Proline

Other names:	(+)-(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
Inchi:	InChI=1S/C5H9NO2/c7-5(8)4-2-1-3-6-4/h4,6H,1-3H2,(H,7,8)/t4-/m1/s1
InchiKey:	ONIBWKKTOPOVIA-SCSAIBSYSA-N
Formula:	C5H9NO2
SMILES:	O=C(O)C1CCCN1
Mol. weight [g/mol]:	115.13
CAS:	147-85-3

Physical Properties

Property code	Value	Unit	Source
affp	936.00	kJ/mol	NIST Webbook
affp	925.90 ± 1.60	kJ/mol	NIST Webbook
affp	938.90	kJ/mol	NIST Webbook
affp	920.10	kJ/mol	NIST Webbook
affp	920.50	kJ/mol	NIST Webbook
basg	886.00	kJ/mol	NIST Webbook
basg	895.70 ± 1.60	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	9.00	eV	NIST Webbook
ie	8.30	eV	NIST Webbook
ie	9.36	eV	NIST Webbook
log10ws	-0.21		Crippen Method
logp	-0.177		Crippen Method
mcvol	87.870	ml/mol	McGowan Method
pc	5585.83	kPa	Joback Method
ss	170.70	J/mol×K	NIST Webbook
ss	164.06	J/mol×K	NIST Webbook
tb	523.68	K	Joback Method
tc	729.91	K	Joback Method
tf	372.79	K	Joback Method
vc	0.319	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	255.23	J/mol×K	729.91	Joback Method
cpg	211.92	J/mol×K	558.05	Joback Method
cpg	221.63	J/mol×K	592.42	Joback Method
cpg	230.81	J/mol×K	626.80	Joback Method
cpg	239.45	J/mol×K	661.17	Joback Method
cpg	247.59	J/mol×K	695.54	Joback Method
cpg	201.66	J/mol×K	523.68	Joback Method
cps	150.40	J/mol×K	298.15	NIST Webbook
cps	151.17	J/mol×K	298.15	NIST Webbook
cps	149.12	J/mol×K	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(Pvp) = A + B/T + C*ln(T) + D*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

