

3«alpha»,4«beta», 7«alpha»-trihydroxy-5«beta»-cholanoic acid, methyl ester-trimethylsilyl-ether derivative

InChI: InChI=1S/C34H66O5Si3/c1-13(14-17-20(35)36-4)24-15-16-25-31-26(18-20-33(24,25)2)3
InChIKey: XLJGJNLLTFGMTE-OLPRANIPSA-N
Formula: C34H66O5Si3
SMILES: COC(=O)CCC(C)C1CCC2C3C(O[Si](C)(C)C)CC4C(O[Si](C)(C)C)C(O[Si](C)(C)C)CCC4
Mol. weight [g/mol]: 639.14

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.31		Crippen Method
logp	9.115		Crippen Method
rinpol	3384.00		NIST Webbook
rinpol	3384.00		NIST Webbook
rinpol	3384.00		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=R493131&Units=SI>

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.cheméo.com/cid/31-293-2/3-alpha-4-beta-7-alpha-trihydroxy-5-beta-cholanoic-acid-methyl-ester-trimethylsilyl-ether-derivative>

Generated by Cheméo on 2024-04-23 20:55:11.800834511 +0000 UTC m=+16194960.721411827.

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