

3«beta»,4«beta»-dihydroxy-5«beta»-cholanoic acid, methyl ester-trimethylsilyl-ether derivative

InChI: InChI=1S/C31H58O4Si2/c1-21(11-16-28(32)33-4)23-14-15-24-22-12-13-26-29(35-37(8,9
InChIKey: OSOBSDUNXQOELS-ZJFWGZMQSA-N
Formula: C31H58O4Si2
SMILES: COC(=O)CCC(C)C1CCC2C3CCC4C(O[Si](C)(C)C)C(O[Si](C)(C)C)CCC4(C)C3CCC12O
Mol. weight [g/mol]: 550.96

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.81		Crippen Method
logp	8.285		Crippen Method
rinpol	3281.00		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=R493191&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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