

allo-Cholanic acid, 3«alpha»,7«beta»,12«alpha»-trihydroxy,

Me-TMS

Other names: 3«alpha»,7«beta»,12«alpha»-Trihydroxy-5«alpha»-cholanic acid, methyl ester,
TMS
InChI: InChI=1S/C34H66O5Si3/c1-23(14-17-31(35)36-4)26-15-16-27-32-28(22-30(34(26,27)3)3
InchiKey: DQKFOBXAKZGIPX-QBPZRYSZSA-N
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)C
Mol. weight [g/mol]: 639.14

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.31		Crippen Method
logp	9.115		Crippen Method
rinpola	3262.00		NIST Webbook
rinpola	3262.00		NIST Webbook
rinpola	3262.00		NIST Webbook
ripola	3524.00		NIST Webbook
ripola	3524.00		NIST Webbook

Sources

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=R533452&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci990307l>
Crippen Method: https://www.chemo.com/doc/models/crippen_log10ws

Legend

log10ws: Log10 of Water solubility in mol/l
logp: Octanol/Water partition coefficient
rinpola: Non-polar retention indices
ripola: Polar retention indices

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