

# Estra-1,3,5(10)-triene-3,11,17-triol, (11 «alpha»,17 «beta»)-

<b>Inchi:</b>	InChI=1S/C18H24O3/c1-18-9-15(20)17-12-5-3-11(19)8-10(12)2-4-13(17)14(18)6-7-16(18)
<b>InchiKey:</b>	IGPOPFXCXSGWCLM-UHFFFAOYSA-N
<b>Formula:</b>	C18H24O3
<b>SMILES:</b>	CC12CC(O)C3c4ccc(O)cc4CCC3C1CCC2O
<b>Mol. weight [g/mol]:</b>	288.38
<b>CAS:</b>	1464-61-5

## Physical Properties

Property code	Value	Unit	Source
gf	-95.37	kJ/mol	Joback Method
hf	-511.26	kJ/mol	Joback Method
hfus	37.11	kJ/mol	Joback Method
hvap	102.98	kJ/mol	Joback Method
log10ws	-3.65		Crippen Method
logp	2.580		Crippen Method
mcvol	225.750	ml/mol	McGowan Method
pc	2738.28	kPa	Joback Method
tb	922.87	K	Joback Method
tc	1147.96	K	Joback Method
tf	622.88	K	Joback Method
vc	0.789	m3/kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	816.84	J/molxK	922.87	Joback Method
cpg	835.77	J/molxK	960.38	Joback Method
cpg	855.14	J/molxK	997.90	Joback Method
cpg	875.20	J/molxK	1035.41	Joback Method
cpg	896.22	J/molxK	1072.93	Joback Method
cpg	918.44	J/molxK	1110.44	Joback Method
cpg	942.13	J/molxK	1147.96	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=C1464615&amp;Mask=8">http://webbook.nist.gov/cgi/cbook.cgi?ID=C1464615&amp;Mask=8</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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