Chenodeoxycholic acid, trimethylsilyl ether-methyl ester

Other names: Chenodeoxycholic acid, methyl ester, TMS
Methyl 3-«alpha»,7-«alpha»-dihydroxy-5-«beta»-cholanoate, TMS
3-«alpha»,7-«alpha»-Dihydroxy-5-«beta»-cholanoic acid, MeTMS
3«alpha»,7«alpha»-Dihydroxy-5«beta»-cholanoic acid, methyl ester-trimethylsilyl ether
5-«beta»-Cholanoic acid, 3-«alpha»-7-«alpha»-diydroxy, methyl ester, TMS

Inchi: InChI=1S/C31H58O4Si2/c1-21(11-14-28(32)33-4)24-12-13-25-29-26(16-18-31(24,25)3)3

InchiKey: FUVKOFYYHKWFJK-CPENPXANSA-N

Formula: C31H58O4Si2

SMILES: COC(=O)CCC(C)C1CCC2C3C(O[Si](C)(C)C)CC4CC(O[Si](C)(C)C)CCC4(C)C3CCC12C

Mol. weight [g/mol]: 550.96

CAS: 52759-80-5

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.81		Crippen Method
logp	8.285		Crippen Method
rinpol	3195.00		NIST Webbook
rinpol	3216.00		NIST Webbook
rinpol	3244.00		NIST Webbook
rinpol	3198.00		NIST Webbook
rinpol	3225.00		NIST Webbook
rinpol	3199.00		NIST Webbook
rinpol	3199.00		NIST Webbook
rinpol	3225.00		NIST Webbook
rinpol	3225.00		NIST Webbook
ripol	3624.00		NIST Webbook
ripol	3624.00		NIST Webbook

Sources

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

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C52759805&Units=SI

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

Legend

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