7«alpha»,25-Dihydroxycholesterol, TMS

Inchi: InChI=1S/C36H70O3Si3/c1-26(16-15-21-34(2,3)39-42(12,13)14)29-17-18-30-33-31(20-2
InchiKey: GPCULFSWTJUQIN-USYHRLOOSA-N
Formula: C36H70O3Si3
SMILES: CC(CCCC(C)(C)O[Si](C)(C)C)C1CCC2C3C(O[Si](C)(C)C)C=C4CC(O[Si](C)(C)C)CCC4(
Mol. weight [g/mol]: 635.20

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.38		Crippen Method
logp	11.052		Crippen Method
rinpol	3390.00		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=R264463&Units=SI

Legend

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