

# 16Beta-hydroxymethyl-5alpha,17alpha-pregnan-3

<b>Inchi:</b>	InChI=1S/C22H34O3/c1-13(24)20-14(12-23)10-19-17-5-4-15-11-16(25)6-8-21(15,2)18(1
<b>InchiKey:</b>	YPNOLIWRANPJKU-UHFFFAOYSA-N
<b>Formula:</b>	C22H34O3
<b>SMILES:</b>	CC(=O)C1C(CO)CC2C3CCC4CC(=O)CCC4(C)C3CCC21C
<b>Mol. weight [g/mol]:</b>	346.50
<b>CAS:</b>	96707-44-7

## Physical Properties

Property code	Value	Unit	Source
gf	-113.29	kJ/mol	Joback Method
hf	-690.40	kJ/mol	Joback Method
hfus	31.66	kJ/mol	Joback Method
hvap	89.21	kJ/mol	Joback Method
log10ws	-4.50		Crippen Method
logp	4.022		Crippen Method
mcvol	286.410	ml/mol	McGowan Method
pc	1553.67	kPa	Joback Method
tb	946.74	K	Joback Method
tc	1179.59	K	Joback Method
tf	601.67	K	Joback Method
vc	1.079	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1093.02	J/molxK	946.74	Joback Method
cpg	1120.11	J/molxK	985.55	Joback Method
cpg	1147.62	J/molxK	1024.36	Joback Method
cpg	1175.84	J/molxK	1063.17	Joback Method
cpg	1205.08	J/molxK	1101.98	Joback Method
cpg	1235.65	J/molxK	1140.79	Joback Method
cpg	1267.85	J/molxK	1179.59	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=C96707447&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C96707447&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>

# 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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