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

Inchi: InChI=1S/C36H72O5Si4/c1-26(16-19-32(37)40-44(10,11)12)28-17-18-29-33-30(21-22-34

InchiKey: MDBKTZNAHUOHSH-UBJCKJILSA-N

Formula: C36H72O5Si4

SMILES: CC(CCC(=O)O[Si](C)(C)C)C1CCC2C3C(O[Si](C)(C)C)CC4(O[Si](C)(C)C)CC(O[Si](C)(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	3347.00		NIST Webbook
rinpol	3406.00		NIST Webbook
rinpol	3347.00		NIST Webbook

Sources

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

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R279831&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