

# 3«alpha»,17«alpha»,21-trihydroxy-5«alpha»-pregn

**Inchi:** InChI=1S/C19H28O5/c20-9-17(23)19(24)6-5-13-14-3-1-10-7-11(21)2-4-12(10)18(14)16(2)  
**InchiKey:** OHOZNBWGXMNTTI-GCSXCLADSA-N  
**Formula:** C19H28O5  
**SMILES:** O=C1CC2C(CCC2(O)C(=O)CO)C2CCC3CC(O)CCC3C12  
**Mol. weight [g/mol]:** 336.42

## Physical Properties

Property code	Value	Unit	Source
gf	-406.70	kJ/mol	Joback Method
hf	-948.18	kJ/mol	Joback Method
hfus	38.37	kJ/mol	Joback Method
hvap	117.04	kJ/mol	Joback Method
log10ws	-2.48		Crippen Method
logp	1.081		Crippen Method
mvol	255.880	ml/mol	McGowan Method
pc	2246.13	kPa	Joback Method
rinpol	3030.00		NIST Webbook
rinpol	3030.00		NIST Webbook
tb	1062.22	K	Joback Method
tc	1300.50	K	Joback Method
tf	665.60	K	Joback Method
vc	0.952	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1037.83	J/mol×K	1062.22	Joback Method
cpg	1058.28	J/mol×K	1101.93	Joback Method
cpg	1078.85	J/mol×K	1141.65	Joback Method
cpg	1099.75	J/mol×K	1181.36	Joback Method
cpg	1121.17	J/mol×K	1221.07	Joback Method
cpg	1143.34	J/mol×K	1260.79	Joback Method
cpg	1166.47	J/mol×K	1300.50	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=R248941&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=R248941&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.cheméo.com/doc/models/crippen_log10ws">https://www.cheméo.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>h vap:</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>r in pol:</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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