

13,14-Dihydro-15-keto-PGE2, BO-TMS, isomer # 3

Inchi: InChI=1S/C34H66N2O5Si2/c1-10-13-18-21-29(35-38-26-14-11-2)24-25-31-30(22-19-16-17-12-8-9-3-4-5-6-7)32-33-34-36-37-39-40-41-42-43-44-45-46-47-48-49-50-51-52-53-54-55-56-57-58-59-60-61-62-63-64-65-66-67-68-69-70-71-72-73-74-75-76-77-78-79-80-81-82-83-84-85-86-87-88-89-90-91-92-93-94-95-96-97-98-99-100
InchiKey: GVSHYYIQRKPSGU-ORGQUXCYSA-N
Formula: C34H66N2O5Si2
SMILES: CCCCC(CCC1C(O[Si](C)(C)C)CC(=NOCCCC)C1CC=CCCC(=O)O[Si](C)(C)C)=NOCCCC
Mol. weight [g/mol]: 639.07

Physical Properties

Property code	Value	Unit	Source
log10ws	-5.97		Crippen Method
logp	10.043		Crippen Method
rinpol	3118.00		NIST Webbook
rinpol	3118.00		NIST Webbook

Sources

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=R580542&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>
Crippen Method: https://www.cheméo.com/doc/models/crippen_log10ws

Legend

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

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