24R,25-Dihydroxycholecalciferol, tris-TMS, # 2

Inchi: InChI=1S/C36H68O3Si3/c1-27-17-21-31(37-40(6,7)8)26-30(27)20-19-29-16-15-25-36(5)
InchiKey: QYCXEPMWUJWGBH-JKBKWPTRSA-N
Formula: C36H68O3Si3
SMILES: C=C1CCC(O[Si](C)(C)C)CC1=CC=C1CCCC2(C)C1CCC2C(C)CCC(O[Si](C)(C)C)C(C)(C
Mol. weight [g/mol]: 633.18

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.92		Crippen Method
logp	11.282		Crippen Method
rinpol	3579.00		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=R529309&Units=SI

Legend

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