

27-nor-5-«beta»-Cholestan-3-«alpha»,7-«alpha»,12-«alpha»-pentol-TMS, # 2

InChIKey: CMINBFHOBVCVDAD-ZPDGHADMSA-N
Formula: C₄₁H₈₄O₇Si₅
SMILES: COC(=O)C(O[Si](C)(C)C)C(CC(C)C1CCC2C3C(O[Si](C)(C)C)CC4CC(O[Si](C)(C)C)CCO
Mol. weight [g/mol]: 829.53

Physical Properties

Property code	Value	Unit	Source
logp	11.165		Crippen Method
rinpol	3486.00		NIST Webbook
rinpol	3486.00		NIST Webbook

Sources

Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci990307l>
Crippen Method: https://www.cheméo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):
Cheméo Relay (1.0, beta):
NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=R393774&Units=SI>

Legend

logp: Octanol/Water partition coefficient
rinpol: Non-polar retention indices

Latest version available from:

<https://www.cheméo.com/cid/114-953-7/27-nor-5-beta-Cholestan-3-alpha-7-alpha-12-alpha-24-25-pentol-TMS-2.pdf>

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