5-«beta»-Cholestan-3-«beta»,7-«alpha»,12-«alpha TMS

InChI: InChI=1S/C36H72O3Si3/c1-25(2)16-15-17-26(3)29-18-19-30-34-31(24-33(36(29,30)5)39

InchiKey: YKRYUGIYGGLKAS-MRDZOKLWSA-N

Formula: C36H72O3Si3

SMILES: CC(C)CCCC(C)C1CCC2C3C(O[Si](C)(C)C)CC4CC(O[Si](C)(C)C)CCC4(C)C3CC(O[Si](C

Mol. weight [g/mol]: 637.21

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.05		Crippen Method
logp	10.988		Crippen Method
rinpol	3138.00		NIST Webbook
rinpol	3138.00		NIST Webbook

Sources

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R390111&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