6,15-Diketo-PGF1A, MO-TMS

Inchi: InChI=1S/C32H64N2O5Si3/c1-13-14-15-18-27(33-36-2)21-22-29-26(25-40(4,5)6)23-31(3
InchiKey: SNUWFDLNIIRKFD-HTXCKNOQSA-N
Formula: C32H64N2O5Si3
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]: 641.12

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.36		Crippen Method
logp	9.267		Crippen Method
rinpol	2836.00		NIST Webbook
rinpol	2836.00		NIST Webbook

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R581476&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