

3«alpha»,7«alpha»,12«alpha»-Trihydroxycholestan-23-en-26-oic acid, isomer # 1,

Inchi:
Me-TMS

InchiKey:

Formula:

SMILES:

Mol. weight [g/mol]:

InChI=1S/C37H70O5Si3/c1-25(16-15-17-26(2)35(38)39-5)29-18-19-30-34-31(24-33(37(2

OPVGZYZXJGHWQK-GYHRYELVSA-N

C37H70O5Si3

COC(=O)C(C)C=CCC(C)C1CCC2C3C(O[Si](C)(C)C)CC4CC(O[Si](C)(C)C)CCC4(C)C3C

679.21

Physical Properties

Property code	Value	Unit	Source
logp	9.917		Crippen Method
rinpol	3386.00		NIST Webbook
rinpol	3386.00		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=R584915&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/56-912-7/3-alpha-7-alpha-12-alpha-Trihydroxy-cholestan-23-en-26-oic-acid-isomer-1-M>

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