

# Trans-androsterone, octanoate

**Inchi:** InChI=1S/C27H44O3/c1-4-5-6-7-8-9-25(29)30-20-14-16-26(2)19(18-20)10-11-21-22-12-3  
**InchiKey:** BTEOMWNRKOOBJV-UHFFFAOYSA-N  
**Formula:** C27H44O3  
**SMILES:** CCCCCCCC(=O)OC1CCC2(C)C(CCC3C4CCC(=O)C4(C)CCC32)C1  
**Mol. weight [g/mol]:** 416.64

## Physical Properties

Property code	Value	Unit	Source
gf	-31.66	kJ/mol	Joback Method
hf	-753.25	kJ/mol	Joback Method
hfus	40.64	kJ/mol	Joback Method
hvap	86.38	kJ/mol	Joback Method
log10ws	-7.51		Crippen Method
logp	6.870		Crippen Method
mvol	356.860	ml/mol	McGowan Method
pc	1045.30	kPa	Joback Method
rinpol	2788.00		NIST Webbook
rinpol	2788.00		NIST Webbook
tb	996.05	K	Joback Method
tc	1230.12	K	Joback Method
tf	623.67	K	Joback Method
vc	1.359	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1378.22	J/molxK	996.05	Joback Method
cpg	1409.86	J/molxK	1035.06	Joback Method
cpg	1441.96	J/molxK	1074.07	Joback Method
cpg	1474.84	J/molxK	1113.09	Joback Method
cpg	1508.81	J/molxK	1152.10	Joback Method
cpg	1544.21	J/molxK	1191.11	Joback Method
cpg	1581.33	J/molxK	1230.12	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=U368385&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U368385&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>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>r in pol:</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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