PGA1, EO-TMS, isomer # 1

Inchi:	InChI=1S/C28H53NO4Si2/c1-9-11-14-17-25(32-34(3,4)5)22-20-24-21-23-27(29-31-10-2)
InchiKey:	AEJQJLKSHLXDED-WDMRMWGLSA-N
Formula:	C28H53NO4Si2
SMILES:	CCCCCC(C=CC1C=CC(=NOCC)C1CCCCCCC(=O)O[Si](C)(C)C)O[Si](C)(C)C
Mol. weight [g/mol]:	523.90

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.07		Crippen Method
logp	8.256		Crippen Method
rinpol	2595.00		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=R581550&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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