

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

MO-TMS, # 1

InchiKey:

ChI=1S/C28H52N2O4Si2/c1-28-17-25(29-31-2)27-21-13-11-20(34-36(7,8)9)16-19(21)10-22-23-24-26N2KMLMUNKFRHGOS-KLPAPNPOSA-N

Formula:

C28H52N2O4Si2

SMILES:

CON=C1C[C@@]2(C)C(CC[C@@H]2C(CO[Si](C)(C)C)=NOC)C2CC[C@H]3C[C@H](O

Mol. weight [g/mol]:

536.91

Physical Properties

Property code	Value	Unit	Source
logp	6.941		Crippen Method

Sources

Cheméo Relay (1.0, beta):

NIST Webbook:

<http://webbook.nist.gov/cgi/cbook.cgi?ID=R526875&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/70-912-1/5-alpha-Pregnane-11-20-dione-3-alpha-21-diol-MO-TMS-1.pdf>

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