

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

Inchi: InChI=1S/C28H52N2O4Si2/c1-28-17-25(29-31-2)27-21-13-11-20(34-36(7,8)9)16-19(21)1
InchiKey: NKMLMUNKFRHGOS-IHCSGJPESA-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]
Mol. weight [g/mol]: 536.91

Physical Properties

Property code	Value	Unit	Source
logp	6.941		Crippen Method

Sources

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=R527036&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/70-913-0/5-beta-Pregnane-11-20-dione-3-alpha-21-diol-MO-TMS-2.pdf>

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