

# Proline

<b>Other names:</b>	(+)-(R)-proline (-)-(S)-Proline (R)-2-carboxypyrrolidine (S)-2-PYRRALIDINECARBOXYLIC ACID (S)-2-pyrrolidinecarboxylic acid 2-Pyrrolidinecarboxylic acid 2-Pyrrolidinecarboxylic acid, (S)- D-proline L-(-)-Proline L-PROLINE Proline, L- R-proline
<b>Inchi:</b>	InChI=1S/C5H9NO2/c7-5(8)4-2-1-3-6-4/h4,6H,1-3H2,(H,7,8)/t4-/m1/s1
<b>InchiKey:</b>	ONIBWKKTOPOVIA-SCSAIBSYSA-N
<b>Formula:</b>	C5H9NO2
<b>SMILES:</b>	O=C(O)C1CCCN1
<b>Mol. weight [g/mol]:</b>	115.13
<b>CAS:</b>	147-85-3

## Physical Properties

Property code	Value	Unit	Source
affp	920.10	kJ/mol	NIST Webbook
affp	938.90	kJ/mol	NIST Webbook
affp	920.50	kJ/mol	NIST Webbook
affp	925.90 ± 1.60	kJ/mol	NIST Webbook
affp	936.00	kJ/mol	NIST Webbook
basg	895.70 ± 1.60	kJ/mol	NIST Webbook
basg	886.00	kJ/mol	NIST Webbook
chs	-2738.60 ± 0.40	kJ/mol	NIST Webbook
chs	-2746.20 ± 2.50	kJ/mol	NIST Webbook
gf	-150.26	kJ/mol	Joback Method
hf	-366.20 ± 4.00	kJ/mol	NIST Webbook
hfs	-507.60 ± 2.60	kJ/mol	NIST Webbook
hfs	-515.18 ± 0.52	kJ/mol	NIST Webbook
hfus	17.92	kJ/mol	Joback Method
hsub	149.00 ± 2.00	kJ/mol	NIST Webbook
hvap	57.16	kJ/mol	Joback Method

ie	9.36	eV	NIST Webbook
ie	9.00	eV	NIST Webbook
ie	8.30	eV	NIST Webbook
log10ws	-0.21		Crippen Method
logp	-0.177		Crippen Method
mvol	87.870	ml/mol	McGowan Method
pc	5585.83	kPa	Joback Method
ss	170.70	J/molxK	NIST Webbook
ss	164.06	J/molxK	NIST Webbook
tb	523.68	K	Joback Method
tc	729.91	K	Joback Method
tf	372.79	K	Joback Method
vc	0.319	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	255.23	J/molxK	729.91	Joback Method
cpg	211.92	J/molxK	558.05	Joback Method
cpg	221.63	J/molxK	592.42	Joback Method
cpg	230.81	J/molxK	626.80	Joback Method
cpg	239.45	J/molxK	661.17	Joback Method
cpg	247.59	J/molxK	695.54	Joback Method
cpg	201.66	J/molxK	523.68	Joback Method
cps	150.40	J/molxK	298.15	NIST Webbook
cps	151.17	J/molxK	298.15	NIST Webbook
cps	149.12	J/molxK	300.40	NIST Webbook
hsubt	127.00 ± 1.00	kJ/mol	406.00	NIST Webbook
hsubt	149.00 ± 4.00	kJ/mol	400.00	NIST Webbook
hsubt	96.70 ± 0.80	kJ/mol	455.00	NIST Webbook

## Correlations

Information	Value
Property code	pvap
Equation	$\ln(P_{vp}) = A + B/T + C \cdot \ln(T) + D \cdot T^2$
Coeff. A	3.00080e+01
Coeff. B	-1.23246e+04

Coeff. C	3.09086e-02
Coeff. D	-2.47929e-08
Temperature range (K), min.	441.15
Temperature range (K), max.	466.15

## Sources

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Viscosities of L-Phenylalanine,  
L-Leucine, L-Glutamic Acid, or L-Proline  
+ 2.0 mol<sup>+</sup>dm<sup>-3</sup> Aqueous NaCl or 2.0  
mol<sup>+</sup>dm<sup>-3</sup> Aqueous NaNO<sub>3</sub> Solutions at  
T = (298.15 to 328.15) K:

<https://www.doi.org/10.1021/je1000878>

## Legend

<b>affp:</b>	Proton affinity
<b>basg:</b>	Gas basicity
<b>chs:</b>	Standard solid enthalpy of combustion
<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>hfs:</b>	Solid phase enthalpy of formation at standard conditions
<b>hfus:</b>	Enthalpy of fusion at standard conditions
<b>hsub:</b>	Enthalpy of sublimation at standard conditions
<b>hsubt:</b>	Enthalpy of sublimation at a given temperature
<b>hvap:</b>	Enthalpy of vaporization at standard conditions
<b>ie:</b>	Ionization energy
<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>pvap:</b>	Vapor 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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