

5.alpha.-Pregnan-3,20-dione, MO, # 2

Inchi: InChI=1S/C22H36N2O2/c1-14(23-25-3)20-9-10-21-19-7-5-15-13-16(24-26-4)6-8-17(15)1
InchiKey: OMMFWSIWKVMITH-FJRBLVNISA-N
Formula: C22H36N2O2
SMILES: CON=C1CCC2C3CC[C@@]4(C)C(CC[C@@H]4C(C)=NOC)C3CC[C@H]2C1
Mol. weight [g/mol]: 360.54

Physical Properties

Property code	Value	Unit	Source
logp	5.280		Crippen Method
mcvol	300.500	ml/mol	McGowan Method

Sources

Cheméo Relay (1.0, beta):

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=R523361&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.cheméo.com/doc/models/crippen_log10ws

Cheméo Relay (1.0):

Legend

logp: Octanol/Water partition coefficient

mcvol: McGowan's characteristic volume

Latest version available from:

<https://www.cheméo.com/cid/58-927-9/5-alpha-Pregnan-3-20-dione-MO-2.pdf>

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