

# 5-Pregnen-3«beta»-ol-20-one, propionate

<b>Inchi:</b>	InChI=1S/C24H36O3/c1-5-22(26)27-17-10-12-23(3)16(14-17)6-7-18-20-9-8-19(15(2)25)2
<b>InchiKey:</b>	YDVRGLSUPTYULK-UHFFFAOYSA-N
<b>Formula:</b>	C24H36O3
<b>SMILES:</b>	CCC(=O)OC1CCC2(C)C(=CCC3C2CCC2(C)C(C(C)=O)CCC32)C1
<b>Mol. weight [g/mol]:</b>	372.54

## Physical Properties

Property code	Value	Unit	Source
gf	-42.92	kJ/mol	Joback Method
hf	-619.90	kJ/mol	Joback Method
hfus	35.79	kJ/mol	Joback Method
hvap	83.16	kJ/mol	Joback Method
log10ws	-6.11		Crippen Method
logp	5.476		Crippen Method
mcvol	310.290	ml/mol	McGowan Method
pc	1316.56	kPa	Joback Method
rinqol	2487.00		NIST Webbook
tb	917.60	K	Joback Method
tc	1152.04	K	Joback Method
tf	584.85	K	Joback Method
vc	1.177	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1123.33	J/molxK	917.60	Joback Method
cpg	1151.07	J/molxK	956.67	Joback Method
cpg	1179.11	J/molxK	995.75	Joback Method
cpg	1207.77	J/molxK	1034.82	Joback Method
cpg	1237.41	J/molxK	1073.89	Joback Method
cpg	1268.34	J/molxK	1112.97	Joback Method
cpg	1300.92	J/molxK	1152.04	Joback Method

# Sources

<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=U368371&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U368371&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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