

13,14-Dihydro-15-keto-PGE2, MO-TMS, isomer # 1

Inchi:	InChI=1S/C28H54N2O5Si2/c1-10-11-14-17-23(29-32-2)20-21-25-24(26(30-33-3)22-27(2
InchiKey:	RPPMUWLTPOHJQW-XYXRJUCCSA-N
Formula:	C28H54N2O5Si2
SMILES:	CCCCC(CCC1C(O[Si](C)(C)C)CC(=NOC)C1CC=CCCC(=O)O[Si](C)(C)C)=NOC
Mol. weight [g/mol]:	554.91

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.46		Crippen Method
logp	7.703		Crippen Method
rinpol	2704.00		NIST Webbook

Sources

Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R580606&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
rinpol:	Non-polar retention indices

Latest version available from:

<https://www.chemeo.com/cid/50-804-3/13-14-Dihydro-15-keto-PGE2-MO-TMS-isomer-1.pdf>

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