5-Cholesten-3-«beta»,7-«alpha»,12-«alpha»,25,26-TMS

InChI: InChI=1S/C42H86O5Si5/c1-31(21-20-25-40(2,47-52(17,18)19)30-43-48(5,6)7)34-22-23-3

InchiKey: OUHBGNOOOYIUFA-GRNOMWHUSA-N

Formula: C42H86O5Si5

SMILES: CC(CCCC(C)(CO[Si](C)(C)C)O[Si](C)(C)C)C1CCC2C3C(O[Si](C)(C)C)C=C4CC(O[Si](C

Mol. weight [g/mol]: 811.56

Physical Properties

Property code	Value	Unit	Source
log10ws	-1.28		Crippen Method
logp	12.714		Crippen Method
rinpol	3644.00		NIST Webbook
rinpol	3644.00		NIST Webbook

Sources

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

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R390191&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