

# Pregnane-3,20-diol, (3«alpha»,5«beta»)-

<b>Other names:</b>	Pregnan-3«alpha»,20-diol, (5«beta»)- 5«beta»-Pregnane-3«alpha»,20-diol 5«beta»-Pregnan-3«alpha»,20-diol
<b>Inchi:</b>	InChI=1S/C21H36O2/c1-13(22)17-6-7-18-16-5-4-14-12-15(23)8-10-20(14,2)19(16)9-11-2
<b>InchiKey:</b>	YWYQTGBBEZQBGO-UHFFFAOYSA-N
<b>Formula:</b>	C21H36O2
<b>SMILES:</b>	CC(O)C1CCC2C3CCC4CC(O)CCC4(C)C3CCC12C
<b>Mol. weight [g/mol]:</b>	320.51
<b>CAS:</b>	55569-11-4

## Physical Properties

Property code	Value	Unit	Source
gf	-9.46	kJ/mol	Joback Method
hf	-576.99	kJ/mol	Joback Method
hfus	28.53	kJ/mol	Joback Method
hvap	92.28	kJ/mol	Joback Method
log10ws	-5.25		Crippen Method
logp	4.387		Crippen Method
mcvol	275.050	ml/mol	McGowan Method
pc	1681.03	kPa	Joback Method
tb	893.91	K	Joback Method
tc	1109.08	K	Joback Method
tf	518.07	K	Joback Method
vc	1.024	m3/kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1035.23	J/molxK	893.91	Joback Method
cpg	1060.13	J/molxK	929.77	Joback Method
cpg	1085.24	J/molxK	965.63	Joback Method
cpg	1110.84	J/molxK	1001.50	Joback Method
cpg	1137.20	J/molxK	1037.36	Joback Method
cpg	1164.59	J/molxK	1073.22	Joback Method

## Sources

<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>
<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=C55569114&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C55569114&amp;Units=SI</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>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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