PGA2, BO-TMS, isomer # 1

Inchi: InChI=1S/C30H55NO4Si2/c1-9-11-15-18-27(34-36(3,4)5)23-21-26-22-24-29(31-33-25-12
InchiKey: JLXZPPNHDUATET-VHBSRNPFSA-N
Formula: C30H55NO4Si2
SMILES: CCCCCC(C=CC1C=CC(=NOCCCC)C1CC=CCCCC(=O)O[Si](C)(C)C)O[Si](C)(C)C
Mol. weight [g/mol]: 549.93

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.76		Crippen Method
logp	8.813		Crippen Method
rinpol	2745.00		NIST Webbook
rinpol	2745.00		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=R581590&Units=SI

Legend

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