DL-Phenylalanine

Other names:	(.+-.)-phenylalanine (.+/-.)-Phenylalanine (S)-(-)-phenylalanine 2-Amino-3-phenylpropionic acid, dl- DL-2-Amino-3-phenylpropanoic acid DL-2-amino-3-phenylpropionic acid DL-3-Phenylalanine DL-«alpha»-Amino-«beta»-phenylpropionic acid DL-«beta»-Phenyl-«alpha»-alanine DL-«beta»-Phenylalanine DLPA L-phenylalanine NSC 9959 Phenylalanine alanine, phenyl-, DL- propanoic acid, 2-amino-3-phenyl-, DL- «beta»-Phenylalanine, dl-
Inchi:	InChI=1S/C9H11NO2/c10-8(9(11)12)6-7-4-2-1-3-5-7/h1-5,8H,6,10H2,(H,11,12)
InchiKey:	COLNVLDHVKWLRT-UHFFFAOYSA-N
Formula:	C9H11NO2
SMILES:	NC(Cc1ccccc1)C(=O)O
Mol. weight [g/mol]:	165.19
CAS:	150-30-1

Physical Properties

Property code	Value	Unit	Source
chs	-4653.00 ± 2.50	kJ/mol	NIST Webbook
chs	-4664.30	kJ/mol	NIST Webbook
gf	-64.42	kJ/mol	Joback Method
hf	-228.86	kJ/mol	Joback Method
hfs	-460.60 ± 2.60	kJ/mol	NIST Webbook
hfus	18.46	kJ/mol	Solubility of L-Phenylalanine Anhydrous and Monohydrate Forms: Experimental Measurements and Predictions
hvap	71.58	kJ/mol	Joback Method

ie	9.40	eV	NIST Webbook
ie	8.90	eV	NIST Webbook
ie	8.40	eV	NIST Webbook
ie	8.40	eV	NIST Webbook
ie	8.50	eV	NIST Webbook
ie	8.40	eV	NIST Webbook
log10ws	-1.34		Crippen Method
logp	0.641		Crippen Method
mcvol	131.330	ml/mol	McGowan Method
pc	4266.28	kPa	Joback Method
tb	650.14	K	Joback Method
tc	865.09	K	Joback Method
tf	396.62	K	Joback Method
vc	0.479	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	335.03	J/mol×K	650.14	Joback Method
cpg	345.39	J/mol×K	685.97	Joback Method
cpg	355.04	J/mol×K	721.79	Joback Method
cpg	363.99	J/mol×K	757.62	Joback Method
cpg	372.30	J/mol×K	793.44	Joback Method
cpg	379.99	J/mol×K	829.27	Joback Method
cpg	387.10	J/mol×K	865.09	Joback Method

Sources

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

Interactions in (L-phenylalanine/L-histidine + 0.01 mol kg-1 aqueous beta-cyclodextrin) systems at T = (293.15, 298.15, 303.15 and 308.15) K: https://www.doi.org/10.1016/j.jct.2012.03.029

Joback Method: https://en.wikipedia.org/wiki/Joback_method

Solubility of L-phenylalanine in water and different binary mixtures from 298.15 to 318.15 K: https://www.doi.org/10.1016/j.fluid.2011.08.029

Solubility of L-Phenylalanine Anhydrous and Monohydrate Forms: Experimental Measurements and Predictions: https://www.doi.org/10.1021/je201354k

Solute-solvent interactions of amino acid L-phenylalanine in aqueous 1-butyl-2,3-dimethylimidazolium bromide ionic liquid solutions: https://www.doi.org/10.1016/j.jct.2017.06.006

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C150301&Units=SI

Physicochemical Behavior of Some Amino Acids/Glycylglycine in Aqueous D-Galactose Solutions at Different Temperatures: https://www.doi.org/10.1007/s10765-010-0742-8

Binary Diffusion Coefficients of Aqueous Phenylalanine, Tyrosine Isomers, and Anthobiotic Acids at Infinitesimal Concentration and Temperatures from (298.2 to 338.2) K: https://www.doi.org/10.1021/je3012698

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

Ultrasonic Velocities and Densities of l-Phenylalanine, l-Leucine, l-Glutamic Acid, and l-Proline + 2 mol*L-1 Aqueous NaCl and 2 mol*L-1 Aqueous NaNO3 Solutions from (298.15 to 328.15) K: https://www.doi.org/10.1021/je900909s

McGowan Method: http://link.springer.com/article/10.1007/BF02311772

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Physicochemical study of solute-solute and solute-solvent interactions of l-Phenylalanine in Water + (Methanol and Ethanol) Binary Solvent Mixtures from 278.15 to 318.15 K: https://www.doi.org/10.1016/j.jct.2013.09.008

Solubility of l-Phenylalanine in Water + (Monosaccharide/Disaccharide) Solutions at Different Temperatures: https://www.doi.org/10.1021/acs.jced.9b00004

Legend

chs:	Standard solid enthalpy of combustion
cpg:	Ideal gas 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
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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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