

5-Cholesten-3-«beta»,7-«alpha»,12-«alpha»,25,26-

TMS

InchiKey:

Formula:

SMILES:

Mol. weight [g/mol]:

InChI=1S/C42H86O5Si5/c1-31(21-20-25-40(2,47-52(17,18)19)30-43-48(5,6)7)34-22-23-

OUHBGNOOOYIUFA-GRNOMWHUSA-N

C42H86O5Si5

CC(CCCC(C)(CO[Si](C)(C)C)O[Si](C)(C)C)C1CCC2C3C(O[Si](C)(C)C)C=C4CC(O[Si](C)

811.56

Physical Properties

Property code	Value	Unit	Source
log10ws	-1.28		Crippen Method
logp	12.714		Crippen Method
rinpol	3644.00		NIST Webbook
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Sources

Crippen Method:

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

NIST Webbook:

<http://webbook.nist.gov/cgi/cbook.cgi?ID=R390191&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/67-385-1/5-Cholesten-3-beta-7-alpha-12-alpha-25-26-pentol-TMS.pdf>

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