

Cholan-24-oic acid, 3,7,12-tri(trimethylsilyloxy)-, trimethylsilyl ester, (3«alpha», 5«beta», 7«alpha», 12«alpha»)-

Other names: (3«alpha», 5«beta», 7«alpha», 12«alpha»)-tri(trimethylsilyloxy)-trimethylsilyl ester, (3«alpha», 5«beta», 7«alpha», 12«alpha»)-cholanic acid, TMS

InChI: InChI=1S/C36H72O5Si4/c1-25(16-19-33(37)41-45(13,14)15)28-17-18-29-34-30(24-32(36)35)31

InChIKey: FUBDSUQXLCQNJD-UHFFFAOYSA-N

Formula: C36H72O5Si4

SMILES: CC(CCC(=O)O[Si](C)(C)C)C1CCC2C3C(O[Si](C)(C)C)CC4CC(O[Si](C)(C)C)CCC4(C)C3

Mol. weight [g/mol]: 697.30

Physical Properties

Property code	Value	Unit	Source
log10ws	-1.20		Crippen Method
logp	10.320		Crippen Method
rinpol	3214.00		NIST Webbook
rinpol	3219.00		NIST Webbook
rinpol	3214.00		NIST Webbook

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=U365566&Units=SI>

Legend

log10ws: Log10 of Water solubility in mol/l

logp: Octanol/Water partition coefficient

rinpol: Non-polar retention indices

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