

# Androst-2-en-4-one, 17-(tetrahydropyran-3-yl)oxy-

Inchi:	InChI=1S/C24H36O3/c1-23-12-3-6-21(25)20(23)8-7-17-18-9-10-22(24(18,2)13-11-19(17
InchiKey:	KFFGVJSLJVBNAO-UHFFFAOYSA-N
Formula:	C24H36O3
SMILES:	CC12CCC3C(CCC4C(=O)C=CCC43C)C1CCC2OC1CCCOC1
Mol. weight [g/mol]:	372.54

## Physical Properties

Property code	Value	Unit	Source
gf	40.29	kJ/mol	Joback Method
hf	-598.65	kJ/mol	Joback Method
hfus	32.31	kJ/mol	Joback Method
hvap	78.19	kJ/mol	Joback Method
log10ws	-5.42		Crippen Method
logp	4.938		Crippen Method
mcvol	303.730	ml/mol	McGowan Method
pc	1439.16	kPa	Joback Method
rinpol	2609.00		NIST Webbook
rinpol	2609.00		NIST Webbook
rinpol	2609.00		NIST Webbook
tb	919.20	K	Joback Method
tc	1178.14	K	Joback Method
tf	574.64	K	Joback Method
vc	1.125	m3/kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1152.04	J/molxK	919.20	Joback Method
cpg	1183.52	J/molxK	962.36	Joback Method
cpg	1214.95	J/molxK	1005.51	Joback Method
cpg	1246.74	J/molxK	1048.67	Joback Method
cpg	1279.31	J/molxK	1091.83	Joback Method
cpg	1313.09	J/molxK	1134.99	Joback Method
cpg	1348.50	J/molxK	1178.14	Joback Method

# Sources

<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=U195615&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U195615&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>

# 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>rinpolar:</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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