Simvastatin, trimethylsilyl ether

Other names: Simvastatin, tms derivative
Inchi: InChI=1S/C28H46O5Si/c1-9-28(4,5)27(30)32-24-15-18(2)14-20-11-10-19(3)23(26(20)24)
InchiKey: SUEDSISDIUMYSI-UHFFFAOYSA-N
Formula: C28H46O5Si
SMILES: CCC(C)(C)C(=O)OC1CC(C)C=C2C=CC(C)C(CCC3CC(O[Si](C)(C)C)CC(=O)O3)C21
Mol. weight [g/mol]: 490.75

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.93		Crippen Method
logp	6.445		Crippen Method
rinpol	3142.00		NIST Webbook
rinpol	3142.00		NIST Webbook

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=U334006&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

Legend

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