

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

InChI: InChI=1S/C37H74O6Si4/c1-25(17-20-34(38)39-4)28-18-19-29-35-30(24-33(37(28,29)3)4)NSPWFCYVNJGODS-XMNUVXEUSA-N
Formula: C37H74O6Si4
SMILES: COC(=O)CCC(C)C1CCC2C3C(O[Si](C)(C)C)CC4CC(O[Si](C)(C)C)CC(O[Si](C)(C)C)C4
Mol. weight [g/mol]: 727.32

Physical Properties

Property code	Value	Unit	Source
logp	9.945		Crippen Method
rinpol	3320.00		NIST Webbook
rinpol	3320.00		NIST Webbook
rinpol	3320.00		NIST Webbook

Sources

Cheméo Relay (1.0, beta):

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=R499535&Units=SI>

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

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

Cheméo Relay (1.0):

Legend

logp: Octanol/Water partition coefficient

rinpol: Non-polar retention indices

Latest version available from:

<https://www.chemeo.com/cid/123-845-7/1-beta-3-alpha-7-alpha-12-alpha-Tetrahydroxy-5-beta-cholanoic-acid-MeTMS>

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