

5«beta»-Cholestane-3«alpha»,7«alpha»,12«alpha»

TMS

InChI=1S/C41H86O5Si5/c1-29(25-36(44-49(12,13)14)39(2,3)46-51(18,19)20)32-21-22-3
InChIKey: OOAPDDQLBPWGEZ-XHLRRERNSA-N

Formula:

C41H86O5Si5

SMILES:

CC(CC(O[Si](C)(C)C)C(C)(C)O[Si](C)(C)C)C1CCC2C3C(O[Si](C)(C)C)CC4CC(O[Si](C)(C)C)C

Mol. weight [g/mol]:

799.55

Physical Properties

Property code	Value	Unit	Source
log10ws	-0.88		Crippen Method
logp	12.402		Crippen Method
rinpol	3607.00		NIST Webbook

Sources

Crippen Method:

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

NIST Webbook:

<http://webbook.nist.gov/cgi/cbook.cgi?ID=R271664&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/60-632-3/5-beta-Cholestane-3-alpha-7-alpha-12-alpha-24S-25-pentol-TMS.pdf>

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