DL-PHENYLALANINE

Other names: (.+/-.)-Phenylalanine
(S)-(-)-phenylalanine
2-Amino-3-phenylpropionic acid, dl-
Alanine, phenyl-, DL-
DL-2-Amino-3-phenylpropanoic acid
DL-3-Phenylalanine
DL-«alpha»-Amino-«beta»-phenylpropionic acid
DL-«beta»-Phenyl-«alpha»-alanine
DL-«beta»-Phenylalanine
DLPA
L-phenylalanine
NSC 9959
Phenylalanine
«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)/t8-/m0/s1

InchiKey: COLNVLDHVKWLRT-UHFFFAOYSA-N

Formula: C9H11NO2

SMILES: NC(Cc1ccccc1)C(=O)O

Mol. weight [g/mol]: 165.19

Physical Properties

Property code	Value	Unit	Source
af	0.7043		Cheméo Relay (1.0)
chs	-4653.00 ± 2.50	kJ/mol	NIST Webbook
chs	-4664.30	kJ/mol	NIST Webbook
hf	-292.82	kJ/mol	Cheméo Relay (1.0)
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	87.54	kJ/mol	Cheméo Relay (1.0)
ie	8.40	eV	NIST Webbook
ie	8.50	eV	NIST Webbook
ie	8.40	eV	NIST Webbook
ie	8.90	eV	NIST Webbook

ie	9.40	eV	NIST Webbook
ie	8.40	eV	NIST Webbook
log10ws	-1.02		Cheméo Relay (1.0)
logp	0.641		Crippen Method
mcvol	131.330	ml/mol	McGowan Method
pc	4266.28	kPa	Joback Method
tb	567.57	K	Cheméo Relay (1.0)
tc	791.07	K	Cheméo Relay (1.0)
tf	488.93	K	Cheméo Relay (1.0)
vc	0.448	m3/kmol	Cheméo Relay (1.0)

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

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C150301&Units=SI
Physicochemical study of solute-solute and solute-solvent interactions of l-Phenylalanine in (Water + Arabinose/Glucose/Sucrose) Solutions at different temperatures:	https://www.doi.org/10.1016/j.jct.2013.09.008
Solubility of L-Phenylalanine Anhydrous and Monohydrate Forms: Influence of the Composition of Aqueous Alcohol Solvents on the Thermodynamic Characteristics of Dissolution at 298.15K:	https://www.doi.org/10.1021/je201354k
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/10.1016/j.tca.2011.08.022
Amino acid behavior in aqueous amide solutions: Temperature dependence of the l-phenylalanine N,N-dimethylformamide interaction:	https://www.doi.org/10.1021/je900909s
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):	
McGowan Method:	https://www.doi.org/10.1016/j.tca.2013.05.014
Crippen Method:	http://link.springer.com/article/10.1007/BF02311772
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:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Joback Method:	https://www.doi.org/10.1021/je1000878
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://en.wikipedia.org/wiki/Joback_method
Cheméo Relay (1.0, beta):	https://www.doi.org/10.1016/j.jct.2012.03.029

Solubility of L-phenylalanine in water and different binary mixtures from 288.15 to 318.15 K: https://www.doi.org/10.1016/j.fluid.2011.08.029

Physicochemical and friccohesity study of glycine, L-alanine and https://www.doi.org/10.1016/j.jct.2013.05.037

Enthalpies of solution of L-phenylalanine with aqueous https://www.doi.org/10.1016/j.tca.2012.11.004

L-phenylalanine in aqueous solution of https://www.doi.org/10.1021/je3012698

Aqueous Phenylalanine, Tyrosine https://www.doi.org/10.1016/j.jct.2017.06.006

1-butyl-2,3-dimethylimidazolium bromide ionic liquid solutions:

Legend

af:	Acentric Factor
chs:	Standard solid enthalpy of combustion
cpg:	Ideal gas heat capacity
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