4-Cholesten-7-.alpha.,12-.alpha.-diol-3-one, TMS

Inchi: InChI=1S/C33H60O3Si2/c1-22(2)13-12-14-23(3)26-15-16-27-31-28(21-30(33(26,27)5)36

InchiKey: UKDIIDZTZTYWAS-MHRMCLNXSA-N

Formula: C33H60O3Si2

SMILES: CC(C)CCC[C@@H](C)[C@H]1CCC2C3C(C[C@H](O[Si](C)(C)C)[C@@]21C)[C@@]1(C

Mol. weight [g/mol]: 561.01

Physical Properties

Property code	Value	Unit	Source
logp	9.257		Crippen Method

Sources

Cheméo Relay (1.0):

Cheméo Relay (1.0, beta):

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?Str2File=R396431

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

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

Legend

logp: Octanol/Water partition coefficient