

# 3Beta,6alpha-dihydroxy-5alpha-pregn-16-en-20-one

<b>Inchi:</b>	InChI=1S/C21H32O3/c1-12(22)15-4-5-16-14-11-19(24)18-10-13(23)6-8-21(18,3)17(14)7
<b>InchiKey:</b>	QLXYXLYKQOXYXNA-UHFFFAOYSA-N
<b>Formula:</b>	C21H32O3
<b>SMILES:</b>	CC(=O)C1=CCC2C3CC(O)C4CC(O)CCC4(C)C3CCC12C
<b>Mol. weight [g/mol]:</b>	332.48
<b>CAS:</b>	14424-67-0

## Physical Properties

Property code	Value	Unit	Source
gf	-115.61	kJ/mol	Joback Method
hf	-637.98	kJ/mol	Joback Method
hfus	34.48	kJ/mol	Joback Method
hvap	100.37	kJ/mol	Joback Method
log10ws	-4.63		Crippen Method
logp	3.486		Crippen Method
mcvol	272.320	ml/mol	McGowan Method
pc	1790.91	kPa	Joback Method
tb	952.36	K	Joback Method
tc	1175.14	K	Joback Method
tf	596.28	K	Joback Method
vc	1.022	m3/kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1031.69	J/molxK	952.36	Joback Method
cpg	1056.70	J/molxK	989.49	Joback Method
cpg	1082.46	J/molxK	1026.62	Joback Method
cpg	1109.28	J/molxK	1063.75	Joback Method
cpg	1137.44	J/molxK	1100.88	Joback Method
cpg	1167.25	J/molxK	1138.01	Joback Method
cpg	1198.99	J/molxK	1175.14	Joback Method

# Sources

<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=C14424670&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C14424670&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>

# 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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