

# 17Alpha-ethyl-3-methoxyestra-1,3,5(10)-trien-17b

<b>Other names:</b>	3-methoxy-19-nor-17-«alpha»-pregna-1,3,5(10)-trien-17-«beta»-ol
<b>Inchi:</b>	InChI=1S/C21H30O2/c1-4-21(22)12-10-19-18-7-5-14-13-15(23-3)6-8-16(14)17(18)9-11-2
<b>InchiKey:</b>	NVYBDSYHTNOJSQ-UHFFFAOYSA-N
<b>Formula:</b>	C21H30O2
<b>SMILES:</b>	CCC1(O)CCC2C3CCc4cc(OC)ccc4C3CCC21C
<b>Mol. weight [g/mol]:</b>	314.46
<b>CAS:</b>	17550-03-7

## Physical Properties

Property code	Value	Unit	Source
gf	108.92	kJ/mol	Joback Method
hf	-351.75	kJ/mol	Joback Method
hfus	28.44	kJ/mol	Joback Method
hvap	82.19	kJ/mol	Joback Method
log10ws	-5.68		Crippen Method
logp	4.692		Crippen Method
mcvol	262.150	ml/mol	McGowan Method
pc	1744.82	kPa	Joback Method
tb	851.02	K	Joback Method
tc	1074.69	K	Joback Method
tf	547.04	K	Joback Method
vc	0.990	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	892.71	J/molxK	851.02	Joback Method
cpg	915.50	J/molxK	888.30	Joback Method
cpg	938.47	J/molxK	925.58	Joback Method
cpg	961.92	J/molxK	962.86	Joback Method
cpg	986.14	J/molxK	1000.13	Joback Method
cpg	1011.43	J/molxK	1037.41	Joback Method
cpg	1038.09	J/molxK	1074.69	Joback Method

# Sources

<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=C17550037&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C17550037&amp;Units=SI</a>
<b>Crippen Method:</b>	<a href="http://pubs.acs.org/doi/abs/10.1021/ci990307l">http://pubs.acs.org/doi/abs/10.1021/ci990307l</a>
<b>Crippen Method:</b>	<a href="https://www.cheméo.com/doc/models/crippen_log10ws">https://www.cheméo.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>

# 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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