

# 5-«alpha»-Pregnan-3,11-dione, MO

**Inchi:** InChI=1S/C23H38N2O2/c1-6-15-8-10-19-18-9-7-16-13-17(24-26-4)11-12-22(16,2)21(18)  
**InchiKey:** ACPIXOASZHBQJM-MXIPSPLNSA-N  
**Formula:** C23H38N2O2  
**SMILES:** CCC1CCC2C3CCC4CC(=NOC)CCC4(C)C3C(=NOC)CC12C  
**Mol. weight [g/mol]:** 374.56

## Physical Properties

Property code	Value	Unit	Source
hf	-470.57	kJ/mol	Joback Method
hvap	77.18	kJ/mol	Joback Method
log10ws	-5.82		Crippen Method
logp	5.670		Crippen Method
mcvol	314.590	ml/mol	McGowan Method
pc	1054.14	kPa	Joback Method
rinpol	2592.00		NIST Webbook
rinpol	2592.00		NIST Webbook
tb	963.58	K	Joback Method
tc	1204.81	K	Joback Method

## Sources

**Crippen Method:** <http://pubs.acs.org/doi/abs/10.1021/ci9903071>  
**Crippen Method:** [https://www.chemeo.com/doc/models/crippen\\_log10ws](https://www.chemeo.com/doc/models/crippen_log10ws)  
**Joback Method:** [https://en.wikipedia.org/wiki/Joback\\_method](https://en.wikipedia.org/wiki/Joback_method)  
**McGowan Method:** <http://link.springer.com/article/10.1007/BF02311772>  
**NIST Webbook:** <http://webbook.nist.gov/cgi/cbook.cgi?ID=R486534&Units=SI>

## Legend

**hf:** Enthalpy of formation at standard conditions  
**hvap:** Enthalpy of vaporization at standard conditions

<b>log10ws:</b>	Log10 of Water solubility in mol/l
<b>logp:</b>	Octanol/Water partition coefficient
<b>mcvol:</b>	McGowan's characteristic volume
<b>pc:</b>	Critical Pressure
<b>rinpola:</b>	Non-polar retention indices
<b>tb:</b>	Normal Boiling Point Temperature
<b>tc:</b>	Critical Temperature

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