

# 3Beta-hydroxyandrost-4-en-17-one

<b>Inchi:</b>	InChI=1S/C19H28O2/c1-18-9-7-13(20)11-12(18)3-4-14-15-5-6-17(21)19(15,2)10-8-16(14)
<b>InchiKey:</b>	VMYTXBKVYDESSJ-UHFFFAOYSA-N
<b>Formula:</b>	C19H28O2
<b>SMILES:</b>	CC12CCC3C(CCC4=CC(O)CCC43C)C1CCC2=O
<b>Mol. weight [g/mol]:</b>	288.42
<b>CAS:</b>	571-44-8

## Physical Properties

Property code	Value	Unit	Source
gf	26.12	kJ/mol	Joback Method
hf	-428.91	kJ/mol	Joback Method
hfus	20.98	kJ/mol	Joback Method
hvap	77.36	kJ/mol	Joback Method
log10ws	-4.66		Crippen Method
logp	3.879		Crippen Method
mcvol	238.270	ml/mol	McGowan Method
pc	2019.95	kPa	Joback Method
tb	837.71	K	Joback Method
tc	1074.12	K	Joback Method
tf	539.69	K	Joback Method
vc	0.893	m3/kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	839.35	J/molxK	837.71	Joback Method
cpg	863.19	J/molxK	877.11	Joback Method
cpg	887.01	J/molxK	916.51	Joback Method
cpg	911.12	J/molxK	955.91	Joback Method
cpg	935.84	J/molxK	995.32	Joback Method
cpg	961.51	J/molxK	1034.72	Joback Method
cpg	988.44	J/molxK	1074.12	Joback Method

# Sources

<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>
<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=C571448&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C571448&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>

# 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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