

# 1,3,5(10)-Oestratriene

<b>Inchi:</b>	InChI=1S/C18H24/c1-18-11-4-7-17(18)16-9-8-13-5-2-3-6-14(13)15(16)10-12-18/h2-3,5-6
<b>InchiKey:</b>	HLCRYAZDZCJZFG-WNRNVDISSA-N
<b>Formula:</b>	C18H24
<b>SMILES:</b>	CC12CCCC1C1CCc3ccccc3C1CC2
<b>Mol. weight [g/mol]:</b>	240.38

## Physical Properties

Property code	Value	Unit	Source
gf	348.31	kJ/mol	Joback Method
hf	11.19	kJ/mol	Joback Method
hfus	21.01	kJ/mol	Joback Method
hvap	57.22	kJ/mol	Joback Method
log10ws	-5.35		Crippen Method
logp	4.933		Crippen Method
mvol	208.140	ml/mol	McGowan Method
pc	2108.07	kPa	Joback Method
rinpol	2075.00		NIST Webbook
rinpol	2020.00		NIST Webbook
tb	667.23	K	Joback Method
tc	915.18	K	Joback Method
tf	398.00	K	Joback Method
vc	0.787	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	616.13	J/mol×K	667.23	Joback Method
cpg	640.17	J/mol×K	708.55	Joback Method
cpg	662.68	J/mol×K	749.88	Joback Method
cpg	683.93	J/mol×K	791.20	Joback Method
cpg	704.25	J/mol×K	832.53	Joback Method
cpg	723.92	J/mol×K	873.85	Joback Method
cpg	743.26	J/mol×K	915.18	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=R523801&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=R523801&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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