

3«beta»,5«alpha»,6«beta»-trihydroxystigmastano

TMS

InchiKey:

Formula:

SMILES:

Mol. weight [g/mol]:

InChI=1S/C38H74O3Si3/c1-16-29(27(2)3)18-17-28(4)32-19-20-33-31-25-35(40-43(10,11

HKXDONLTXDRWFO-FMANNOCJSA-N

C38H74O3Si3

CCC(C=CC(C)C1CCC2C3CC(O[Si](C)(C)C)C4(O[Si](C)(C)C)CC(O[Si](C)(C)C)CCC4(C)

663.25

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.74		Crippen Method
logp	11.544		Crippen Method
rinpol	3446.00		NIST Webbook
rinpol	3446.00		NIST Webbook

Sources

Crippen Method:

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

Crippen Method:

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

NIST Webbook:

<http://webbook.nist.gov/cgi/cbook.cgi?ID=R395334&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.chemeo.com/cid/13-400-2/3-beta-5-alpha-6-beta-trihydroxystigmastanol-TMS.pdf>

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