6,15-Diketo-PGF1A, EO-TMS, isomer # 2

Inchi: InChI=1S/C34H68N2O5Si3/c1-13-16-17-20-29(35-38-14-2)23-24-31-28(27-42(4,5)6)25-3
InchiKey: WHYVOPATRJWSGY-XHFBHPQOSA-N
Formula: C34H68N2O5Si3
SMILES: CCCCCC(C=CC1C(C[Si](C)(C)C)CC(O[Si](C)(C)C)C1CC(CCCCC(=O)O[Si](C)(C)C)=NO
Mol. weight [g/mol]: 669.17

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.19		Crippen Method
logp	10.047		Crippen Method
rinpol	2899.00		NIST Webbook
rinpol	2899.00		NIST Webbook

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R581456&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