

3-«beta»,7-«alpha»-Dihydroxy-4-cholenoic acid, methyl ester, TMS

Inchi: InChI=1S/C31H56O4Si2/c1-21(11-14-28(32)33-4)24-12-13-25-29-26(16-18-31(24,25)3)3
InchiKey: KHYMDYRSKURYAZ-QMTMEVIGSA-N
Formula: C31H56O4Si2
SMILES: COC(=O)CCC(C)C1CCC2C3C(O[Si](C)(C)C)CC4=CC(O[Si](C)(C)C)CCC4(C)C3CCC12
Mol. weight [g/mol]: 548.94

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.90		Crippen Method
logp	8.205		Crippen Method
rinpol	3188.00		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=R390082&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/44-331-5/3-beta-7-alpha-Dihydroxy-4-cholenoic-acid-methyl-ester-TMS.pdf>

Generated by Cheméo on 2024-04-18 15:31:16.884892974 +0000 UTC m=+15743525.805470289.

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