

# Trans-androsterone, hexanoate

**Inchi:** InChI=1S/C25H40O3/c1-4-5-6-7-23(27)28-18-12-14-24(2)17(16-18)8-9-19-20-10-11-22(2)  
**InchiKey:** SMYVCRCXPSLNDH-UHFFFAOYSA-N  
**Formula:** C25H40O3  
**SMILES:** CCCCCC(=O)OC1CCC2(C)C(CCC3C4CCC(=O)C4(C)CCC32)C1  
**Mol. weight [g/mol]:** 388.58

## Physical Properties

Property code	Value	Unit	Source
gf	-48.50	kJ/mol	Joback Method
hf	-711.97	kJ/mol	Joback Method
hfus	35.46	kJ/mol	Joback Method
hvap	81.93	kJ/mol	Joback Method
log10ws	-6.67		Crippen Method
logp	6.090		Crippen Method
mvol	328.680	ml/mol	McGowan Method
pc	1188.24	kPa	Joback Method
rinpol	2597.00		NIST Webbook
rinpol	2597.00		NIST Webbook
tb	950.29	K	Joback Method
tc	1185.02	K	Joback Method
tf	601.13	K	Joback Method
vc	1.248	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1240.37	J/molxK	950.29	Joback Method
cpg	1270.15	J/molxK	989.41	Joback Method
cpg	1300.14	J/molxK	1028.53	Joback Method
cpg	1330.65	J/molxK	1067.65	Joback Method
cpg	1361.99	J/molxK	1106.77	Joback Method
cpg	1394.47	J/molxK	1145.89	Joback Method
cpg	1428.41	J/molxK	1185.02	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>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=U368383&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U368383&amp;Units=SI</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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