

5.alpha.-Pregnane-11,20-dione-3.alpha.,21-diol,

TMSO-TMS, # 2

InChIKey:

InChI=1S/C32H64N2O4Si4/c1-32-21-29(33-37-41(8,9)10)31-25-17-15-24(36-40(5,6)7)20
SGEJXYYPQSHIRL-ULPLONHSA-N

Formula:

C32H64N2O4Si4

SMILES:

C[C@]12CC(=NO[Si](C)(C)C)C3C(CC[C@H]4C[C@H](O[Si](C)(C)C)CCC34)C1CC[C@]

Mol. weight [g/mol]:

653.22

Physical Properties

Property code	Value	Unit	Source
logp	9.352		Crippen Method

Sources

NIST Webbook:

<http://webbook.nist.gov/cgi/cbook.cgi?ID=R526904&Units=SI>

Crippen Method:

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

Crippen Method:

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

Cheméo Relay (1.0):

Cheméo Relay (1.0, beta):

Legend

logp: Octanol/Water partition coefficient

Latest version available from:

<https://www.cheméo.com/cid/71-139-9/5-alpha-Pregnane-11-20-dione-3-alpha-21-diol-TMSO-TMS-2.pdf>

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