

13,14-Dihydro-6,15-diketo-PGF1A, BO-TMS, isomer # 1

Inchi: InChI=1S/C37H76N2O6Si3/c1-13-16-19-22-31(38-41-27-17-14-2)25-26-33-34(36(44-47(48-49-50)51)52)53
InchiKey: LQTFTWUJGAVZNV-SKXFTCKDSA-N
Formula: C37H76N2O6Si3
SMILES: CCCCCC(CCC1C(O[Si](C)(C)C)CC(O[Si](C)(C)C)C1CC(CCCCC(=O)O[Si](C)(C)C)=NO
Mol. weight [g/mol]: 729.27

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.62		Crippen Method
logp	11.097		Crippen Method
rinpol	3155.00		NIST Webbook

Sources

Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>
Crippen Method: https://www.cheméo.com/doc/models/crippen_log10ws
NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=R580824&Units=SI>

Legend

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

Latest version available from:

<https://www.cheméo.com/cid/66-565-2/13-14-Dihydro-6-15-diketo-PGF1A-BO-TMS-isomer-1.pdf>

Generated by Cheméo on 2024-05-01 16:06:55.617371868 +0000 UTC m=+16868864.537949178.

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