

# 3-Hydroxy-17alpha-oxa-d-homoestra-1,3,5(10),6,8

<b>Inchi:</b>	InChI=1S/C18H18O3/c1-18-9-8-14-13-5-3-12(19)10-11(13)2-4-15(14)16(18)6-7-17(20)2
<b>InchiKey:</b>	CNAZCZPBIZXVKY-UHFFFAOYSA-N
<b>Formula:</b>	C18H18O3
<b>SMILES:</b>	CC12CCc3c(ccc4cc(O)ccc34)C1CCC(=O)O2
<b>Mol. weight [g/mol]:</b>	282.33
<b>CAS:</b>	101790-02-7

## Physical Properties

Property code	Value	Unit	Source
gf	28.96	kJ/mol	Joback Method
hf	-308.68	kJ/mol	Joback Method
hfus	31.70	kJ/mol	Joback Method
hvap	81.69	kJ/mol	Joback Method
log10ws	-4.83		Crippen Method
logp	3.671		Crippen Method
mcvol	212.850	ml/mol	McGowan Method
pc	2859.68	kPa	Joback Method
tb	864.51	K	Joback Method
tc	1136.77	K	Joback Method
tf	636.03	K	Joback Method
vc	0.748	m3/kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	684.87	J/molxK	864.51	Joback Method
cpg	704.28	J/molxK	909.89	Joback Method
cpg	723.96	J/molxK	955.26	Joback Method
cpg	744.30	J/molxK	1000.64	Joback Method
cpg	765.71	J/molxK	1046.02	Joback Method
cpg	788.57	J/molxK	1091.40	Joback Method
cpg	813.28	J/molxK	1136.77	Joback Method

# Sources

<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=C101790027&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C101790027&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.chemeo.com/doc/models/crippen_log10ws">https://www.chemeo.com/doc/models/crippen_log10ws</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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