13,14-Dihydro-15-keto-PGF1A, BO-TMS, isomer # 1

Inchi: InChI=1S/C33H69NO5Si3/c1-12-14-18-21-28(34-36-26-15-13-2)24-25-30-29(22-19-16-1

InchiKey: HVPUTDTWEIYAQD-IHZBLBIESA-N

Formula: C33H69NO5Si3

SMILES: CCCCCC(CCC1C(O[Si](C)(C)C)CC(O[Si](C)(C)C)C1CCCCCCC(=O)O[Si](C)(C)C)=NOC

Mol. weight [g/mol]: 644.16

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.70		Crippen Method
logp	10.315		Crippen Method
rinpol	2922.00		NIST Webbook
rinpol	2922.00		NIST Webbook

Sources

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

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R580651&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