

# 3-Oxa-a-nor-5alpha-androstane-2-one, 5,17beta-dihydroxy-

<b>Inchi:</b>	InChI=1S/C17H26O4/c1-15-7-6-12-10(11(15)3-4-13(15)18)5-8-17(20)16(12,2)9-14(19)21
<b>InchiKey:</b>	WAJSBKRXXSZNLG-UHFFFAOYSA-N
<b>Formula:</b>	C17H26O4
<b>SMILES:</b>	CC12CCC3C(CCC4(O)OC(=O)CC34C)C1CCC2O
<b>Mol. weight [g/mol]:</b>	294.39
<b>CAS:</b>	3656-95-9

## Physical Properties

Property code	Value	Unit	Source
gf	-235.09	kJ/mol	Joback Method
hf	-717.11	kJ/mol	Joback Method
hfus	23.91	kJ/mol	Joback Method
hvap	91.51	kJ/mol	Joback Method
log10ws	-3.42		Crippen Method
logp	2.225		Crippen Method
mcvol	226.130	ml/mol	McGowan Method
pc	2540.49	kPa	Joback Method
tb	898.24	K	Joback Method
tc	1125.37	K	Joback Method
tf	614.44	K	Joback Method
vc	0.841	m3/kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	850.72	J/molxK	898.24	Joback Method
cpg	875.42	J/molxK	936.09	Joback Method
cpg	901.48	J/molxK	973.95	Joback Method
cpg	929.28	J/molxK	1011.80	Joback Method
cpg	959.19	J/molxK	1049.66	Joback Method
cpg	991.60	J/molxK	1087.51	Joback Method
cpg	1026.89	J/molxK	1125.37	Joback Method

# Sources

<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=C3656959&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C3656959&amp;Units=SI</a>
<b>Crippen Method:</b>	<a href="http://pubs.acs.org/doi/abs/10.1021/ci990307I">http://pubs.acs.org/doi/abs/10.1021/ci990307I</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>mccvol:</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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