

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

TMS

InchiKey:

InChI=1S/C38H78O4Si4/c1-27(26-39-43(5,6)7)17-18-28(2)31-19-20-32-36-33(25-35(38)

LTWMNVRMBRXNLW-HLAIWXDNSA-N

Formula:

C38H78O4Si4

SMILES:

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

Mol. weight [g/mol]:

711.37

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.02		Crippen Method
logp	11.429		Crippen Method
rinpol	3314.00		NIST Webbook

Sources

Crippen Method:

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

NIST Webbook:

<http://webbook.nist.gov/cgi/cbook.cgi?ID=R271302&Units=SI>

Crippen Method:

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

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/29-967-7/24-Nor-5-beta-cholestane-3-alpha-7-alpha-12-alpha-25-tetrol-TMS.pdf>

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