7-«beta»-Hydroxycholesterol, TMS

Other names: Cholesterol, 7«beta»-hydroxy, TMS
Inchi: InChI=1S/C33H64O2Si2/c1-23(2)13-12-14-24(3)27-15-16-28-31-29(18-20-33(27,28)5)32
InchiKey: SABSXFHUKZVEMF-ADOKZBEXSA-N
Formula: C33H64O2Si2
SMILES: CC(C)CCCC(C)C1CCC2C3C(O[Si](C)(C)C)CC4CC(O[Si](C)(C)C)CCC4(C)C3CCC12C
Mol. weight [g/mol]: 549.03

Physical Properties

Property code	Value	Unit	Source
log10ws	-5.54		Crippen Method
logp	10.158		Crippen Method
rinpol	3235.00		NIST Webbook
rinpol	3228.00		NIST Webbook
rinpol	3235.00		NIST Webbook

Sources

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R150082&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