

13,14-Dihydro-15-keto-PGE2, EO-TMS, isomer # 4

Inchi:	InChI=1S/C30H58N2O5Si2/c1-10-13-16-19-25(31-34-11-2)22-23-27-26(20-17-14-15-18-
InchiKey:	UWXDFULQJFGIIN-OPNXPFFOSA-N
Formula:	C30H58N2O5Si2
SMILES:	CCCCC(CCC1C(O[Si](C)(C)C)CC(=NOCC)C1CC=CCCC(=O)O[Si](C)(C)C)=NOCC
Mol. weight [g/mol]:	582.96

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.29		Crippen Method
logp	8.483		Crippen Method
rinpol	2832.00		NIST Webbook
rinpol	2832.00		NIST Webbook

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R580597&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.cheméo.com/doc/models/crippen_log10ws

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.cheméo.com/cid/69-860-1/13-14-Dihydro-15-keto-PGE2-EO-TMS-isomer-4.pdf>

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