

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

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