

15-Keto-PGE2, BO-TMS, isomer # 4

Inchi: InChI=1S/C34H64N2O5Si2/c1-10-13-18-21-29(35-38-26-14-11-2)24-25-31-30(22-19-16-17-20)32-33-34-36-37
InchiKey: RMJAGIVEDWGGNH-WVFFVVGEFSA-N
Formula: C34H64N2O5Si2
SMILES: CCCCC(C=CC1C(O[Si](C)(C)C)CC(=NOCCCC)C1CC=CCCC(=O)O[Si](C)(C)C=NO
Mol. weight [g/mol]: 637.05

Physical Properties

Property code	Value	Unit	Source
log10ws	-5.82		Crippen Method
logp	9.819		Crippen Method
rincpol	3144.00		NIST Webbook
rincpol	3144.00		NIST Webbook

Sources

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=R581169&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci990307l>
Crippen Method: https://www.cheméo.com/doc/models/crippen_log10ws

Legend

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

Latest version available from:

<https://www.cheméo.com/cid/23-837-7/15-Keto-PGE2-BO-TMS-isomer-4.pdf>

Generated by Cheméo on 2024-05-01 06:42:36.506184717 +0000 UTC m=+16835005.426762028.

Cheméo (<https://www.cheméo.com>) is the biggest free database of chemical and physical data for the process industry.