6-Keto-PGF1A, MO-TMS

Inchi: InChI=1S/C34H71NO5Si4/c1-15-16-17-21-30(38-42(6,7)8)23-24-31-28(27-41(3,4)5)25-3
InchiKey: AQGAIGJYJZDSGB-MIGCGHNUSA-N
Formula: C34H71NO5Si4
SMILES: CCCCCC(C=CC1C(C[Si](C)(C)C)CC(O[Si](C)(C)C)C1CC(CCCCC(=O)O[Si](C)(C)C)=NC
Mol. weight [g/mol]: 686.27

Physical Properties

Property code	Value	Unit	Source
log10ws	-1.20		Crippen Method
logp	10.485		Crippen Method
rinpol	2823.00		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=R581525&Units=SI

Legend

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