

3«beta»,4«beta»,7«alpha»,12«alpha»-tetrahydroxy-5-beta-cholanoic acid, methyl ester-trimethylsilyl-ether derivative

Inchi: nChI=1S/C37H74O6Si4/c1-25(17-20-33(38)39-4)26-18-19-27-34-28(24-32(37(26,27)3)4

InchiKey: QKSYQONADMPPHH-ULZXMGCHSA-N

Formula: C37H74O6Si4

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

Mol. weight [g/mol]: 727.32

Physical Properties

Property code	Value	Unit	Source
log10ws	-0.82		Crippen Method
logp	9.945		Crippen Method
rinpol	3334.00		NIST Webbook
rinpol	3334.00		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=R493171&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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