

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

Inchi: CCCCC(C)(C=CC1C(O[Si](C)(C)C)CC(=NOC)C1CCCCCCC(=O)O[Si](C)(C)C)O[Si](C)(C)C
InchiKey: MCAIMDFXQSDXPD-ATQBCQKVSA-N
Formula: C31H63NO5Si3
SMILES: CCCCC(C)(C=CC1C(O[Si](C)(C)C)CC(=NOC)C1CCCCCCC(=O)O[Si](C)(C)C)O[Si](C)(C)C
Mol. weight [g/mol]: 614.09

Physical Properties

Property code	Value	Unit	Source
logp	9.310		Crippen Method
rinpol	2860.00		NIST Webbook
rinpol	2860.00		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=R385525&Units=SI>

Legend

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

Latest version available from:
<https://www.cheméo.com/cid/116-953-5/11-alpha-15-alpha-dihydroxy-9-ketoprost-13-enoic-acid-MO-TMS-1.pdf>
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