

3«alpha»,7«alpha»,12«alpha»-trihydroxy-5«beta»-bile acid, methyl ester, TMS

InChI: InChI=1S/C37H72O5Si3/c1-25(16-15-17-26(2)35(38)39-5)29-18-19-30-34-31(24-33(37)28)/36,32,34,35,37,38,39,40,41,42,43,44,45,46,47,48,49,50,51,52,53,54,55,56,57,58,59,60,61,62,63,64,65,66,67,68,69,70,71,72/s1-3,1-3,1-3

InChIKey: GRUORWHHLRJRJ-GYHRYELVSA-N

Formula: C37H72O5Si3

SMILES: COC(=O)C(C)CCCC(C)C1CCC2C3C(O[Si](C)(C)C)CC4CC(O[Si](C)(C)C)CCC4(C)C3C

Mol. weight [g/mol]: 681.22

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.33		Crippen Method
logp	10.141		Crippen Method
rinpol	3455.00		NIST Webbook
rinpol	3455.00		NIST Webbook

Sources

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=R534915&Units=SI>

Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>

Crippen Method: https://www.cheméo.com/doc/models/crippen_log10ws

Legend

log10ws: Log10 of Water solubility in mol/l

logp: Octanol/Water partition coefficient

rinpol: Non-polar retention indices

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