

15-Keto-PGA1A, BO-TMS, isomer # 1

Inchi: InChI=1S/C31H56N2O4Si/c1-7-10-15-18-28(32-35-25-11-8-2)23-21-27-22-24-30(33-36-2)
InchiKey: LSOMCPVJIKZVAL-VPSOQQPASA-N
Formula: C31H56N2O4Si
SMILES: CCCCCC(C=CC1C=CC(=NOCCCC)C1CCCCCCC(=O)O[Si](C)(C)C)=NOCCCC
Mol. weight [g/mol]: 548.87

Physical Properties

Property code	Value	Unit	Source
log10ws	-7.31		Crippen Method
logp	8.989		Crippen Method
rinpol	2926.00		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=R581030&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/123-196-8/15-Keto-PGA1A-BO-TMS-isomer-1.pdf>

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