

(24S)-24-ethyl-5«alpha»-cholestan-3«beta»,24-diol-TMS

TMS

InChI=1S/C35H68O2Si2/c1-13-35(25(2)3,37-39(10,11)12)23-18-26(4)30-16-17-31-29-15

InchiKey:

NHGLLGYKQQEFMP-RZLQZIACSA-N

Formula:

C35H68O2Si2

SMILES:

CCC(CCC(C)C1CCC2C3CCC4CC(O[Si](C)(C)C)CCC4(C)C3CCC12C)(O[Si](C)(C)C)C(C)C

Mol. weight [g/mol]:

577.08

Physical Properties

Property code	Value	Unit	Source
log10ws	-6.38		Crippen Method
logp	10.938		Crippen Method
rinpol	3572.00		NIST Webbook
rinpol	3574.00		NIST Webbook
rinpol	3572.00		NIST Webbook

Sources

NIST Webbook:

<http://webbook.nist.gov/cgi/cbook.cgi?ID=R279717&Units=SI>

Crippen Method:

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

Crippen Method:

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

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/64-675-2/24S-24-ethyl-5-alpha-cholestan-3-beta-24-diol-TMS.pdf>

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