

allo-Cholanic acid, 3«alpha»,7«alpha»,12«beta»-trihydroxy, Me-TMS

Other names: 3«alpha»,7«alpha»,12«beta»-Trihydroxy-5«alpha»-cholanic acid, methyl ester,
Inchi: TMS
InChI=1S/C34H66O5Si3/c1-23(14-17-31(35)36-4)26-15-16-27-32-28(22-30(34(26,27)3)3
InchiKey: DQKFOBAXKZGIPX-YHPCAMAXSA-N
Formula: C34H66O5Si3
SMILES: COC(=O)CCC(C)C1CCC2C3C(O[Si](C)(C)C)CC4CC(O[Si](C)(C)C)CCC4(C)C3CC(O[Si](C)(C)C)C
Mol. weight [g/mol]: 639.14

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.31		Crippen Method
logp	9.115		Crippen Method
rinpol	3211.00		NIST Webbook
rinpol	3211.00		NIST Webbook
ripol	3416.00		NIST Webbook
ripol	3416.00		NIST Webbook

Sources

Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci990307l>
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=R533412&Units=SI>

Legend

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

Latest version available from:

<https://www.chemeo.com/cid/30-948-6/allo-Cholanic-acid-3-alpha-7-alpha-12-beta-trihydroxy-Me-TMS.pdf>

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