

# DL-Proline, 5-oxo-

<b>Other names:</b>	DL-Pyroglutamic acid 2-Pyrrolidone-5-carboxylic acid DL-5-Oxoproline 5-oxo-DL-proline
<b>Inchi:</b>	InChI=1S/C5H7NO3/c7-4-2-1-3(6-4)5(8)9/h3H,1-2H2,(H,6,7)(H,8,9)
<b>InchiKey:</b>	ODHCTXKNWHHXJC-UHFFFAOYSA-N
<b>Formula:</b>	C5H7NO3
<b>SMILES:</b>	O=C1CCC(C(=O)O)N1
<b>Mol. weight [g/mol]:</b>	129.11
<b>CAS:</b>	149-87-1

## Physical Properties

Property code	Value	Unit	Source
gf	-272.85	kJ/mol	Joback Method
hf	-450.75	kJ/mol	Joback Method
hfus	17.43	kJ/mol	Joback Method
hvap	61.41	kJ/mol	Joback Method
log10ws	0.01		Crippen Method
logp	-0.650		Crippen Method
mcvol	89.440	ml/mol	McGowan Method
pc	5889.94	kPa	Joback Method
tb	591.50	K	Joback Method
tc	811.70	K	Joback Method
tf	441.01	K	Joback Method
vc	0.326	m3/kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	264.47	J/molxK	775.00	Joback Method
cpg	220.24	J/molxK	591.50	Joback Method
cpg	230.15	J/molxK	628.20	Joback Method
cpg	239.54	J/molxK	664.90	Joback Method
cpg	248.40	J/molxK	701.60	Joback Method

cpg	256.72	J/mol×K	738.30	Joback Method
cpg	271.63	J/mol×K	811.70	Joback Method
hsubt	133.00 ± 1.00	kJ/mol	405.00	NIST Webbook

## Sources

<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>
<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=C149871&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C149871&amp;Units=SI</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>hsubt:</b>	Enthalpy of sublimation at a given temperature
<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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