3«beta»,7«beta»-Dihydroxy-5«beta»-cholanoic acid, MeTMS

Other names: Ursodeoxycholic acid, trimethylsilyl ether-methyl ester
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-MLZFRZJBSA-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: 78964-21-3

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.81		Crippen Method
logp	8.285		Crippen Method
rinpol	3316.00		NIST Webbook
rinpol	3268.00		NIST Webbook
rinpol	3316.00		NIST Webbook
rinpol	3268.00		NIST Webbook
ripol	3687.00		NIST Webbook
ripol	3687.00		NIST Webbook

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C78964213&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

Legend

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