

11«alpha»,15«alpha»-dihydroxy-9-ketoprost-13-enoic acid, 19-hydroxy, EO-TMS # 2

InChI: InChI=1S/C35H73NO6Si4/n11-38-36-2-28-33(40-44(7,8)9)31(30(32)23-19-17-18-20-21)35-34-33-32-31-30-29-28-27-26-25-24-23-22-21-20-19-18-17-16-15-14-13-12-11-10-9-8-7-6-5-4-3-2-1
InChIKey: PCJNNCJCCXDURPT-MYDRTQKRSA-N

Formula: C35H73NO6Si4

SMILES: CCON=C1CC(O[Si](C)(C)C)C(C=CC(C)(CCCC(C)O[Si](C)(C)C)O[Si](C)(C)C)C1CCCCO

Mol. weight [g/mol]: 716.30

Physical Properties

Property code	Value	Unit	Source
log10ws	-1.64		Crippen Method
logp	10.530		Crippen Method
rinpol	3130.00		NIST Webbook
rinpol	3130.00		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=R385476&Units=SI>

Legend

log10ws: Log10 of Water solubility in mol/l

logp: Octanol/Water partition coefficient

rinpol: Non-polar retention indices

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