

# Androsten-17-(beta)-ol-3-one, 17(alpha)-methyl-delta<sup>4</sup>-

<b>Other names:</b>	Androsten-17-(beta)-ol-3-one, 17(alpha)-methyl-delta
<b>Inchi:</b>	InChI=1S/C20H30O2/c1-18-9-6-14(21)12-13(18)4-5-15-16(18)7-10-19(2)17(15)8-11-20(1)
<b>InchiKey:</b>	GCKMFJBGXUYNAG-UHFFFAOYSA-N
<b>Formula:</b>	C20H30O2
<b>SMILES:</b>	CC12CCC(=O)C=C1CCC1C2CCC2(C)C1CCC2(C)O
<b>Mol. weight [g/mol]:</b>	302.45
<b>CAS:</b>	2607-14-9

## Physical Properties

Property code	Value	Unit	Source
gf	29.05	kJ/mol	Joback Method
hf	-434.31	kJ/mol	Joback Method
hfus	17.28	kJ/mol	Joback Method
hvap	78.43	kJ/mol	Joback Method
log10ws	-5.07		Crippen Method
logp	4.269		Crippen Method
mcvol	252.360	ml/mol	McGowan Method
pc	1930.44	kPa	Joback Method
tb	860.83	K	Joback Method
tc	1100.51	K	Joback Method
tf	574.86	K	Joback Method
vc	0.948	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	898.24	J/molxK	860.83	Joback Method
cpg	925.32	J/molxK	900.78	Joback Method
cpg	953.37	J/molxK	940.72	Joback Method
cpg	982.85	J/molxK	980.67	Joback Method
cpg	1014.21	J/molxK	1020.62	Joback Method
cpg	1047.90	J/molxK	1060.56	Joback Method
cpg	1084.38	J/molxK	1100.51	Joback Method

# Sources

<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=C2607149&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C2607149&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>hvp:</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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