3-«alpha»,5-«beta»,7-«beta»-Trihydroxy-5-«beta»-acid, methyl ester, TMS

Inchi: InChI=1S/C34H66O5Si3/c1-24(14-17-30(35)36-4)26-15-16-27-31-28(19-20-32(26,27)2)3
InchiKey: DFIHHDPWZQDJQM-IIHIQKLTSA-N
Formula: C34H66O5Si3
SMILES: COC(=O)CCC(C)C1CCC2C3C(O[Si](C)(C)C)CC4(O[Si](C)(C)C)CC(O[Si](C)(C)C)CCC4(
Mol. weight [g/mol]: 639.14

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.55		Crippen Method
logp	9.259		Crippen Method
rinpol	3367.00		NIST Webbook
rinpol	3367.00		NIST Webbook

Sources

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R393016&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