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

Inchi: InChI=1S/C35H70O3Si3/c1-24(2)15-16-25(3)28-17-18-29-33-30(23-32(35(28,29)5)38-41

InchiKey: ADZXHKTUEUYJJL-ZVPGYCKJSA-N

Formula: C35H70O3Si3

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

Mol. weight [g/mol]: 623.18

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.63		Crippen Method
logp	10.598		Crippen Method
rinpol	3195.00		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=R271699&Units=SI

Legend

log10ws: Log10 of Water solubility in mol/l

logp: Octanol/Water partition coefficient

rinpol: Non-polar retention indices