

# 14-Nor-cadin-5-en-4-one isomer A

<b>Inchi:</b>	InChI=1S/C14H22O/c1-9(2)12-6-4-10(3)13-7-5-11(15)8-14(12)13/h8-10,12-13H,4-7H2,1
<b>InchiKey:</b>	AQNMVDGKNNYA EW-LQN XFFKNSA-N
<b>Formula:</b>	C14H22O
<b>SMILES:</b>	CC(C)C1CCC(C)C2CCC(=O)C=C12
<b>Mol. weight [g/mol]:</b>	206.32

## Physical Properties

Property code	Value	Unit	Source
gf	27.69	kJ/mol	Joback Method
hf	-328.34	kJ/mol	Joback Method
hfus	17.78	kJ/mol	Joback Method
hvap	51.78	kJ/mol	Joback Method
log10ws	-3.64		Crippen Method
logp	3.594		Crippen Method
mvol	183.670	ml/mol	McGowan Method
pc	2121.68	kPa	Joback Method
ripol	2324.00		NIST Webbook
ripol	2324.00		NIST Webbook
tb	617.13	K	Joback Method
tc	846.53	K	Joback Method
tf	331.60	K	Joback Method
vc	0.688	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	511.90	J/mol×K	617.13	Joback Method
cpg	534.67	J/mol×K	655.36	Joback Method
cpg	556.06	J/mol×K	693.60	Joback Method
cpg	576.08	J/mol×K	731.83	Joback Method
cpg	594.76	J/mol×K	770.06	Joback Method
cpg	612.12	J/mol×K	808.30	Joback Method
cpg	628.19	J/mol×K	846.53	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=R420094&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=R420094&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>ripol:</b>	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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