

11«alpha»,15«alpha»-dihydroxy-9-ketoprost-5,13-dienoic acid, 19-hydroxy, EO-TMS # 2

Inchi: InChI=1S/C35H71NO6Si4/c1-10-38-36-32-28-33(40-44(7,8)9)31(30(32)23-19-17-18-20-21)29-34-35-37-39-41-42-43-45-46-47-48-49-50-51-52-53-54-55-56-57-58-59-60-61-62-63-64-65-66-67-68-69-70-71-72-73-74-75-76-77-78-79-80-81-82-83-84-85-86-87-88-89-90-91-92-93-94-95-96-97-98-99-100/h1-10,38,36,32,28,33(40-44(7,8)9)31(30(32)23-19-17-18-20-21)29-34-35-37-39-41-42-43-45-46-47-48-49-50-51-52-53-54-55-56-57-58-59-60-61-62-63-64-65-66-67-68-69-70-71-72-73-74-75-76-77-78-79-80-81-82-83-84-85-86-87-88-89-90-91-92-93-94-95-96-97-98-99-100/t1,10,38,36,32,28,33(40-44(7,8)9)31(30(32)23-19-17-18-20-21)29-34-35-37-39-41-42-43-45-46-47-48-49-50-51-52-53-54-55-56-57-58-59-60-61-62-63-64-65-66-67-68-69-70-71-72-73-74-75-76-77-78-79-80-81-82-83-84-85-86-87-88-89-90-91-92-93-94-95-96-97-98-99-100/m-1/s-1

InchiKey: WPMVWUJJQGVFLNU-DIQWJETCSA-N

Formula: C35H71NO6Si4

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

Mol. weight [g/mol]: 714.28

Physical Properties

Property code	Value	Unit	Source
logp	10.307		Crippen Method
rinpol	3145.00		NIST Webbook
rinpol	3145.00		NIST Webbook

Sources

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):

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=R385550&Units=SI>

Legend

logp: Octanol/Water partition coefficient

rinpol: Non-polar retention indices

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