Cholan-24-oic acid, 3-oxo-7,12-bis[(trimethylsilyl)oxy]-, methyl ester, (5«beta»,7«alpha»,12«alpha»)-

Othernames: 5«beta»-Cholan-24-oic acid, 3-oxo-7«alpha»,12«alpha»-bis(trimethylsiloxy)-, methyl ester, Methyl 7-«alpha»,12-«alpha»-dihydroxy-3-keto-5-«beta»-cholanoate, TMS

Inchi: InChI=1S/C31H56O5Si2/c1-20(11-14-28(33)34-4)23-12-13-24-29-25(19-27(31(23,24)3)3

InchiKey: LYEQLVCCHOHXEJ-QUUIAQLXSA-N

Formula: C31H56O5Si2

SMILES: COC(=O)CCC(C)C1CCC2C3C(O[Si](C)(C)C)CC4CC(=O)CCC4(C)C3CC(O[Si](C)(C)C)C

Mol. weight [g/mol]: 564.94

CAS: 15093-99-9

Physical Properties

Property code	Value	Unit	Source
logp	7.464		Crippen Method
rinpol	3300.00		NIST Webbook
rinpol	3300.00		NIST Webbook

Sources

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

Cheméo Relay (1.0):

Cheméo Relay (1.0, beta):

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C15093999&Units=SI

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

logp: Octanol/Water partition coefficient

rinpol: Non-polar retention indices

Latest version available from:
https://www.chemeo.com/cid/117-696-0/Cholan-24-oic-acid-3-oxo-7-12-bis-trimethylsilyl-oxy-methyl-ester-5-beta-7-al
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