

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

<b>Inchi:</b>	InChI=1S/C25H38O3/c1-5-6-23(27)28-18-11-13-24(3)17(15-18)7-8-19-21-10-9-20(16(2)2)
<b>InchiKey:</b>	DTHSTPZCWGYBFE-UHFFFAOYSA-N
<b>Formula:</b>	C25H38O3
<b>SMILES:</b>	CCCC(=O)OC1CCC2(C)C(=CCC3C2CCC2(C)C(C(C)=O)CCC3)C1
<b>Mol. weight [g/mol]:</b>	386.57

## Physical Properties

Property code	Value	Unit	Source
gf	-34.50	kJ/mol	Joback Method
hf	-640.54	kJ/mol	Joback Method
hfus	38.38	kJ/mol	Joback Method
hvap	85.38	kJ/mol	Joback Method
log10ws	-6.52		Crippen Method
logp	5.866		Crippen Method
mcvol	324.380	ml/mol	McGowan Method
pc	1229.42	kPa	Joback Method
rinpol	2546.00		NIST Webbook
tb	940.48	K	Joback Method
tc	1173.36	K	Joback Method
tf	596.12	K	Joback Method
vc	1.232	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1189.78	J/mol×K	940.48	Joback Method
cpg	1218.37	J/mol×K	979.29	Joback Method
cpg	1247.39	J/mol×K	1018.11	Joback Method
cpg	1277.17	J/mol×K	1056.92	Joback Method
cpg	1308.04	J/mol×K	1095.73	Joback Method
cpg	1340.33	J/mol×K	1134.54	Joback Method
cpg	1374.39	J/mol×K	1173.36	Joback Method

# Sources

<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=U368372&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U368372&amp;Units=SI</a>
<b>Crippen Method:</b>	<a href="http://pubs.acs.org/doi/abs/10.1021/ci990307I">http://pubs.acs.org/doi/abs/10.1021/ci990307I</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>hvac:</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>mccol:</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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