

3«alpha»,6«alpha»,7«beta»,12«alpha»-Tetrahydroxy-5«beta»-cholanoic acid, methyl ester-trimethylsilyl ether

Other names:

3«alpha»,6«alpha»,7«beta»,12«alpha»-tetrahydroxy-5«beta»-cholanoic acid,

Inchi:

InChI=1S/C37H74O6Si4/c1-25(17-20-32(39)39-4)27-18-19-28-33-29(24-31(37(27,28)3)4

InchiKey: CAHBNWKLQVHQBQ-FNPTXHGCSA-N

Formula: C37H74O6Si4

SMILES: COC(=O)CCC(C)C1CCC2C3C(O[Si](C)(C)C)C(O[Si](C)(C)C)C4CC(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	3447.00		NIST Webbook
rinpol	3447.00		NIST Webbook
rinpol	3447.00		NIST Webbook

Sources

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=R271362&Units=SI>

Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>

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/10-068-5/3-alpha-6-alpha-7-beta-12-alpha-Tetrahydroxy-5-beta-cholanoic-acid-methyl->

Generated by Cheméo on 2024-04-23 15:59:25.165689538 +0000 UTC m=+16177214.086266848.

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