

# trans-Androsterone, pentafluoropropionate

**Inchi:** InChI=1S/C22H29F5O3/c1-19-9-7-13(30-18(29)21(23,24)22(25,26)27)11-12(19)3-4-14-1  
**InchiKey:** MDOSQUKLWNVMRK-UHFFFAOYSA-N  
**Formula:** C22H29F5O3  
**SMILES:** CC12CCC3C(CCC4CC(OC(=O)C(F)(F)C(F)(F)F)CCC43C)C1CCC2=O  
**Mol. weight [g/mol]:** 436.46

## Physical Properties

Property code	Value	Unit	Source
gf	-1042.13	kJ/mol	Joback Method
hf	-1648.10	kJ/mol	Joback Method
hfus	28.26	kJ/mol	Joback Method
hvap	68.58	kJ/mol	Joback Method
log10ws	-6.39		Crippen Method
logp	5.708		Crippen Method
mvol	295.260	ml/mol	McGowan Method
pc	1275.51	kPa	Joback Method
rmpol	2481.60		NIST Webbook
rmpol	2481.60		NIST Webbook
tb	871.54	K	Joback Method
tc	1094.33	K	Joback Method
tf	575.11	K	Joback Method
vc	1.147	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1077.09	J/molxK	871.54	Joback Method
cpg	1101.49	J/molxK	908.67	Joback Method
cpg	1125.80	J/molxK	945.80	Joback Method
cpg	1150.32	J/molxK	982.93	Joback Method
cpg	1175.37	J/molxK	1020.07	Joback Method
cpg	1201.25	J/molxK	1057.20	Joback Method
cpg	1228.26	J/molxK	1094.33	Joback Method

# Sources

<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=U352220&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U352220&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.cheméo.com/doc/models/crippen_log10ws">https://www.cheméo.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>

# 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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