22-Hydroxycholesterol, di-TMS

Inchi: InChI=1S/C33H62O2Si2/c1-23(2)12-17-31(35-37(9,10)11)24(3)28-15-16-29-27-14-13-25
InchiKey: YCJOXUPPUMVNFF-RQCBSPJQSA-N
Formula: C33H62O2Si2
SMILES: CC(C)CCC(O[Si](C)(C)C)C(C)C1CCC2C3CC=C4CC(O[Si](C)(C)C)CCC4(C)C3CCC12C
Mol. weight [g/mol]: 547.02

Physical Properties

Property code	Value	Unit	Source
log10ws	-5.64		Crippen Method
logp	10.078		Crippen Method
rinpol	3275.00		NIST Webbook

Sources

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R11684&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