

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

Inchi: InChI=1S/C29H53NO4Si2/c1-10-12-17-23-29(3,34-36(7,8)9)24-22-25-20-21-27(30-32-11)
InchiKey: ISRTXSKMZPSKTM-INJRARDFSA-N
Formula: C29H53NO4Si2
SMILES: CCCCCC(C)(C=CC1C=CC(=NOCC)C1CC=CCCCC(=O)O[Si](C)(C)C)O[Si](C)(C)C
Mol. weight [g/mol]: 535.91

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.34		Crippen Method
logp	8.422		Crippen Method
rinpol	2661.00		NIST Webbook
rinpol	2661.00		NIST Webbook

Sources

Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=R581298&Units=SI>

Legend

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

Latest version available from:

<https://www.chemeo.com/cid/47-192-7/15-S-15-Methyl-PGA2-EO-TMS-isomer-2.pdf>

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