

5-Cholesten-3-«beta»,7-«alpha»,12-«alpha»,24,25-pentol-TMS, # 3

InChI=1S/C42H86O5Si5/c1-30(21-24-37(45-50(12,13)14)40(2,3)47-52(18,19)20)33-22-23
InChIKey: WIWBKHSEMSTCKV-ZMNROGEKSA-N

Formula: C42H86O5Si5

SMILES: CC(CCC(O[Si](C)(C)C)C(C)(C)O[Si](C)(C)C)C1CCC2C3C(O[Si](C)(C)C)C=C4CC(O[Si](C)(C)C)C5

Mol. weight [g/mol]: 811.56

Physical Properties

Property code	Value	Unit	Source
logp	12.712		Crippen Method
rinpol	3593.00		NIST Webbook
rinpol	3593.00		NIST Webbook

Sources

Cheméo Relay (1.0):

Cheméo Relay (1.0, beta):

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=R390171&Units=SI>

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

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

Legend

logp: Octanol/Water partition coefficient

rinpol: Non-polar retention indices

Latest version available from:

<https://www.chemeo.com/cid/124-083-2/5-Cholesten-3-beta-7-alpha-12-alpha-24-25-pentol-TMS-3.pdf>

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