

# N-L-alanyl-L-valine

<b>Other names:</b>	L-alanyl-L-valine ala-val
<b>Inchi:</b>	InChI=1S/C8H16N2O3/c1-4(2)6(8(12)13)10-7(11)5(3)9/h4-6H,9H2,1-3H3,(H,10,11)(H,12)
<b>InchiKey:</b>	LIWMQSWFLXEGMA-WDSKDSINSA-N
<b>Formula:</b>	C8H16N2O3
<b>SMILES:</b>	CC(N)C(=O)NC(C(=O)O)C(C)C
<b>Mol. weight [g/mol]:</b>	188.22
<b>CAS:</b>	3303-45-5

## Physical Properties

Property code	Value	Unit	Source
basg	874.10	kJ/mol	NIST Webbook
gf	-229.66	kJ/mol	Joback Method
hf	-514.42	kJ/mol	Joback Method
hfus	23.49	kJ/mol	Joback Method
hvap	79.49	kJ/mol	Joback Method
log10ws	-0.65		Crippen Method
logp	-0.441		Crippen Method
mcvol	152.550	ml/mol	McGowan Method
pc	3568.53	kPa	Joback Method
tb	703.74	K	Joback Method
tc	900.15	K	Joback Method
tf	431.52	K	Joback Method
vc	0.560	m3/kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	430.34	J/molxK	703.74	Joback Method
cpg	440.75	J/molxK	736.48	Joback Method
cpg	450.52	J/molxK	769.21	Joback Method
cpg	459.68	J/molxK	801.95	Joback Method
cpg	468.26	J/molxK	834.68	Joback Method
cpg	476.26	J/molxK	867.42	Joback Method

## Sources

<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=C3303455&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C3303455&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.chemeo.com/doc/models/crippen_log10ws">https://www.chemeo.com/doc/models/crippen_log10ws</a>
<b>Solvation behaviour of dipeptides of alanine in aqueous solutions of ampicillin at different temperatures:</b>	<a href="https://www.doi.org/10.1016/j.tca.2013.09.006">https://www.doi.org/10.1016/j.tca.2013.09.006</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>

## Legend

<b>basg:</b>	Gas basicity
<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>m cvol:</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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