

Other names

trisochoic acid, trimethylsilyl ether-methyl ester

Inchi:

InChI=1S/C34H66O5Si3/c1-23(14-17-

InchiKey:

DQKFOB XAKZ

Formula:

C₃₄H₆₆O₅Si₃

SMILES:

COC(=O)CCC(C)C1CCC2C3C(O[Si](C)(C)C)CC4CC(O[Si](C)(C)C)CCC4(C)C3CC(O[Si](C)(C)C)C1

Mol. weight [g/mol]:

639.14

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.31		Crippen Method
logp	9.115		Crippen Method
rinpol	3332.00		NIST Webbook
rinpol	3332.00		NIST Webbook

Sources

Crippen Method:

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

Crippen Method:

<https://www.chemeo.com/doc/models/crippen> log10ws

NIST Webbook:

<http://webbook.nist.gov/cgi/cbook.cgi?ID=R182806&Units=SI>

Legend

log10ws:

Log10 of Water solubility in mol/l

logp:

Octanol/Water partition coefficient

rinpol:

Non-polar retention indices

Latest version available from:

<https://www.chemeo.com/cid/20-364-5/3-alpha-7-beta-12-alpha-Trihydroxy-5-beta-cholanoic-acid-MeTMS.pdf>

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