

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

**Inchi:** InChI=1S/C23H31F3O3/c1-13(27)17-6-7-18-16-5-4-14-12-15(29-20(28)23(24,25)26)8-10  
**InchiKey:** XMFYUFNYYIKKQW-UHFFFAOYSA-N  
**Formula:** C23H31F3O3  
**SMILES:** CC(=O)C1CCC2C3CC=C4CC(OC(=O)C(F)(F)F)CCC4(C)C3CCC12C  
**Mol. weight [g/mol]:** 412.49

## Physical Properties

Property code	Value	Unit	Source
gf	-632.93	kJ/mol	Joback Method
hf	-1196.34	kJ/mol	Joback Method
hfus	35.03	kJ/mol	Joback Method
hvap	77.18	kJ/mol	Joback Method
log10ws	-6.35		Crippen Method
logp	5.628		Crippen Method
mcvol	301.510	ml/mol	McGowan Method
pc	1297.66	kPa	Joback Method
tb	889.30	K	Joback Method
tc	1113.79	K	Joback Method
tf	577.77	K	Joback Method
vc	1.163	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1079.05	J/mol×K	889.30	Joback Method
cpg	1103.88	J/mol×K	926.71	Joback Method
cpg	1128.87	J/mol×K	964.13	Joback Method
cpg	1154.35	J/mol×K	1001.54	Joback Method
cpg	1180.62	J/mol×K	1038.96	Joback Method
cpg	1208.03	J/mol×K	1076.37	Joback Method
cpg	1236.87	J/mol×K	1113.79	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=U352614&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U352614&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>mcvol:</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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