

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

Inchi: CC(C)(C)C(=O)O[C@H]1CC[C@@H]2[C@H]3CC[C@H]4[C@@H]1CC[C@@H](C(=O)OC)[C@H]5[C@@H](C)[C@H](C)[C@@H](C)[C@H]5C[C@H](C)[C@H]4O[C@@H]3C[C@H]2O
InchiKey: SNBYLKJWRXVZKO-ZECCVNMMSA-N

Formula: C34H62O5Si3
SMILES: COC(=O)CCC(C)C1CCC2C3C(O[Si](C)(C)C)CC4=CC(O[Si](C)(C)C)=CCC4(C)C3CC(O[Si](C)(C)C)C2C1
Mol. weight [g/mol]: 635.11

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.65		Crippen Method
logp	9.160		Crippen Method
rinpol	3360.00		NIST Webbook

Sources

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=R493968&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci990307l>

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/55-613-0/7-alpha-12-alpha-dihydroxy-3-oxy-4-cholenoate-methyl-ester-trimethylsilyl-eth>

Generated by Cheméo on 2025-12-18 15:59:53.592372931 +0000 UTC m=+5821791.122413591.

Cheméo (<https://www.chemeo.com>) is the biggest free database of chemical and physical data for the process industry.