

5.beta.-Pregnane-11,20-dione-3.alpha.,21-diol, EO-TMS, # 2

Inchi: InChI=1S/C30H56N2O4Si2/c1-10-33-31-27-19-30(3)25(16-17-26(30)28(32-34-11-2)20-3
InchiKey: OIKBPBVQNHABES-UWIYIKSCSA-N
Formula: C30H56N2O4Si2
SMILES: CCON=C1C[C@@]2(C)C(CC[C@@H]2C(CO[Si](C)(C)C)=NOCC)C2CC[C@@H]3C[C@]
Mol. weight [g/mol]: 564.96

Physical Properties

Property code	Value	Unit	Source
logp	7.722		Crippen Method

Sources

Cheméo Relay (1.0, beta):

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=R527016&Units=SI>

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

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

Cheméo Relay (1.0):

Legend

logp: Octanol/Water partition coefficient

Latest version available from:

<https://www.chemeo.com/cid/67-172-7/5-beta-Pregnane-11-20-dione-3-alpha-21-diol-EO-TMS-2.pdf>

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