

13,14-Dihydro-15-keto-PGF1A, BO-TMS, isomer # 2

Inchi:	InChI=1S/C33H69NO5Si3/c1-12-14-18-21-28(34-36-26-15-13-2)24-25-30-29(22-19-16-1
InchiKey:	HVPUTDTWEIYAQD-IHZBLBIESA-N
Formula:	C33H69NO5Si3
SMILES:	CCCCC(CCC1C(O[Si](C)(C)C)CC(O[Si](C)(C)C)C1CCCCC(=O)O[Si](C)(C)C)=NO
Mol. weight [g/mol]:	644.16

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.70		Crippen Method
logp	10.315		Crippen Method
rinpol	2937.00		NIST Webbook

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.cheméo.com/doc/models/crippen_log10ws
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R580666&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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