

(24E)-Trihydroxy-24-coprostenic acid, Me-TMS

Inchi: InChI=1S/C38H72O5Si3/c1-26(2)17-16-18-27(3)29-19-20-30-34-31(23-33(37(29,30)5)43
InchiKey: ZUIBNORDRCDWLW-AKZDMUSASA-N
Formula: C38H72O5Si3
SMILES: COC(=O)C12CC(O[Si](C)(C)C)CCC1(C)C1CC(O[Si](C)(C)C)C3(C)C(C(C)CC=CC(C)C)C
Mol. weight [g/mol]: 693.23

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.60		Crippen Method
logp	10.307		Crippen Method
rinpol	3478.00		NIST Webbook
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Sources

Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=R584871&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/13-765-8/24E-Trihydroxy-24-coprostenic-acid-Me-TMS.pdf>

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