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

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-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