

# N-cyano-n-methyl-5alpha-pregnan-18-amine

<b>Inchi:</b>	InChI=1S/C23H38N2/c1-4-17-9-11-21-19-10-8-18-7-5-6-13-22(18,2)20(19)12-14-23(17,2
<b>InchiKey:</b>	LFUCSBAKSOGICG-UHFFFAOYSA-N
<b>Formula:</b>	C23H38N2
<b>SMILES:</b>	CCC1CCC2C3CCC4CCCCC4(C)C3CCC12CN(C)C#N
<b>Mol. weight [g/mol]:</b>	342.56
<b>CAS:</b>	76938-41-5

## Physical Properties

Property code	Value	Unit	Source
gf	535.13	kJ/mol	Joback Method
hf	-55.78	kJ/mol	Joback Method
hfus	32.51	kJ/mol	Joback Method
hvap	76.60	kJ/mol	Joback Method
log10ws	-6.27		Crippen Method
logp	5.838		Crippen Method
mcvol	302.850	ml/mol	McGowan Method
pc	1260.16	kPa	Joback Method
tb	874.94	K	Joback Method
tc	1108.80	K	Joback Method
tf	535.67	K	Joback Method
vc	1.149	m3/kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1091.53	J/molxK	874.94	Joback Method
cpg	1119.74	J/molxK	913.92	Joback Method
cpg	1148.05	J/molxK	952.89	Joback Method
cpg	1176.82	J/molxK	991.87	Joback Method
cpg	1206.43	J/molxK	1030.85	Joback Method
cpg	1237.25	J/molxK	1069.83	Joback Method
cpg	1269.65	J/molxK	1108.80	Joback Method

# Sources

<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=C76938415&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C76938415&amp;Units=SI</a>
<b>Crippen Method:</b>	<a href="http://pubs.acs.org/doi/abs/10.1021/ci9903071">http://pubs.acs.org/doi/abs/10.1021/ci9903071</a>
<b>Crippen Method:</b>	<a href="https://www.chemeo.com/doc/models/crippen_log10ws">https://www.chemeo.com/doc/models/crippen_log10ws</a>
<b>Joback Method:</b>	<a href="https://en.wikipedia.org/wiki/Joback_method">https://en.wikipedia.org/wiki/Joback_method</a>
<b>McGowan Method:</b>	<a href="http://link.springer.com/article/10.1007/BF02311772">http://link.springer.com/article/10.1007/BF02311772</a>

# Legend

<b>cpg:</b>	Ideal gas heat capacity
<b>gf:</b>	Standard Gibbs free energy of formation
<b>hf:</b>	Enthalpy of formation at standard conditions
<b>hfus:</b>	Enthalpy of fusion at standard conditions
<b>hvap:</b>	Enthalpy of vaporization at standard conditions
<b>log10ws:</b>	Log10 of Water solubility in mol/l
<b>logp:</b>	Octanol/Water partition coefficient
<b>mccvol:</b>	McGowan's characteristic volume
<b>pc:</b>	Critical Pressure
<b>tb:</b>	Normal Boiling Point Temperature
<b>tc:</b>	Critical Temperature
<b>tf:</b>	Normal melting (fusion) point
<b>vc:</b>	Critical Volume

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