

# 5-«alpha»-Pregnane-20-«beta»,21-diol

<b>Inchi:</b>	InChI=1S/C21H36O2/c1-20-11-4-3-5-14(20)6-7-15-16-8-9-18(19(23)13-22)21(16,2)12-10
<b>InchiKey:</b>	QUQBOXYLXZAONE-JJCUVKMUSA-N
<b>Formula:</b>	C21H36O2
<b>SMILES:</b>	CC12CCCCC1CCC1C2CCC2(C)C(C(O)CO)CCC12
<b>Mol. weight [g/mol]:</b>	320.51

## Physical Properties

Property code	Value	Unit	Source
gf	-1.75	kJ/mol	Joback Method
hf	-556.65	kJ/mol	Joback Method
hfus	27.46	kJ/mol	Joback Method
hvap	92.59	kJ/mol	Joback Method
log10ws	-5.14		Crippen Method
logp	4.389		Crippen Method
mcvol	275.050	ml/mol	McGowan Method
pc	1727.46	kPa	Joback Method
rinpol	2700.00		NIST Webbook
tb	898.58	K	Joback Method
tc	1114.14	K	Joback Method
tf	522.31	K	Joback Method
vc	1.024	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1032.05	J/mol×K	898.58	Joback Method
cpg	1056.87	J/mol×K	934.51	Joback Method
cpg	1081.99	J/mol×K	970.43	Joback Method
cpg	1107.71	J/mol×K	1006.36	Joback Method
cpg	1134.30	J/mol×K	1042.29	Joback Method
cpg	1162.06	J/mol×K	1078.21	Joback Method
cpg	1191.26	J/mol×K	1114.14	Joback Method

# Sources

<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=R149894&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=R149894&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>
<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>

# 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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