

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

Inchi: InChI=1S/C33H68N2O6Si3/c1-13-16-17-20-27(34-37-14-2)23-24-29-30(32(40-43(7,8)9)2
InchiKey: NFECWVKGLYDHML-RTNMLALUSA-N
Formula: C33H68N2O6Si3
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]: 673.16

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.94		Crippen Method
logp	9.537		Crippen Method
rinpol	2905.00		NIST Webbook
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Sources

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=R580884&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci990307I>

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/61-689-0/13-14-Dihydro-6-15-diketo-PGF1A-EO-TMS-isomer-3.pdf>

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