

13,14-Dihydro-6,15-diketo-PGF1A, BO-TMS, isomer # 3

Inchi: InChI=1S/C37H76N2O6Si3/c1-13-16-19-22-31(38-41-27-17-14-2)25-26-33-34(36(44-47)
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	3178.00		NIST Webbook
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Sources

Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=R580844&Units=SI>

Legend

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

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<https://www.chemeo.com/cid/30-368-0/13-14-Dihydro-6-15-diketo-PGF1A-BO-TMS-isomer-3.pdf>

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