

# 4-Pregnen-3,20-dione, MO

**Inchi:** InChI=1S/C23H36N2O2/c1-15(24-26-4)19-8-9-20-18-7-6-16-14-17(25-27-5)10-12-22(16,  
**InchiKey:** WCBFSBXYZBTGBQ-JYVPLEQZSA-N  
**Formula:** C23H36N2O2  
**SMILES:** CON=C1C=C2CCC3C(CCC4(C)C(C(C)=NOC)CCC34)C2(C)CC1  
**Mol. weight [g/mol]:** 372.54

## Physical Properties

Property code	Value	Unit	Source
hf	-372.52	kJ/mol	Joback Method
hvap	77.70	kJ/mol	Joback Method
log10ws	-5.92		Crippen Method
logp	5.590		Crippen Method
mcvol	310.290	ml/mol	McGowan Method
pc	1112.59	kPa	Joback Method
rinpol	2800.00		NIST Webbook
rinpol	2765.00		NIST Webbook
tb	969.79	K	Joback Method
tc	1217.22	K	Joback Method

## Sources

**NIST Webbook:** <http://webbook.nist.gov/cgi/cbook.cgi?ID=R486227&Units=SI>  
**Crippen Method:** <http://pubs.acs.org/doi/abs/10.1021/ci990307l>  
**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

<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>rinpol:</b>	Non-polar retention indices
<b>tb:</b>	Normal Boiling Point Temperature
<b>tc:</b>	Critical Temperature

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