

# 17-«beta»-Hydroxy-7-«alpha»,17-«alpha»-dimethyl

<b>Inchi:</b>	InChI=1S/C21H34O2/c1-13-11-14-12-15(22)5-8-19(14,2)16-6-9-20(3)17(18(13)16)7-10-2
<b>InchiKey:</b>	OXGWMWXYFIDNLU-JJQLRENSA-N
<b>Formula:</b>	C21H34O2
<b>SMILES:</b>	CC1CC2CC(=O)CCC2(C)C2CCC3(C)C(CCC3(C)O)C12
<b>Mol. weight [g/mol]:</b>	318.49

## Physical Properties

Property code	Value	Unit	Source
gf	1.72	kJ/mol	Joback Method
hf	-541.94	kJ/mol	Joback Method
hfus	21.17	kJ/mol	Joback Method
hvap	79.09	kJ/mol	Joback Method
log10ws	-5.16		Crippen Method
logp	4.595		Crippen Method
mcvol	270.750	ml/mol	McGowan Method
pc	1653.80	kPa	Joback Method
rinsol	2657.00		NIST Webbook
tb	870.23	K	Joback Method
tc	1104.48	K	Joback Method
tf	564.37	K	Joback Method
vc	1.016	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	997.14	J/molxK	870.23	Joback Method
cpg	1026.10	J/molxK	909.27	Joback Method
cpg	1055.81	J/molxK	948.31	Joback Method
cpg	1086.69	J/molxK	987.36	Joback Method
cpg	1119.15	J/molxK	1026.40	Joback Method
cpg	1153.61	J/molxK	1065.44	Joback Method
cpg	1190.49	J/molxK	1104.48	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=R257415&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=R257415&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>
<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>hvac:</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>mccol:</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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