2-Oxacholesterol, TMS

Inchi: InChI=1S/C29H54O2Si/c1-20(2)10-9-11-21(3)24-14-15-25-23-13-12-22-18-27(31-32(6,7)
InchiKey: IJELOPGGEBSQFW-PUHYIDFYSA-N
Formula: C29H54O2Si
SMILES: CC(C)CCCC(C)C1CCC2C3CCC4CC(O[Si](C)(C)C)OCC4(C)C3CCC12C
Mol. weight [g/mol]: 462.82

Physical Properties

Property code	Value	Unit	Source
log10ws	-6.20		Crippen Method
logp	8.522		Crippen Method
rinpol	3070.00		NIST Webbook
rinpol	3070.00		NIST Webbook

Sources

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R528737&Units=SI

Legend

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