6-Keto-PGF1A, BO-TMS, isomer # 1

Inchi: InChI=1S/C37H77NO5Si4/c1-15-17-19-23-33(41-45(6,7)8)25-26-34-31(30-44(3,4)5)28-3
InchiKey: MHPMXOMGJCDOJX-JGNWWJDASA-N
Formula: C37H77NO5Si4
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]: 728.35

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.46		Crippen Method
logp	11.655		Crippen Method
rinpol	2988.00		NIST Webbook
rinpol	2988.00		NIST Webbook

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R581481&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