

# L-Alanine, N-[N-(N-L-alanyl-L-alanyl)-L-alanyl]-

<b>Other names:</b>	tetra-L-alanine N-L-alanyl-N-L-alanyl-N-L-alanyl-L-alanine
<b>Inchi:</b>	InChI=1S/C12H22N4O5/c1-5(13)9(17)14-6(2)10(18)15-7(3)11(19)16-8(4)12(20)21/h5-8H
<b>InchiKey:</b>	ZHRZLXZJVUFLNY-WCTZXKLSA-N
<b>Formula:</b>	C12H22N4O5
<b>SMILES:</b>	CC(N)C(O)=NC(C)C(O)=NC(C)C(O)=NC(C)C(=O)O
<b>Mol. weight [g/mol]:</b>	302.33
<b>CAS:</b>	926-79-4

## Physical Properties

Property code	Value	Unit	Source
basg	944.60	kJ/mol	NIST Webbook
hf	-782.55	kJ/mol	Joback Method
hvap	135.04	kJ/mol	Joback Method
log10ws	-0.78		Crippen Method
logp	0.453		Crippen Method
mcvol	232.010	ml/mol	McGowan Method
pc	2163.33	kPa	Joback Method
tb	1197.00	K	Joback Method
tc	1487.42	K	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=C926794&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C926794&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>
<b>Crippen Method:</b>	<a href="https://www.chemeo.com/doc/models/crippen_log10ws">https://www.chemeo.com/doc/models/crippen_log10ws</a>

## Legend

<b>basg:</b>	Gas basicity
<b>hf:</b>	Enthalpy of formation at standard conditions
<b>hvac:</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>tb:</b>	Normal Boiling Point Temperature
<b>tc:</b>	Critical Temperature

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