5«alpha»-Cholestan-3«alpha»,6«beta»-diol, TMS

Inchi: InChI=1S/C33H64O2Si2/c1-23(2)13-12-14-24(3)27-15-16-28-26-22-31(35-37(9,10)11)30

InchiKey: UBHDPUUHTCWMLG-YXOPIZLTSA-N

Formula: C33H64O2Si2

SMILES: CC(C)CCCC(C)C1CCC2C3CC(O[Si](C)(C)C)C4CC(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	3143.00		NIST Webbook

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R529369&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