

Prosta-5,11-dien-1-oic acid, 9-oxo-11,15-bis[(trimethylsilyl)oxy]-, trimethylsilyl ester, (5Z,11«alpha»,13E,15S)-

Other names:

Prostaglandin E2, O, 9-bis(trimethylsilyl)-, trimethylsilyl ester
PGE2 TMS

Inchi:	InChI=1S/C29H56O5Si3/c1-11-12-15-18-24(32-35(2,3)4)21-22-26-25(27(30)23-28(26)33
InchiKey:	UHIZANMZAQLJAR-LBWJEKIOSA-N
Formula:	C29H56O5Si3
SMILES:	CCCCC(C=CC1C(O[Si](C)(C)C)CC(=O)C1CC=CCCC(=O)O[Si](C)(C)C)O[Si](C)(C)C
Mol. weight [g/mol]:	569.01
CAS:	39003-20-8

Physical Properties

Property code	Value	Unit	Source
log10ws	-1.77		Crippen Method
logp	8.263		Crippen Method
rinpol	2788.50		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=C39003208&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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<https://www.chemeo.com/cid/32-611-7/Prosta-5-11-dien-1-oic-acid-9-oxo-11-15-bis-trimethylsilyl-oxy-trimethylsilyl-es>

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