

6,15-Diketo-PGF1A, BO-TMS, isomer # 1

Inchi: InChI=1S/C38H76N2O5Si3/c1-13-16-19-22-33(39-42-27-17-14-2)25-26-35-32(31-46(4,5
InchiKey: NKWDLQMGTICIYIA-DZPYAQHZSA-N
Formula: C38H76N2O5Si3
SMILES: CCCCCC(C=CC1C(C[Si](C)(C)C)CC(O[Si](C)(C)C)C1CC(CCCCC(=O)O[Si](C)(C)C)=NO
Mol. weight [g/mol]: 725.28

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.87		Crippen Method
logp	11.607		Crippen Method
rinpol	3105.00		NIST Webbook

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=R581401&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/56-166-6/6-15-Diketo-PGF1A-BO-TMS-isomer-1.pdf>

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