

# Androsterone, TFA

**Inchi:** InChI=1S/C21H29F3O3/c1-19-9-7-13(27-18(26)21(22,23)24)11-12(19)3-4-14-15-5-6-17(20)  
**InchiKey:** NTPCFTHVUCOBOX-PGPSKLPQSA-N  
**Formula:** C21H29F3O3  
**SMILES:** CC12CCC3C(CCC4CC(OC(=O)C(F)(F)F)CCC43C)C1CCC2=O  
**Mol. weight [g/mol]:** 386.45

## Physical Properties

Property code	Value	Unit	Source
gf	-663.77	kJ/mol	Joback Method
hf	-1226.49	kJ/mol	Joback Method
hfus	26.93	kJ/mol	Joback Method
hvap	69.28	kJ/mol	Joback Method
log10ws	-5.66		Crippen Method
logp	5.072		Crippen Method
mvol	277.630	ml/mol	McGowan Method
pc	1442.44	kPa	Joback Method
rinpol	2372.00		NIST Webbook
tb	853.35	K	Joback Method
tc	1083.86	K	Joback Method
tf	560.24	K	Joback Method
vc	1.067	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	999.23	J/mol×K	853.35	Joback Method
cpg	1024.27	J/mol×K	891.77	Joback Method
cpg	1049.07	J/mol×K	930.19	Joback Method
cpg	1073.95	J/mol×K	968.60	Joback Method
cpg	1099.21	J/mol×K	1007.02	Joback Method
cpg	1125.16	J/mol×K	1045.44	Joback Method
cpg	1152.12	J/mol×K	1083.86	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=R305287&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=R305287&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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