

# 5-«beta»-Pregnan-11-one, MO

**Inchi:** InChI=1S/C22H37NO/c1-5-15-10-12-18-17-11-9-16-8-6-7-13-21(16,2)20(17)19(23-24-4)  
**InchiKey:** HKQXLBHDHDHGOK-DMLAZZSJSA-N  
**Formula:** C22H37NO  
**SMILES:** CCC1CCC2C3CCC4CCCCC4(C)C3C(=NOC)CC12C  
**Mol. weight [g/mol]:** 331.54

## Physical Properties

Property code	Value	Unit	Source
hf	-358.74	kJ/mol	Joback Method
hvap	68.40	kJ/mol	Joback Method
log10ws	-6.16		Crippen Method
logp	6.058		Crippen Method
mcvol	288.950	ml/mol	McGowan Method
pc	1240.71	kPa	Joback Method
rinpol	2266.00		NIST Webbook
tb	839.12	K	Joback Method
tc	1075.45	K	Joback Method

## Sources

**NIST Webbook:** <http://webbook.nist.gov/cgi/cbook.cgi?ID=R486816&Units=SI>  
**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>

## Legend

**hf:** Enthalpy of formation at standard conditions  
**hvap:** Enthalpy of vaporization at standard conditions  
**log10ws:** 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>rinpol:</b>	Non-polar retention indices
<b>tb:</b>	Normal Boiling Point Temperature
<b>tc:</b>	Critical Temperature

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