15-Keto-PGF 1A, TMS

Inchi:	InChI=1S/C29H58O5Si3/c1-11-12-15-18-24(30)21-22-26-25(19-16-13-14-17-20-29(31)34
InchiKey:	VKHUWWDVDKWLQM-JHYFEYLISA-N
Formula:	C29H58O5Si3
SMILES:	CCCCCC(=O)C=CC1C(O[Si](C)(C)C)CC(O[Si](C)(C)C)C1CCCCCCC(=O)O[Si](C)(C)C
Mol. weight [g/mol]:	571.02

Physical Properties

Property code	Value	Unit	Source
log10ws	-1.92		Crippen Method
logp	8.487		Crippen Method
rinpol	2803.00		NIST Webbook
rinpol	2803.00		NIST Webbook

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R581243&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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