Densities, Speeds of Sound, and Viscosities of (L-Proline + Aqueous Glucose), and (L-Proline + Aqueous Sucrose). Solutions in the Temperature Range (298.15 to 323.15) K:	https://www.doi.org/10.1021/je2000205
KDB:	https://www.cheric.org/research/kdb/hcprop/showprop.php?cmpid=1468
Volumetric and compressibility behaviour of poly(propylene glycol) - Amino acid aqueous solutions at Different Temperatures:	https://www.doi.org/10.1016/j.jct.2015.06.024
Effect of KCl and KNO3 on Partial Molal Volumes and Partial Molal Compressibilities of Some Amino Acids at Different Temperatures:	https://www.doi.org/10.1007/s10765-008-0514-x
Interactions in L-alanine / L-proline / L-valine / L-leucine aqueous KCl/KNO3 systems at different temperatures: An Isentropic compressibility study:	https://www.doi.org/10.1016/j.tca.2008.10.023
Apparent molar volumes and apparent molar isentropic compressibilities of Amino Acids in Water, Ethanol and Ethanol–Water Mixtures:	https://www.doi.org/10.1021/acs.jced.7b00486
Intermolecular interactions in L-isoleucine-, L-proline-, and L-glutamine aqueous electrolyte systems:	https://www.doi.org/10.1016/j.jct.2006.03.009
Temperature Dependences and Enthalpic Discrimination of Homochiral Pairwise Interactions of Dilute Amino Acid Enantiomers in Pure Water:	https://www.doi.org/10.1021/je500825a
Measuring and modeling aqueous electrolyte/amino acid solutions with SPCE-SAFT:	https://www.doi.org/10.1016/j.jct.2013.08.018
Calorimetric interactions of PAMAM-NH2 G4 dendrimer with selected natural amino acids in aqueous solutions:	https://www.doi.org/10.1016/j.jct.2013.10.022
Salting-out effect in aqueous polypropylene glycol–amino acid solutions revealed by vapor pressure osmometry:	https://www.doi.org/10.1016/j.fluid.2016.05.025
Physical properties of seven deep eutectic solvents based on L-proline or betaine:	https://www.doi.org/10.1016/j.jct.2018.12.017
Activity coefficients of CaCl2 in (serine or proline + water) mixtures at T = 298.15 K:	https://www.doi.org/10.1016/j.jct.2010.01.002
Solubility and Thermodynamic Properties of (2S)-1-Oxo-2-carboxylic Acid in (Phenylalanine, Leucine) Glutamic Mixtures:	https://www.doi.org/10.1021/je5007949
Ultrasonic Velocities and Densities of (2S)-1-Oxo-2-carboxylic Acid in Water, Alcohols, and Water + Alcohol Mixtures:	https://www.doi.org/10.1021/je900909s
Solubility Behavior and Data Modeling of L-Proline in Different Neat and Binary Solvents:	https://www.doi.org/10.1021/acs.jced.9b00802
Effect of temperature on solvation behaviour of diclofenac sodium salt in aqueous glycine and L-proline solutions:	https://www.doi.org/10.1016/j.jct.2014.11.007
Thermodynamic approach to the interaction of L-Proline in aqueous Metformin Hydrochloride Solutions for temperature range 298.15-318.15 K:	https://www.doi.org/10.1016/j.jct.2019.02.012
4-hydroxyproline atdifferent temperatures:	https://www.doi.org/10.1016/j.jct.2009.11.017
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
KDB Vapor Pressure Data:	https://www.cheric.org/research/kdb/hcprop/showprop.php?cmpid=1468
Volumetric property of glycine, L-serine, L-alanine and L-proline in aqueous solutions of 1-phenylpiperazinium tetrafluoroborate:	https://www.doi.org/10.1016/j.jct.2016.03.045
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Viscosity studies of (L-alanine-, L-proline, L-valine, L-leucine + aqueous KCl/KNO3) solutions at different temperatures:	https://www.doi.org/10.1016/j.jct.2008.07.019
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C147853&Units=SI
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Vapor pressure osmometry determination of vapor-liquid equilibria for mixtures of L-Proline + 2 mol·L−1 aqueous NaNO3 solutions from (298.15 to 328.15) K:	https://www.doi.org/10.1016/j.fluid.2017.05.019
Solubilities of L-Proline in Subcritical HFC-134a and Supercritical CO2 Fluids:	https://www.doi.org/10.1021/je801009z
Imidazolium-Based Ionic Liquid + Amino acid systems:	https://www.doi.org/10.1021/acs.jced.9b00026
Surface Tension of Aqueous Solutions of Small-Chain Amino and Organic Acids:	https://en.wikipedia.org/wiki/Joback_method
Joback Method:	https://www.doi.org/10.1016/j.tca.2012.02.035
THE STANDARD ENTHALPIES OF FORMATION OF PROLINE ISOMERS:	https://www.doi.org/10.1016/j.fluid.2007.01.043
Volumetric and viscometric behaviour of amino acids in aqueous metal electrolytes solutions at 308K:	https://www.doi.org/10.1021/acs.jced.9b00752
Temperature of Maximum Density for Binary Aqueous Solutions of Five Amino Acids:	https://www.doi.org/10.1021/je0601053
Mutual Coexistence Curve Measurement of Aqueous Biphasic Systems Composed of [bmim][BF4] and Glycine, L-Serine, and L-Proline, Respectively:	

Viscosities of l-Phenylalanine, l-Leucine, l-Glutamic Acid, or l-Proline + 2.0 mol*dm-3 Aqueous NaCl or 2.0 mol*dm-3 Aqueous NaNO3 Solutions at T = (298.15 to 328.15) K: https://www.doi.org/10.1021/je1000878

Legend

affp:	Proton affinity
basg:	Gas basicity
chs:	Standard solid enthalpy of combustion
cpg:	Ideal gas heat capacity
cps:	Solid phase heat capacity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfs:	Solid phase enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hsub:	Enthalpy of sublimation at standard conditions
hsubt:	Enthalpy of sublimation at a given temperature
hvap:	Enthalpy of vaporization at standard conditions
ie:	Ionization energy
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
pvap:	Vapor pressure
ss:	Solid phase molar entropy at standard conditions
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume