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

InChI: InChI=1S/C42H88O5Si5/c1-29(2)40(47-52(18,19)20)37(45-50(12,13)14)25-30(3)33-21-2

InchiKey: XFGLUJVVOKGJOB-KFGALLTASA-N

Formula: C42H88O5Si5

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

Mol. weight [g/mol]: 813.57

Physical Properties

Property code	Value	Unit	Source
logp	12.648		Crippen Method
rinpol	3547.00		NIST Webbook
rinpol	3547.00		NIST Webbook

Sources

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

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

Cheméo Relay (1.0):

Cheméo Relay (1.0, beta):

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R394148&Units=SI

Legend

logp: Octanol/Water partition coefficient

rinpol: Non-polar retention indices