3«alpha»,5«beta»-dihydroxy-5«beta»-cholan-24-oic acid, TMS

Inchi: InChI=1S/C33H64O4Si3/c1-24(13-16-30(34)36-39(7,8)9)27-14-15-28-26-18-22-33(37-40
InchiKey: SFCDXMBGHKELBK-UQLHAXPDSA-N
Formula: C33H64O4Si3
SMILES: CC(CCC(=O)O[Si](C)(C)C)C1CCC2C3CCC4(O[Si](C)(C)C)CC(O[Si](C)(C)C)CCC4(C)C3
Mol. weight [g/mol]: 609.12

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.94		Crippen Method
logp	9.634		Crippen Method
rinpol	3328.00		NIST Webbook
rinpol	3358.00		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=R279851&Units=SI

Legend

log10ws: Log10 of Water solubility in mol/l
logp: Octanol/Water partition coefficient
rinpol: Non-polar retention indices