

# L-Alanine, N-acetyl-

<b>Other names:</b>	Alanine, N-acetyl-, L-Acetylalanine N-Acetyl-L-alanine N-Acetyl-S-alanine N-Acetylalanine CH <sub>3</sub> CONHCH(CH <sub>3</sub> )COOH N-Acetyl-L-«alpha»-alanine 2-acetamidopropionic acid
<b>Inchi:</b>	InChI=1S/C5H9NO3/c1-3(5(8)9)6-4(2)7/h3H,1-2H3,(H,6,7)(H,8,9)/t3-/m1/s1
<b>InchiKey:</b>	KTHDTJVBEPMMGL-GSVUOUGTGSA-N
<b>Formula:</b>	C <sub>5</sub> H <sub>9</sub> NO <sub>3</sub>
<b>SMILES:</b>	CC(=O)NC(C)C(=O)O
<b>Mol. weight [g/mol]:</b>	131.13
<b>CAS:</b>	97-69-8

## Physical Properties

Property code	Value	Unit	Source
gf	-316.49	kJ/mol	Joback Method
hf	-475.73	kJ/mol	Joback Method
hfus	17.57	kJ/mol	Joback Method
hvap	62.94	kJ/mol	Joback Method
ie	9.20	eV	NIST Webbook
ie	9.65	eV	NIST Webbook
log10ws	-0.09		Crippen Method
logp	-0.404		Crippen Method
mcvol	100.300	ml/mol	McGowan Method
pc	4697.74	kPa	Joback Method
tb	563.45	K	Joback Method
tc	751.18	K	Joback Method
tf	344.45	K	Joback Method
vc	0.376	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	235.05	J/mol×K	563.45	Joback Method
cpg	242.87	J/mol×K	594.74	Joback Method
cpg	250.29	J/mol×K	626.03	Joback Method
cpg	257.32	J/mol×K	657.31	Joback Method
cpg	263.98	J/mol×K	688.60	Joback Method
cpg	270.25	J/mol×K	719.89	Joback Method
cpg	276.17	J/mol×K	751.18	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=C97698&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C97698&amp;Units=SI</a>
<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>

## 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>ie:</b>	Ionization energy
<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>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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