

7«alpha»,12«alpha»-dihydroxy, 3-oxy-5«beta»-cholanoate, methyl ester-trimethylsilyl ether

Inchi: COC(=O)CCC(C)C1CCC2C3C(O[Si](C)(C)C)CC4C=C(O[Si](C)(C)C)CCC4(C)C3CC(O[Si](C)(C)C)C1
InchiKey: NNW FYLODZ QPGHC-NSGCQEPQSA-N

Formula: C₃₄H₆₄O₅Si₃

SMILES: COC(=O)CCC(C)C1CCC2C3C(O[Si](C)(C)C)CC4C=C(O[Si](C)(C)C)CCC4(C)C3CC(O[Si](C)(C)C)C1

Mol. weight [g/mol]: 637.13

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.55		Crippen Method
logp	9.240		Crippen Method
rinpol	3320.00		NIST Webbook
rinpol	3320.00		NIST Webbook

Sources

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=R493973&Units=SI>

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

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

Legend

log10ws: Log10 of Water solubility in mol/l

logp: Octanol/Water partition coefficient

rinpol: Non-polar retention indices

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