

5«beta»-pregnane-3«alpha»,17,20«alpha»-triol,

MO-TMS

InChIKey:

InChI=1S/C30H60O3Si3/c1-22(31-34(4,5)6)30(33-36(10,11)12)20-17-27-25-14-13-23-21

Formula:

C30H60O3Si3

SMILES:

CC(O[Si](C)(C)C)C1(O[Si](C)(C)C)CCC2C3CCC4CC(O[Si](C)(C)C)CCC4(C)C3CCC21C

Mol. weight [g/mol]:

553.05

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.26		Crippen Method
logp	9.079		Crippen Method
rinpol	2889.00		NIST Webbook
rinpol	2889.00		NIST Webbook

Sources

Crippen Method:

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

Crippen Method:

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

NIST Webbook:

<http://webbook.nist.gov/cgi/cbook.cgi?ID=R488298&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/16-456-8/5-beta-pregnane-3-alpha-17-20-alpha-triol-MO-TMS.pdf>

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