

7«alpha»-Hydroxy-3-oxo-4-cholestenoate, MeTMS

Inchi: InChI=1S/C34H60O4Si2/c1-23(13-12-14-24(2)32(35)36-5)27-15-16-28-31-29(18-20-34(2)
InchiKey: UDKJVEQQSDKFME-LISNPCNLSA-N
Formula: C34H60O4Si2
SMILES: COC(=O)C(C)CCCC(C)C1CCC2C3C(O[Si](C)(C)C)CC4=CC(O[Si](C)(C)C)=CCC4(C)C3
Mol. weight [g/mol]: 589.01

Physical Properties

Property code	Value	Unit	Source
log10ws	-5.15		Crippen Method
logp	9.356		Crippen Method
rinpol	3515.00		NIST Webbook
rinpol	3515.00		NIST Webbook

Sources

Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci990307l>
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=R264498&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/40-696-5/7-alpha-Hydroxy-3-oxo-4-cholestenoate-MeTMS.pdf>

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