

# dl-Citrulline

<b>Other names:</b>	Citrulline Citrulline, (dl) DL-2-amino-5-ureidovaleric acid DL-Ornithine, N(5)-(aminocarbonyl)- L-citruline N5-aminocarbonyl-L-ornithine N5-carbamyl-ornithine Ornithine, N5-carbamoyl-, DL-
<b>Inchi:</b>	InChI=1S/C6H13N3O3/c7-4(5(10)11)2-1-3-9-6(8)12/h4H,1-3,7H2,(H,10,11)(H3,8,9,12)
<b>InchiKey:</b>	RHGKLRLOHDJJDR-UHFFFAOYSA-N
<b>Formula:</b>	C6H13N3O3
<b>SMILES:</b>	NC(=O)NCCCC(N)C(=O)O
<b>Mol. weight [g/mol]:</b>	175.19
<b>CAS:</b>	627-77-0

## Physical Properties

Property code	Value	Unit	Source
gf	-175.17	kJ/mol	Joback Method
hf	-428.79	kJ/mol	Joback Method
hfus	30.55	kJ/mol	Joback Method
hvap	86.45	kJ/mol	Joback Method
log10ws	-0.36		Crippen Method
logp	-1.153		Crippen Method
mcvol	134.350	ml/mol	McGowan Method
pc	4815.84	kPa	Joback Method
ss	254.40	J/molxK	NIST Webbook
tb	731.39	K	Joback Method
tc	932.93	K	Joback Method
tf	522.24	K	Joback Method
vc	0.489	m3/kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
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cpg	382.27	J/mol×K	731.39	Joback Method
cpg	390.63	J/mol×K	764.98	Joback Method
cpg	398.45	J/mol×K	798.57	Joback Method
cpg	405.74	J/mol×K	832.16	Joback Method
cpg	412.52	J/mol×K	865.75	Joback Method
cpg	418.82	J/mol×K	899.34	Joback Method
cpg	424.65	J/mol×K	932.93	Joback Method
cps	232.80	J/mol×K	300.80	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>Solubility and Solution Thermodynamics of the d Form of Joback Method: Water + Ethanol Binary Solvent Mixtures:</b>	<a href="https://www.doi.org/10.1021/acs.jced.5b00585">https://www.doi.org/10.1021/acs.jced.5b00585</a>
<b>McGowan Method:</b>	<a href="https://en.wikipedia.org/wiki/Joback_method">https://en.wikipedia.org/wiki/Joback_method</a>
<b>NIST Webbook:</b>	<a href="http://link.springer.com/article/10.1007/BF02311772">http://link.springer.com/article/10.1007/BF02311772</a>
<b>Crippen Method:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=C627770&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C627770&amp;Units=SI</a>
	<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>mccvol:</b>	McGowan's characteristic volume
<b>pc:</b>	Critical Pressure
<b>ss:</b>	Solid phase molar entropy at standard conditions
<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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