

11«alpha»,15«alpha»-dihydroxy-9-ketoprost-5,13-dienoic acid, MO TMS #1

Inchi: CCCCC(C)(C=CC1C(O[Si](C)(C)C)CC(=NOC)C1CC=CCCCC(=O)O[Si](C)(C)C)O[Si](C)(C)C
InchiKey: XQFHPVCJGCPJIN-QHVDWANMSA-N
Formula: C31H61NO5Si3
SMILES: CCCCC(C)(C=CC1C(O[Si](C)(C)C)CC(=NOC)C1CC=CCCCC(=O)O[Si](C)(C)C)O[Si](C)(C)C
Mol. weight [g/mol]: 612.08

Physical Properties

Property code	Value	Unit	Source
logp	9.086		Crippen Method
rinpol	2830.00		NIST Webbook
rinpol	2830.00		NIST Webbook

Sources

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):
Cheméo Relay (1.0, beta):
NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=R385609&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci990307l>

Legend

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

Latest version available from:

<https://www.chemeo.com/cid/112-617-2/11-alpha-15-alpha-dihydroxy-9-ketoprost-5-13-dienoic-acid-MO-TMS-1.pdf>

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