

5-«alpha»-Cholanoic acid, 3-«alpha»-12-«beta»-dihydroxy, methyl ester,

TMS

InchiKey:

Formula:

SMILES:

Mol. weight [g/mol]:

InChI=1S/C31H58O4Si2/c1-21(11-16-29(32)33-4)25-14-15-26-24-13-12-22-19-23(34-36)

RDYDEBUPRMEHW-QWVOEWKVSA-N

C31H58O4Si2

COC(=O)CCC(C)C1CCC2C3CCC4CC(O[Si](C)(C)C)CCC4(C)C3CC(O[Si](C)(C)C)C12C

550.96

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.81		Crippen Method
logp	8.285		Crippen Method
rinpol	3145.00		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=R393818&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/15-718-8/5-alpha-Cholanoic-acid-3-alpha-12-beta-dihydroxy-methyl-ester-TMS.pdf>

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