PGA1, MO-TMS, isomer # 2

Inchi: InChI=1S/C27H51NO4Si2/c1-9-10-13-16-24(31-33(3,4)5)21-19-23-20-22-26(28-30-2)25(
InchiKey: ZDSXOMLVLPGWHE-SVCXTJLYSA-N
Formula: C27H51NO4Si2
SMILES: CCCCCC(C=CC1C=CC(=NOC)C1CCCCCCC(=O)O[Si](C)(C)C)O[Si](C)(C)C
Mol. weight [g/mol]: 509.87

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.65		Crippen Method
logp	7.866		Crippen Method
rinpol	2604.00		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=R581585&Units=SI

Legend

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