

11.alpha.,15.alpha.-dihydroxy-9-ketoprost-13-enoic acid, MO-TMS # 2

Inchi: CCCC[C@@](C)(/C=C/[C@H]1[C@H](O[Si](C)(C)C)CC(=NOC)[C@@H]1CCCCCCC(=O)O)C
InchiKey: MCAIMDFXQSDXPD-RQGWRDATSA-N
Formula: C₃₁H₆₃NO₅Si₃
SMILES: CCCCC[C@@](C)(/C=C/[C@H]1[C@H](O[Si](C)(C)C)CC(=NOC)[C@@H]1CCCCCCC(=O)O)C
Mol. weight [g/mol]: 614.11

Physical Properties

Property code	Value	Unit	Source
logp	9.310		Crippen Method

Sources

Cheméo Relay (1.0):

Cheméo Relay (1.0, beta):

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?Str2File=R385530>

Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci990307l>

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

Legend

logp: Octanol/Water partition coefficient

Latest version available from:

<https://www.chemeo.com/cid/123-599-1/11-alpha-15-alpha-dihydroxy-9-ketoprost-13-enoic-acid-MO-TMS-2.pdf>

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