS

Inchi: InChI=1S/C31H58O4Si2/c1-21(11-14-29(32)33-4)24-12-13-25-23-20-28(35-37(8,9)10)27
InchiKey: FYDBJLGZNQLQEL-DVYZTLNDSA-N
Formula: C31H58O4Si2
SMILES: COC(=O)CCC(C)C1CCC2C3CC(O[Si](C)(C)C)C4CC(O[Si](C)(C)C)CCC4(C)C3CCC12C
Mol. weight [g/mol]: 550.96

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.81		Crippen Method
logp	8.285		Crippen Method
rinpol	3248.00		NIST Webbook
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Sources

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=R394306&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci990307l>

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/34-186-8/Cholanoic-acid-3-6-dihydroxy-methyl-ester-TMS.pdf>

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