3«alpha»,7«alpha»,17«alpha»-trihydroxy-5«beta»-acid, TMS

Inchi: InChI=1S/C36H72O5Si4/c1-26(16-17-32(37)40-44(10,11)12)36(41-45(13,14)15)23-20-30

InchiKey: CQOCBDHGMLOCMN-GZTKFGANSA-N

Formula: C36H72O5Si4

SMILES: CC(CCC(=O)O[Si](C)(C)C)C1(O[Si](C)(C)C)CCC2C3C(O[Si](C)(C)C)CC4CC(O[Si](C)(C)

Mol. weight [g/mol]: 697.30

Physical Properties

Property code	Value	Unit	Source
log10ws	-1.44		Crippen Method
logp	10.464		Crippen Method
rinpol	3356.00		NIST Webbook
rinpol	3391.00		NIST Webbook

Sources

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

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

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R279891&Units=SI

Legend

log10ws: Log10 of Water solubility in mol/l

logp: Octanol/Water partition coefficient

rinpol: Non-polar retention indices