

5-«alpha»-Pregnan-3-«beta»,16-«alpha»,20-«beta»

InChI:
MeTMS

InChI=1S/C33H68O4Si4/c1-32-19-17-25(35-39(6,7)8)21-24(32)15-16-26-27(32)18-20-33

InChIKey:

USVGSUAGVCXQBV-PZRAEKEQSA-N

Formula:

C33H68O4Si4

SMILES:

CC12CCC(O[Si](C)(C)C)CC1CCC1C2CCC2(C)C1CC(O[Si](C)(C)C)C2C(CO[Si](C)(C)C)

Mol. weight [g/mol]:

641.23

Physical Properties

Property code	Value	Unit	Source
logp	9.767		Crippen Method
rinpol	3087.00		NIST Webbook
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rinpol	3087.00		NIST Webbook

Sources

Cheméo Relay (1.0):

Cheméo Relay (1.0, beta):

NIST Webbook:

<http://webbook.nist.gov/cgi/cbook.cgi?ID=R393378&Units=SI>

Crippen Method:

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

Crippen Method:

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

Legend

logp: Octanol/Water partition coefficient

rinpol: Non-polar retention indices

Latest version available from:

<https://www.chemeo.com/cid/117-731-0/5-alpha-Pregnan-3-beta-16-alpha-20-beta-21-tetrol-MeTMS.pdf>

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