

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

TMS

InchiKey:

InChI=1S/C35H70O3Si3/c1-24(2)15-16-25(3)28-17-18-29-33-30(23-32(35(28,29)5)38-41

ADZXHKTUEUYJLL-ZVPGYCKJSA-N

Formula:

C35H70O3Si3

SMILES:

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

Mol. weight [g/mol]:

623.18

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.63		Crippen Method
logp	10.598		Crippen Method
rinpol	3195.00		NIST Webbook

Sources

Crippen Method:

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

Crippen Method:

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

NIST Webbook:

<http://webbook.nist.gov/cgi/cbook.cgi?ID=R271699&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/31-777-5/5-beta-Cholestane-3-alpha-7-alpha-12-alpha-triol-TMS.pdf>

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