

# Androstane-11,17-dione, 3-hydroxy-, (3«alpha»,5«alpha»)-

Other names:

5«alpha»-Androstane-11,17-dione, 3«alpha»-hydroxy-

Ba 2683

11-Oxoandrosterone

11-Ketoandrosterone

**Inchi:** InChI=1S/C19H28O3/c1-18-8-7-12(20)9-11(18)3-4-13-14-5-6-16(22)19(14,2)10-15(21)17

**InchiKey:** IUNYGQONJQTULL-XROONHRISA-N

**Formula:** C19H28O3

**SMILES:** CC12CC(=O)C3C(CCC4CC(O)CCC43C)C1CCC2=O

**Mol. weight [g/mol]:** 304.42

**CAS:** 1231-82-9

## Physical Properties

Property code	Value	Unit	Source
gf	-124.51	kJ/mol	Joback Method
hf	-633.26	kJ/mol	Joback Method
hfus	20.73	kJ/mol	Joback Method
hvap	80.34	kJ/mol	Joback Method
log10ws	-3.84		Crippen Method
logp	3.138		Crippen Method
mcvol	244.140	ml/mol	McGowan Method
pc	1985.89	kPa	Joback Method
tb	896.72	K	Joback Method
tc	1140.10	K	Joback Method
tf	590.39	K	Joback Method
vc	0.913	m3/kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	913.93	J/molxK	896.72	Joback Method
cpg	939.35	J/molxK	937.28	Joback Method
cpg	964.88	J/molxK	977.85	Joback Method
cpg	990.81	J/molxK	1018.41	Joback Method
cpg	1017.44	J/molxK	1058.97	Joback Method

cpg	1045.09	J/mol×K	1099.53	Joback Method
cpg	1074.05	J/mol×K	1140.10	Joback Method

## Sources

<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=C1231829&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C1231829&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>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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