3«alpha»,7«beta»,14«alpha»-trihydroxy-5«beta»-c acid, TMS

Inchi: InChI=1S/C36H72O5Si4/c1-26(16-17-32(37)40-44(10,11)12)29-20-23-36(41-45(13,14)15
InchiKey: FXIHTYHJAIHHNY-TVIBPRCASA-N
Formula: C36H72O5Si4
SMILES: CC(CCC(=O)O[Si](C)(C)C)C1CCC2(O[Si](C)(C)C)C3C(O[Si](C)(C)C)CC4CC(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	3184.00		NIST Webbook
rinpol	3188.00		NIST Webbook

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R279935&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

Legend

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