13,14-Dihydro-15-keto-PGE2, MO-TMS, isomer # 2

Inchi: InChI=1S/C28H54N2O5Si2/c1-10-11-14-17-23(29-32-2)20-21-25-24(26(30-33-3)22-27(2

InchiKey: RPPMUWLTPOHJQW-XYXRJUCCSA-N

Formula: C28H54N2O5Si2

SMILES: CCCCCC(CCC1C(O[Si](C)(C)C)CC(=NOC)C1CC=CCCCC(=O)O[Si](C)(C)C)=NOC

Mol. weight [g/mol]: 554.91

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.46		Crippen Method
logp	7.703		Crippen Method
rinpol	2750.00		NIST Webbook

Sources

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R580611&Units=SI

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

log10ws: Log10 of Water solubility in mol/l

logp: Octanol/Water partition coefficient

rinpol: Non-polar retention indices