

# methyltestosterone acetate

<b>Inchi:</b>	InChI=1S/C22H32O3/c1-14(23)25-22(4)12-9-19-17-6-5-15-13-16(24)7-10-20(15,2)18(17)
<b>InchiKey:</b>	RLIONZRKXHAVFB-UHFFFAOYSA-N
<b>Formula:</b>	C22H32O3
<b>SMILES:</b>	CC(=O)OC1(C)CCC2C3CCC4=CC(=O)CCC4(C)C3CCC21C
<b>Mol. weight [g/mol]:</b>	344.49

## Physical Properties

Property code	Value	Unit	Source
gf	-51.21	kJ/mol	Joback Method
hf	-568.16	kJ/mol	Joback Method
hfus	21.15	kJ/mol	Joback Method
hvap	75.36	kJ/mol	Joback Method
log10ws	-5.28		Aqueous Solubility Prediction Method
log10ws	-5.28		Estimated Solubility Method
logp	4.840		Crippen Method
mcvol	282.110	ml/mol	McGowan Method
pc	1582.23	kPa	Joback Method
tb	890.70	K	Joback Method
tc	1141.56	K	Joback Method
tf	608.74	K	Joback Method
vc	1.065	m3/kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1007.38	J/molxK	890.70	Joback Method
cpg	1037.89	J/molxK	932.51	Joback Method
cpg	1069.55	J/molxK	974.32	Joback Method
cpg	1102.87	J/molxK	1016.13	Joback Method
cpg	1138.33	J/molxK	1057.94	Joback Method
cpg	1176.45	J/molxK	1099.75	Joback Method
cpg	1217.71	J/molxK	1141.56	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>Joback Method:</b>	<a href="https://en.wikipedia.org/wiki/Joback_method">https://en.wikipedia.org/wiki/Joback_method</a>
<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>

# 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>h vap:</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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