4-Cholesten-7-«beta»-ol-3-one, TMS

Other names: 7-«beta»-Hydroxycholest-4-en-3-one, TMS
Inchi: InChI=1S/C33H60O2Si2/c1-23(2)13-12-14-24(3)27-15-16-28-31-29(18-20-33(27,28)5)32
InchiKey: FEHLHHZINBWGES-VQKHYFMMSA-N
Formula: C33H60O2Si2
SMILES: CC(C)CCCC(C)C1CCC2C3C(O[Si](C)(C)C)CC4=CC(O[Si](C)(C)C)=CCC4(C)C3CCC12
Mol. weight [g/mol]: 545.00

Physical Properties

Property code	Value	Unit	Source
log10ws	-5.87		Crippen Method
logp	10.203		Crippen Method
rinpol	3345.00		NIST Webbook
rinpol	3314.00		NIST Webbook
rinpol	3314.00		NIST Webbook

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R150077&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