

# Pregnanedione, MO TMS

**Inchi:** InChI=1S/C23H38N2O2/c1-15(24-26-4)19-8-9-20-18-7-6-16-14-17(25-27-5)10-12-22(16,  
**InchiKey:** BRBZYVRSVCPKEU-QFSYNTFFSA-N  
**Formula:** C23H38N2O2  
**SMILES:** CON=C1CCC2(C)C(CCC3C2CCC2(C)C(C(C)=NOC)CCC32)C1  
**Mol. weight [g/mol]:** 374.56

## Physical Properties

Property code	Value	Unit	Source
hf	-439.17	kJ/mol	Joback Method
hvap	76.43	kJ/mol	Joback Method
log10ws	-5.82		Crippen Method
logp	5.670		Crippen Method
mcvol	314.590	ml/mol	McGowan Method
pc	1073.57	kPa	Joback Method
rinpol	2868.00		NIST Webbook
tb	960.98	K	Joback Method
tc	1206.29	K	Joback Method

## Sources

**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=R250578&Units=SI>  
**Crippen Method:** <http://pubs.acs.org/doi/abs/10.1021/ci990307I>  
**Crippen Method:** [https://www.chemeo.com/doc/models/crippen\\_log10ws](https://www.chemeo.com/doc/models/crippen_log10ws)

## 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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