

5«beta»-Stigmastanol (24«beta»-ethyl-5«beta»-cholestan-3«beta»-ol), TMS

InChI=1S/C32H60OSi/c1-10-24(22(2)3)12-11-23(4)28-15-16-29-27-14-13-25-21-26(33-3

TZWRPXXRQJDCPG-NBIDMSKMSA-N

Formula:

C32H60OSi

SMILES:

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

Mol. weight [g/mol]:

488.90

Physical Properties

Property code	Value	Unit	Source
log10ws	-7.63		Crippen Method
logp	9.964		Crippen Method
rinpol	3196.00		NIST Webbook
rinpol	3196.00		NIST Webbook

Sources

Crippen Method:

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

NIST Webbook:

<http://webbook.nist.gov/cgi/cbook.cgi?ID=R435695&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/56-112-5/5-beta-Stigmastanol-24-beta-ethyl-5-beta-cholestan-3-beta-ol-TMS.pdf>

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