

3-«alpha»,6-«alpha»,12-«alpha»-Trihydroxy-5-«beta»-Cholanoic acid, 3-«alpha»,6-«alpha»,12-«alpha»-trihydroxy, methyl ester, TMS

Other names: 3-«alpha»,6-«alpha»,12-«alpha»-Trihydroxy-5-«beta»-Cholanoic acid, 3-«alpha»,6-«alpha»,12-«alpha»-trihydroxy, methyl ester, TMS
Inchi: InChI=1S/C34H66O5Si3/c1-23(14-17-32(35)36-4)26-15-16-27-25-21-30(38-41(8,9)10)29
InchiKey: UQGJPQVEFKEVQU-XKDDARQZSA-N
Formula: C34H66O5Si3
SMILES: COC(=O)CCC(C)C1CCC2C3CC(O[Si](C)(C)C)C4CC(O[Si](C)(C)C)CCC4(C)C3CC(O[Si](C)(C)C)C
Mol. weight [g/mol]: 639.14

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.31		Crippen Method
logp	9.115		Crippen Method
rinpol	3280.00		NIST Webbook
rinpol	3280.00		NIST Webbook

Sources

Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci990307l>
Crippen Method: https://www.cheméo.com/doc/models/crippen_log10ws
NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=R393185&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.cheméo.com/cid/50-997-0/3-alpha-6-alpha-12-alpha-Trihydroxy-5-beta-cholanoic-acid-MeTMS.pdf>
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