13,14-Dihydro-15-keto-PGF1A, EO-TMS, isomer # 2

Inchi: InChI=1S/C31H65NO5Si3/c1-12-14-17-20-26(32-34-13-2)23-24-28-27(21-18-15-16-19-2

InchiKey: ZRIXZDUAXLAJTG-ZXYZSCNASA-N

Formula: C31H65NO5Si3

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]: 616.11

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.87		Crippen Method
logp	9.534		Crippen Method
rinpol	2799.00		NIST Webbook
rinpol	2799.00		NIST Webbook

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R580686&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