

# Estrone, formate

<b>Inchi:</b>	InChI=1S/C19H22O3/c1-19-9-8-15-14-5-3-13(22-11-20)10-12(14)2-4-16(15)17(19)6-7-18
<b>InchiKey:</b>	GOZPPZIUYYOIF-UHFFFAOYSA-N
<b>Formula:</b>	C19H22O3
<b>SMILES:</b>	CC12CCC3c4ccc(OC=O)cc4CCC3C1CCC2=O
<b>Mol. weight [g/mol]:</b>	298.38

## Physical Properties

Property code	Value	Unit	Source
gf	19.99	kJ/mol	Joback Method
hf	-376.42	kJ/mol	Joback Method
hfus	26.19	kJ/mol	Joback Method
hvap	73.49	kJ/mol	Joback Method
log10ws	-4.52		Crippen Method
logp	3.647		Crippen Method
mcvol	231.240	ml/mol	McGowan Method
pc	2071.76	kPa	Joback Method
rinqol	2359.00		NIST Webbook
tb	833.99	K	Joback Method
tc	1083.50	K	Joback Method
tf	554.24	K	Joback Method
vc	0.885	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	761.43	J/molxK	833.99	Joback Method
cpg	781.95	J/molxK	875.58	Joback Method
cpg	801.79	J/molxK	917.16	Joback Method
cpg	821.15	J/molxK	958.75	Joback Method
cpg	840.27	J/molxK	1000.33	Joback Method
cpg	859.38	J/molxK	1041.92	Joback Method
cpg	878.71	J/molxK	1083.50	Joback Method

# Sources

<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=U368352&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U368352&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>

# 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>rinpola:</b>	Non-polar retention indices
<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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