

5-«beta»-Cholanoic acid, 3-«alpha»,4-«beta»,12-«alpha»-trihydroxy, methyl ester, TMS

Other names: 3-«alpha»,4-«beta»,12-«alpha»-Trihydroxy-5-«beta»-cholanoic acid, MeTMS
Inchi: InChI=1S/C34H66O5Si3/c1-23(14-19-31(35)36-4)25-17-18-26-24-15-16-27-32(39-42(11,12,13)40-41)33-34/s1-3,1-3,1-3

InchiKey: HUODHVYTPOSCBY-HHBLUBSASA-N

Formula: C34H66O5Si3

SMILES: COC(=O)CCC(C)C1CCC2C3CCC4C(O[Si](C)(C)C)C(O[Si](C)(C)C)CCC4(C)C3CC(O[Si](C)(C)C)C1

Mol. weight [g/mol]: 639.14

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.31		Crippen Method
logp	9.115		Crippen Method
rinpol	3390.00		NIST Webbook
rinpol	3390.00		NIST Webbook
rinpol	3390.00		NIST Webbook

Sources

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

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=R393150&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/47-312-3/5-beta-Cholanoic-acid-3-alpha-4-beta-12-alpha-trihydroxy-methyl-ester-TMS>

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