

5.beta.-Pregnane-11,20-dione-3.alpha.,21-diol, TMSO-TMS, # 1

Inchi: InChI=1S/C32H64N2O4Si4/c1-32-21-29(33-37-41(8,9)10)31-25-17-15-24(36-40(5,6)7)20
InchiKey: SGEJXYYPQSHIRL-UPOKHZKQSA-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@H]2
Mol. weight [g/mol]: 653.22

Physical Properties

Property code	Value	Unit	Source
logp	9.352		Crippen Method

Sources

Cheméo Relay (1.0):

Cheméo Relay (1.0, beta):

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=R527041&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

Latest version available from:

<https://www.chemeo.com/cid/70-405-4/5-beta-Pregnane-11-20-dione-3-alpha-21-diol-TMSO-TMS-1.pdf>

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