

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

Inchi: InChI=1S/C31H64N2O6Si3/c1-13-14-15-18-25(32-35-2)21-22-27-28(30(38-41(7,8)9)24-2
InchiKey: VIPQHXLXJXFOZ-GCXHJFECSA-N
Formula: C31H64N2O6Si3
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]: 645.11

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.11		Crippen Method
logp	8.757		Crippen Method
rinsol	2849.00		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=R580899&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>

Legend

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

Latest version available from:

<https://www.chemeo.com/cid/118-182-9/13-14-Dihydro-6-15-diketo-PGF1A-MO-TMS-isomer-1.pdf>

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