

allo-Cholanic acid, 7«alpha»,12«beta»-dihydroxy, Me-TMS

Other names: 7«alpha»,12«beta»-Dihydroxy-5«alpha»-cholanic acid, methyl ester, TMS
Inchi: InChI=1S/C31H58O4Si2/c1-21(14-17-28(32)33-4)23-15-16-24-29-25(20-27(31(23,24)3)3)3
InchiKey: WLOQXQFDQGTWNC-HZNNNNMJSA-N
Formula: C31H58O4Si2
SMILES: COC(=O)CCC(C)C1CCC2C3C(O[Si](C)(C)C)CC4CCCCC4(C)C3CC(O[Si](C)(C)C)C12O
Mol. weight [g/mol]: 550.96

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.81		Crippen Method
logp	8.285		Crippen Method
rinpole	3043.00		NIST Webbook
rinpole	3043.00		NIST Webbook
rinpole	3043.00		NIST Webbook
ripole	3324.00		NIST Webbook
ripole	3324.00		NIST Webbook

Sources

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=R533734&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

Legend

log10ws: Log10 of Water solubility in mol/l
logp: Octanol/Water partition coefficient
rinpole: Non-polar retention indices
ripole: Polar retention indices

Latest version available from:

<https://www.cheméo.com/cid/70-539-6/allo-Cholanic-acid-7-alpha-12-beta-dihydroxy-Me-TMS.pdf>

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