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

Other names: 5«beta»-Cholan-24-oic acid, 3«alpha»,7«alpha»,12«alpha»-tris(trimethylsiloxy)-, methyl ester

Methyl 3,7,12-tris[(trimethylsilyl)oxy]cholan-24-oate, (3«alpha»,5«beta»,7«alpha»,12«alpha»)-

3«alpha»,7«alpha»,12«alpha»-Trihydroxy-5«beta»-cholanoic acid, methyl ester-trimethylsilyl ether

3-«alpha»,7-«alpha»,12-«alpha»-Trihydroxy-5-«beta»-cholanoic acid, MeTMS

5-«beta»-Cholanoic acid, 3-«alpha»-7-«alpha»12-«alpha»-trihydroxy, methyl ester, TMS

Cholic acid, methyl ester, TMS

Cholic acid, trimethylsilyl ether-methyl ester

3«alpha»,7«alpha»,12«alpha»-trihydroxy-5«beta»-cholestanoic acid, trimethylsilyl ether-methyl ester

Methyl cholate, 3tms derivative

Inchi: 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: DQKFOBXAKZGIPX-UHFFFAOYSA-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]

Mol. weight [g/mol]: 639.14

CAS: 6818-43-5

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.31		Crippen Method
logp	9.115		Crippen Method
rinpol	3261.00		NIST Webbook
rinpol	3212.00		NIST Webbook
rinpol	3212.00		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=C6818435&Units=SI

Legend

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