

# Medrogestone

<b>Inchi:</b>	InChI=1S/C23H32O2/c1-14-12-17-18(21(3)9-6-16(25)13-20(14)21)7-11-23(5)19(17)8-10
<b>InchiKey:</b>	HCFSGRMEE XUOSS-UHFFFAOYSA-N
<b>Formula:</b>	C23H32O2
<b>SMILES:</b>	CC(=O)C1(C)CCC2C3C=C(C)C4=CC(=O)CCC4(C)C3CCC21C
<b>Mol. weight [g/mol]:</b>	340.51

## Physical Properties

Property code	Value	Unit	Source
gf	82.54	kJ/mol	Joback Method
hf	-410.27	kJ/mol	Joback Method
hfus	23.39	kJ/mol	Joback Method
hvap	76.13	kJ/mol	Joback Method
log10ws	-5.27		Aqueous Solubility Prediction Method
log10ws	-5.27		Estimated Solubility Method
logp	5.280		Crippen Method
mvol	286.030	ml/mol	McGowan Method
pc	1511.67	kPa	Joback Method
tb	895.30	K	Joback Method
tc	1147.57	K	Joback Method
tf	611.06	K	Joback Method
vc	1.089	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1008.98	J/molxK	895.30	Joback Method
cpg	1039.84	J/molxK	937.34	Joback Method
cpg	1072.07	J/molxK	979.39	Joback Method
cpg	1106.22	J/molxK	1021.43	Joback Method
cpg	1142.79	J/molxK	1063.48	Joback Method
cpg	1182.33	J/molxK	1105.52	Joback Method
cpg	1225.35	J/molxK	1147.57	Joback Method

# Sources

<b>Aqueous Solubility Prediction Method:</b>	<a href="http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa">http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa</a>
<b>Estimated Solubility Method:</b>	<a href="http://pubs.acs.org/doi/suppl/10.1021/ci034243x/suppl_file/ci034243xsi20040112_053635.txt">http://pubs.acs.org/doi/suppl/10.1021/ci034243x/suppl_file/ci034243xsi20040112_053635.txt</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>Crippen Method:</b>	<a href="http://pubs.acs.org/doi/abs/10.1021/ci990307I">http://pubs.acs.org/doi/abs/10.1021/ci990307I</a>
<b>Joback Method:</b>	<a href="https://en.wikipedia.org/wiki/Joback_method">https://en.wikipedia.org/wiki/Joback_method</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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