PGA1, EO-TMS, isomer # 2

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	2652.00		NIST Webbook
rinpol	2652.00		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=R581565&Units=SI

Legend

log10ws: Log10 of Water solubility in mol/l
logp: Octanol/Water partition coefficient
rinpol: Non-polar retention indices