

15-Keto-PGA2A, BO-TMS, isomer # 1

Inchi: InChI=1S/C31H54N2O4Si/c1-7-10-15-18-28(32-35-25-11-8-2)23-21-27-22-24-30(33-36-2)
InchiKey: ICTMTUUJRSRFCU-SJKBTYSASA-N
Formula: C31H54N2O4Si
SMILES: CCCCCC(C=CC1C=CC(=NOCCCC)C1CC=CCCCC(=O)O[Si](C)(C)C)=NOCCCC
Mol. weight [g/mol]: 546.86

Physical Properties

Property code	Value	Unit	Source
log10ws	-7.17		Crippen Method
logp	8.765		Crippen Method
rinpol	2890.00		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=R581085&Units=SI>

Legend

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

Latest version available from:

<https://www.chemeo.com/cid/118-667-1/15-Keto-PGA2A-BO-TMS-isomer-1.pdf>

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