

# Tibolone

<b>Other names:</b>	19-Norpregn-5(10)-en-20-yn-3-one, 17-hydroxy-7-methyl-, (7«alpha»,17«alpha»)-17-Hydroxy-7«alpha»-methyl-19-nor-17«alpha»-pregn-5(10)-en-20-yn-3-one (1«alpha»,17«alpha»)-17-hydroxy-7-methyl-19-norpregn-5(10)-en-20-yn-3-one (tibolone)
<b>Inchi:</b>	InChI=1S/C21H28O2/c1-4-21(23)10-8-18-19-13(2)11-14-12-15(22)5-6-16(14)17(19)7-9-2
<b>InchiKey:</b>	WZDGZWOAQTVYBX-UHFFFAOYSA-N
<b>Formula:</b>	C21H28O2
<b>SMILES:</b>	C#CC1(O)CCC2C3C(C)CC4=C(CCC(=O)C4)C3CCC21C
<b>Mol. weight [g/mol]:</b>	312.45
<b>CAS:</b>	5630-53-5

## Physical Properties

Property code	Value	Unit	Source
gf	256.40	kJ/mol	Joback Method
hf	-189.76	kJ/mol	Joback Method
hfus	28.75	kJ/mol	Joback Method
hvap	82.33	kJ/mol	Joback Method
log10ws	-5.29		Crippen Method
logp	3.883		Crippen Method
mcvol	257.850	ml/mol	McGowan Method
pc	1916.94	kPa	Joback Method
tb	878.57	K	Joback Method
tc	1120.72	K	Joback Method
tf	621.72	K	Joback Method
vc	0.968	m3/kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	905.12	J/molxK	878.57	Joback Method
cpg	929.95	J/molxK	918.93	Joback Method
cpg	955.15	J/molxK	959.29	Joback Method
cpg	981.07	J/molxK	999.64	Joback Method
cpg	1008.05	J/molxK	1040.00	Joback Method
cpg	1036.46	J/molxK	1080.36	Joback Method

## Sources

<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>
<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=C5630535&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C5630535&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>

## 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>mcvol:</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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