

11«alpha»,15«alpha»-dihydroxy-9-ketoprost-13-enoic acid, 19-hydroxy, MO-TMS # 1

Inchi: InChI=1S/C34H71NO6Si4/c1-28-38-42(4,5)6)21-20-25-34(2,41-45(13,14)15)26-24-30-29
InchiKey: QEOCZWAYQCHHBD-WUJOPPNJSA-N

Formula: C34H71NO6Si4
SMILES: CON=C1CC(O[Si](C)(C)C)C(C=CC(C)(CCCC(C)O[Si](C)(C)C)O[Si](C)(C)C)C1CCCCC
Mol. weight [g/mol]: 702.27

Physical Properties

Property code	Value	Unit	Source
logp	10.140		Crippen Method
rinpol	3040.00		NIST Webbook
rinpol	3040.00		NIST Webbook

Sources

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=R385481&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci990307l>
Crippen Method: https://www.cheméo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):
Cheméo Relay (1.0, beta):

Legend

logp: Octanol/Water partition coefficient
rinpol: Non-polar retention indices

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