

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

<b>Inchi:</b>	InChI=1S/C27H42O3/c1-5-6-7-8-25(29)30-20-13-15-26(3)19(17-20)9-10-21-23-12-11-22
<b>InchiKey:</b>	IBCXWBFTIJYFJY-UHFFFAOYSA-N
<b>Formula:</b>	C27H42O3
<b>SMILES:</b>	CCCCC(=O)OC1CCC2(C)C(=CCC3C2CCC2(C)C(C(C)=O)CCC3)C1
<b>Mol. weight [g/mol]:</b>	414.62

## Physical Properties

Property code	Value	Unit	Source
gf	-17.66	kJ/mol	Joback Method
hf	-681.82	kJ/mol	Joback Method
hfus	43.56	kJ/mol	Joback Method
hvap	89.83	kJ/mol	Joback Method
log10ws	-7.36		Crippen Method
logp	6.647		Crippen Method
mcvol	352.560	ml/mol	McGowan Method
pc	1079.22	kPa	Joback Method
rinpol	2715.00		NIST Webbook
rinpol	2715.00		NIST Webbook
tb	986.24	K	Joback Method
tc	1218.42	K	Joback Method
tf	618.66	K	Joback Method
vc	1.345	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1326.10	J/mol×K	986.24	Joback Method
cpg	1356.82	J/mol×K	1024.94	Joback Method
cpg	1388.25	J/mol×K	1063.63	Joback Method
cpg	1420.72	J/mol×K	1102.33	Joback Method
cpg	1454.57	J/mol×K	1141.02	Joback Method
cpg	1490.14	J/mol×K	1179.72	Joback Method
cpg	1527.78	J/mol×K	1218.42	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=U368373&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U368373&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>mcvol:</b>	McGowan's characteristic volume
<b>pc:</b>	Critical Pressure
<b>rinpola:</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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