15(S)-15-Methyl-PGA2, MO-TMS, isomer # 2

Inchi: InChI=1S/C28H51NO4Si2/c1-10-11-16-22-28(2,33-35(7,8)9)23-21-24-19-20-26(29-31-3)
InchiKey: BHEWARGZXKXHEQ-RQIMKRAQSA-N
Formula: C28H51NO4Si2
SMILES: CCCCCC(C)(C=CC1C=CC(=NOC)C1CC=CCCCC(=O)O[Si](C)(C)C)O[Si](C)(C)C
Mol. weight [g/mol]: 521.88

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.92		Crippen Method
logp	8.032		Crippen Method
rinpol	2604.00		NIST Webbook
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=R581312&Units=SI

Legend

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