

# 5A-Estran-3-on-17B-ol, 17A-ethyl

<b>Inchi:</b>	InChI=1S/C20H32O2/c1-3-20(22)11-9-18-17-6-4-13-12-14(21)5-7-15(13)16(17)8-10-19(
<b>InchiKey:</b>	IOLODVBMNDJVOP-PPHAMSMSSA-N
<b>Formula:</b>	C20H32O2
<b>SMILES:</b>	CCC1(O)CCC2C3CCC4CC(=O)CCC4C3CCC21C
<b>Mol. weight [g/mol]:</b>	304.47

## Physical Properties

Property code	Value	Unit	Source
gf	6.50	kJ/mol	Joback Method
hf	-516.20	kJ/mol	Joback Method
hfus	23.81	kJ/mol	Joback Method
hvap	78.32	kJ/mol	Joback Method
log10ws	-4.98		Crippen Method
logp	4.349		Crippen Method
mvol	256.660	ml/mol	McGowan Method
pc	1772.85	kPa	Joback Method
rinpol	2535.00		NIST Webbook
tb	851.78	K	Joback Method
tc	1082.72	K	Joback Method
tf	533.44	K	Joback Method
vc	0.963	m3/kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	933.14	J/molxK	851.78	Joback Method
cpg	958.57	J/molxK	890.27	Joback Method
cpg	983.88	J/molxK	928.76	Joback Method
cpg	1009.37	J/molxK	967.25	Joback Method
cpg	1035.35	J/molxK	1005.74	Joback Method
cpg	1062.10	J/molxK	1044.23	Joback Method
cpg	1089.95	J/molxK	1082.72	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=R5548&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=R5548&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>mccvol:</b>	McGowan's characteristic volume
<b>pc:</b>	Critical Pressure
<b>rinpol:</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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