

3-oxy-7«alpha»,12«alpha»-dihydroxy-4-cholesten methyl ester-trimethylsilyl ether

InChI: InChI=1S/C37H68O5Si3/c1-15(16-15-17-26(2)35(38)39-5)29-18-19-30-34-31(24-33(37(2)36-35)38)39-5/si3-1-2-3
InChIKey: RNIFHRKAQFHUNGQ-MJOMMUNASA-N

Formula: C37H68O5Si3
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]: 677.19

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.66		Crippen Method
logp	10.186		Crippen Method
rinpol	3595.00		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=R493859&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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