

5-«beta»-Pregnan-3-«alpha»,11-«beta»,20-«beta»-TMS

TMS

InchiKey:

InChI=1S/C30H60O3Si3/c1-21(31-34(4,5)6)25-15-16-26-24-14-13-22-19-23(32-35(7,8)9)

NWGHICYXPXWBNLK-KDVUPINTSA-N

Formula:

C30H60O3Si3

SMILES:

CC(O[Si](C)(C)C)C1CCC2C3CCC4CC(O[Si](C)(C)C)CCC4(C)C3C(O[Si](C)(C)C)CC12O

Mol. weight [g/mol]:

553.05

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.02		Crippen Method
logp	8.935		Crippen Method
rinpol	2938.00		NIST Webbook
rinpol	2938.00		NIST Webbook

Sources

NIST Webbook:

<http://webbook.nist.gov/cgi/cbook.cgi?ID=R486950&Units=SI>

Crippen Method:

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

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/30-070-0/5-beta-Pregnan-3-alpha-11-beta-20-beta-triol-TMS.pdf>

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