27-nor-5-«beta»-Cholestan-3-«alpha»,7-«alpha»,12
TMS, # 1

InChI: InChI=1S/C41H84O7Si5/c1-28(24-35(46-51(11,12)13)38(39(42)43-4)48-53(17,18)19)31-

InchiKey: CMINBFHOBCVDAD-ZPDGHADMSA-N

Formula: C41H84O7Si5

SMILES: COC(=O)C(O[Si](C)(C)C)C(CC(C)C1CCC2C3C(O[Si](C)(C)C)CC4CC(O[Si](C)(C)C)CC

Mol. weight [g/mol]: 829.53

Physical Properties

Property code	Value	Unit	Source
logp	11.165		Crippen Method
rinpol	3466.00		NIST Webbook
rinpol	3466.00		NIST Webbook

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R393769&Units=SI

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

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

Cheméo Relay (1.0):

Cheméo Relay (1.0, beta):

Legend

logp: Octanol/Water partition coefficient

rinpol: Non-polar retention indices