5-Cholesten-3-«beta»,7-«beta»,27-triol, TMS

Other names: 7«beta»,27-Dihydroxycholesterol, TMS
Inchi: InChI=1S/C36H70O3Si3/c1-26(25-37-40(5,6)7)15-14-16-27(2)30-17-18-31-34-32(20-22-
InchiKey: OIKRTDOOOQVHEN-GQXAZDAQSA-N
Formula: C36H70O3Si3
SMILES: CC(CCCC(C)C1CCC2C3C(O[Si](C)(C)C)C=C4CC(O[Si](C)(C)C)CCC4(C)C3CCC12C)C
Mol. weight [g/mol]: 635.20

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.03		Crippen Method
logp	10.909		Crippen Method
rinpol	3563.00		NIST Webbook
rinpol	3555.00		NIST Webbook

Sources

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R177572&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