

3«beta»,7«alpha»,12«alpha»-Trihydroxy-4-cholenic acid, methyl ester, TMS

Inchi: COC(=O)CCCC(C)C1CCC2C3C(O[Si](C)(C)C)CC4=CC(O[Si](C)(C)C)CCC4(C)C3CC(O[Si](C)(C)C)CC2(C)C1
InchiKey: QVMBQRVPUGQSMQ-YFJAVQHYSA-N

Formula: C34H64O5Si3
SMILES: COC(=O)CCCC(C)C1CCC2C3C(O[Si](C)(C)C)CC4=CC(O[Si](C)(C)C)CCC4(C)C3CC(O[Si](C)(C)C)CC2(C)C1
Mol. weight [g/mol]: 637.13

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.41		Crippen Method
logp	9.035		Crippen Method
rinpol	3214.00		NIST Webbook

Sources

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=R535136&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci990307l>
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

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/47-240-3/3-beta-7-alpha-12-alpha-Trihydroxy-4-cholenic-acid-methyl-ester-TMS.pdf>

Generated by Cheméo on 2025-12-05 16:47:21.092622531 +0000 UTC m=+4701438.622663185.

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