

24-Nor-5«beta»-cholane-3«alpha»,7«alpha»,12«alpha»-TMS

TMS

InchiKey:

InChI=1S/C35H72O4Si4/c1-25(19-21-36-40(4,5)6)28-16-17-29-33-30(24-32(35(28,29)3)

AZJYCBBVNRRNOD-ZVPGYCKJSA-N

Formula:

C35H72O4Si4

SMILES:

CC(CCO[Si](C)(C)C)C1CCC2C3C(O[Si](C)(C)C)CC4CC(O[Si](C)(C)C)CCC4(C)C3CC(O

Mol. weight [g/mol]:

669.29

Physical Properties

Property code	Value	Unit	Source
log10ws	-1.01		Crippen Method
logp	10.403		Crippen Method
rinpol	3186.00		NIST Webbook
rinpol	3186.00		NIST Webbook

Sources

Crippen Method:

<http://pubs.acs.org/doi/abs/10.1021/ci9903071>

Crippen Method:

https://www.cheméo.com/doc/models/crippen_log10ws

NIST Webbook:

<http://webbook.nist.gov/cgi/cbook.cgi?ID=R271288&Units=SI>

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.cheméo.com/cid/70-480-1/24-Nor-5-beta-cholane-3-alpha-7-alpha-12-alpha-23-tetrol-TMS.pdf>

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