

3-«alpha»,4-«beta»,7-«alpha»,12-«alpha»-Tetrahydroxy-5-«alpha»-cholanoic acid, MeTMS

Inchi: InChI=1S/C37H74O6Si4/c1-25(17-20-33(38)39-4)26-18-19-27-34-28(24-32(37(26,27)3)4)QKSYQONADMPPHH-HEPCSLPDSA-N
InchiKey: QKSYQONADMPPHH-HEPCSLPDSA-N
Formula: C37H74O6Si4
SMILES: COC(=O)CCC(C)C1CCC2C3C(O[Si](C)(C)C)CC4C(O[Si](C)(C)C)C(O[Si](C)(C)C)CCC4
Mol. weight [g/mol]: 727.32

Physical Properties

Property code	Value	Unit	Source
log10ws	-0.82		Crippen Method
logp	9.945		Crippen Method
rinpol	3436.00		NIST Webbook
rinpol	3436.00		NIST Webbook

Sources

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=R393165&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/68-633-4/3-alpha-4-beta-7-alpha-12-alpha-Tetrahydroxy-5-alpha-cholanoic-acid-MeTMS>

Generated by Cheméo on 2025-12-05 11:44:15.221467398 +0000 UTC m=+4683252.751508051.

Cheméo (<https://www.chemeo.com>) is the biggest free database of chemical and physical data for the process industry.