5-«beta»-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(16
InchiKey: NUNRMUMDGNQFCZ-HXUNKEQXSA-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	2758.00		NIST Webbook
rinpol	2758.00		NIST Webbook

Sources

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):
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R486910&Units=SI

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/123-300-1/5-beta-Pregnan-3-11-20-trione-MO.pdf