

5-«alpha»-Pregnan-3,11,20-trione, MO

Inchi: InChI=1S/C24H39N3O3/c1-15(25-28-4)19-9-10-20-18-8-7-16-13-17(26-29-5)11-12-23(10-3)-24
InchiKey: NUNRMUMDGNQFCZ-BYFUWVQTSA-N
Formula: C24H39N3O3
SMILES: CON=C1CCC2(C)C(CCC3C4CCC(C(C)=NOC)C4(C)CC(=NOC)C32)C1
Mol. weight [g/mol]: 417.58

Physical Properties

Property code	Value	Unit	Source
logp	5.282		Crippen Method
mcvol	340.230	ml/mol	McGowan Method
rinpol	2813.00		NIST Webbook
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Sources

Cheméo Relay (1.0):

Cheméo Relay (1.0, beta):

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=R486529&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

Legend

logp: Octanol/Water partition coefficient

mcvol: McGowan's characteristic volume

rinpol: Non-polar retention indices

Latest version available from:

<https://www.chemeo.com/cid/121-667-7/5-alpha-Pregnan-3-11-20-trione-MO.pdf>

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