

3«alpha»,5«beta»,7«beta»-trihydroxy-5«beta»-cholanic acid, TMS

InChI: InChI=1S/C36H72O5Si4/c1-26(16-19-32(37)40-44(10,11)12)28-17-18-29-33-30(21-22-34)43-45-46-47-48-49-50-51-52-53-54-55-56-57-58-59-60-61-62-63-64-65-66-67-68-69-70-71-72-73-74-75-76-77-78-79-80-81-82-83-84-85-86-87-88-89-90-91-92-93-94-95-96-97-98-99-100/h1-36,41-43,45-47,49-51,53-55,57-59,61-63,65-67,69-71,73-75,77-79,81-83,85-87,89-91,93-95,97-99,101-102/t1-36,41-43,45-47,49-51,53-55,57-59,61-63,65-67,69-71,73-75,77-79,81-83,85-87,89-91,93-95,97-99,101-102/s1-36,41-43,45-47,49-51,53-55,57-59,61-63,65-67,69-71,73-75,77-79,81-83,85-87,89-91,93-95,97-99,101-102

InChIKey: MDBKTZNAHUOHS-UBJCKJILSA-N

Formula: C₃₆H₇₂O₅Si₄

SMILES: CC(CCC(=O)O[Si](C)(C)C)C1CCC2C3C(O[Si](C)(C)C)CC4(O[Si](C)(C)C)CC(O[Si](C)(C)C)C

Mol. weight [g/mol]: 697.30

Physical Properties

Property code	Value	Unit	Source
log10ws	-1.44		Crippen Method
logp	10.464		Crippen Method
rinpol	3347.00		NIST Webbook
rinpol	3406.00		NIST Webbook
rinpol	3347.00		NIST Webbook

Sources

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

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=R279831&Units=SI>

Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci990307l>

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/44-069-7/3-alpha-5-beta-7-beta-trihydroxy-5-beta-cholan-24-oic-acid-TMS.pdf>

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