

# dl-Alanylglycylglycine

<b>Other names:</b>	Alanylglycylglycine (DL)
<b>Inchi:</b>	InChI=1S/C7H13N3O4/c1-4(8)7(14)10-2-5(11)9-3-6(12)13/h4H,2-3,8H2,1H3,(H,9,11)(H,
<b>InchiKey:</b>	VGPWRRFOPXVGOH-UHFFFAOYSA-N
<b>Formula:</b>	C7H13N3O4
<b>SMILES:</b>	CC(N)C(=O)NCC(=O)NCC(=O)O
<b>Mol. weight [g/mol]:</b>	203.20
<b>CAS:</b>	927-21-9

## Physical Properties

Property code	Value	Unit	Source
gf	-272.73	kJ/mol	Joback Method
hf	-542.33	kJ/mol	Joback Method
hfus	34.64	kJ/mol	Joback Method
hvap	91.22	kJ/mol	Joback Method
log10ws	0.67		Crippen Method
logp	-2.349		Crippen Method
mcvol	150.010	ml/mol	McGowan Method
pc	4339.67	kPa	Joback Method
tb	785.78	K	Joback Method
tc	986.65	K	Joback Method
tf	552.84	K	Joback Method
vc	0.557	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	434.08	J/mol×K	785.78	Joback Method
cpg	442.22	J/mol×K	819.26	Joback Method
cpg	449.77	J/mol×K	852.74	Joback Method
cpg	456.75	J/mol×K	886.21	Joback Method
cpg	463.18	J/mol×K	919.69	Joback Method
cpg	469.08	J/mol×K	953.17	Joback Method
cpg	474.47	J/mol×K	986.65	Joback Method
cps	236.00	J/mol×K	298.00	NIST Webbook

# 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=C927219&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C927219&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>cps:</b>	Solid phase 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>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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