

# Estran-4-on-17B-ol

**Inchi:** InChI=1S/C18H28O2/c1-18-10-9-12-11-3-2-4-16(19)14(11)6-5-13(12)15(18)7-8-17(18)20  
**InchiKey:** LJZJXYCOLLINLR-RYYDINKKSA-N  
**Formula:** C18H28O2  
**SMILES:** CC12CCC3C4CCCC(=O)C4CCC3C1CCC2O  
**Mol. weight [g/mol]:** 276.41

## Physical Properties

Property code	Value	Unit	Source
gf	-4.85	kJ/mol	Joback Method
hf	-490.16	kJ/mol	Joback Method
hfus	24.93	kJ/mol	Joback Method
hvap	75.02	kJ/mol	Joback Method
log10ws	-4.14		Crippen Method
logp	3.569		Crippen Method
mcvol	228.480	ml/mol	McGowan Method
pc	2014.51	kPa	Joback Method
rinpol	2510.00		NIST Webbook
rinpol	2510.00		NIST Webbook
tb	805.78	K	Joback Method
tc	1036.50	K	Joback Method
tf	487.00	K	Joback Method
vc	0.853	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	813.75	J/mol×K	805.78	Joback Method
cpg	836.59	J/mol×K	844.23	Joback Method
cpg	858.43	J/mol×K	882.69	Joback Method
cpg	879.47	J/mol×K	921.14	Joback Method
cpg	899.90	J/mol×K	959.59	Joback Method
cpg	919.91	J/mol×K	998.05	Joback Method
cpg	939.69	J/mol×K	1036.50	Joback Method

# Sources

<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=R5653&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=R5653&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>hvp:</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>rinp:</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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