5«beta»-Homocholane-3«alpha»,7«alpha»,12«alpha»-tetrol-TMS

InChI: InChI=1S/C37H76O4Si4/c1-27(18-16-17-23-38-42(4,5)6)30-19-20-31-35-32(26-34(37(30,31)

InchiKey: XCJMPPVSTROYKS-RLIJUXHNSA-N

Formula: C37H76O4Si4

SMILES: CC(CCCCO[Si](C)(C)C)C1CCC2C3C(O[Si](C)(C)C)CC4CC(O[Si](C)(C)C)CCC4(C)C3CC

Mol. weight [g/mol]: 697.34

Physical Properties

Property code	Value	Unit	Source
log10ws	-1.84		Crippen Method
logp	11.183		Crippen Method
rinpol	3385.00		NIST Webbook
rinpol	3385.00		NIST Webbook

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R271753&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