7«alpha»,27-Dihydroxy-4-cholesten-3-one, TMS

Other names: 4-Cholesten-7-«alpha»,27-diol-3-one, TMS
Inchi: InChI=1S/C36H68O3Si3/c1-26(25-37-40(5,6)7)15-14-16-27(2)30-17-18-31-34-32(20-22-
InchiKey: LVBALRWAXSVALG-RVUDJKPNSA-N
Formula: C36H68O3Si3
SMILES: CC(CCCC(C)C1CCC2C3C(O[Si](C)(C)C)CC4=CC(O[Si](C)(C)C)=CCC4(C)C3CCC12C)
Mol. weight [g/mol]: 633.18

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.27		Crippen Method
logp	11.035		Crippen Method
rinpol	3581.00		NIST Webbook
rinpol	3545.00		NIST Webbook

Sources

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R177418&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

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