5«alpha»-pregnane-3,20-dione, MO-TMS, anti

Inchi: InChI=1S/C23H38N2O2/c1-15(24-26-4)19-8-9-20-18-7-6-16-14-17(25-27-5)10-12-22(16,

InchiKey: BRBZYVRSVCPKEU-ZPEGQXQVSA-N

Formula: C23H38N2O2

SMILES: CON=C1CCC2(C)C(CCC3C2CCC2(C)C(C(C)=NOC)CCC32)C1

Mol. weight [g/mol]: 374.56

Physical Properties

Property code	Value	Unit	Source
log10ws	-5.14		Cheméo Relay (1.0)
logp	5.670		Crippen Method
mcvol	314.590	ml/mol	McGowan Method
rinpol	2881.00		NIST Webbook
tf	388.99	K	Cheméo Relay (1.0)

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R395790&Units=SI

Joback Method: https://en.wikipedia.org/wiki/Joback_method

McGowan Method: http://link.springer.com/article/10.1007/BF02311772

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):

Cheméo Relay (1.0, beta):

Legend

log10ws: Log10 of Water solubility in mol/l

logp: Octanol/Water partition coefficient

mcvol: McGowan's characteristic volume

rinpol: Non-polar retention indices

tf: Normal melting (fusion) point