L-Phenylalanine

Other names:	(-)-Phenylalanine
	(-)-«beta»-Phenylalanine
	(S)-(-)-phenylalanine
	(S)-2-Amino-3-phenylpropanoic acid
	(S)-2-Amino-3-phenylpropionic acid
	(S)-Phenylalanine
	(S)-«alpha»-Aminobenzenepropanoic acid
	3-Phenyl-L-alanine
	3-Phenylalanine
	Alanine, 3-phenyl-
	Alanine, phenyl-
	Alanine, phenyl-, L-
	Antibiotic FN 1636
	Benzenepropanoic acid, «alpha»-amino-, (S)-
	DL-3-PHENYLALANINE
	DL-PHENYLALANINE
	Hydrocinnamic acid, «alpha»-amino-
	L-Alanine, 3-phenyl-
	L-Alanine, phenyl-
	L-Antibiotic FN 1636
	L-«beta»-Phenylalanine
	NSC 79477
	PAL
	Phenyl-«alpha»-alanine
	«alpha»-Amino-«beta»-phenylpropionic acid
	«alpha»-Aminohydrocinnamic acid
	«beta»-Phenyl-L-alanine
	«beta»-Phenyl-«alpha»-alanine
	«beta»-Phenyl-«alpha»-alanine, L-
	«beta»-Phenylalanine
	Phenylalanine
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-QMMMGPOBSA-N
Formula:	C9H11NO2
SMILES:	N[C@@H](Cc1ccccc1)C(=O)O
Mol. weight [g/mol]:	165.19
CAS:	63-91-2

Physical Properties

Property code	Value	Unit	Source
af	0.6937		Cheméo Relay (1.0)
affp	922.90	kJ/mol	NIST Webbook
basg	888.90	kJ/mol	NIST Webbook
chs	-4667.40	kJ/mol	NIST Webbook
chs	-4646.30 ± 0.80	kJ/mol	NIST Webbook
hf	-280.48	kJ/mol	Cheméo Relay (1.0)
hfus	24.92	kJ/mol	Joback Method
hvap	82.60	kJ/mol	Cheméo Relay (1.0)
ie	8.48	eV	Cheméo Relay (1.0)
log10ws	-0.83		Aqueous Solubility Prediction Method
log10ws	-0.92		Aqueous Solubility Prediction Method
logp	0.641		Crippen Method
mcvol	131.330	ml/mol	McGowan Method
pc	3920.94	kPa	Joback Method
ss	213.64	J/mol×K	NIST Webbook
tb	576.85	K	Cheméo Relay (1.0)
tc	792.40	K	Cheméo Relay (1.0)
tf	497.84	K	Cheméo Relay (1.0)
vc	0.463	m3/kmol	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cps	203.10	J/mol×K	298.15	NIST Webbook
cps	203.01	J/mol×K	298.15	NIST Webbook
hsubt	154.00 ± 0.80	kJ/mol	455.00	NIST Webbook
hsubt	154.00 ± 8.00	kJ/mol	455.00	NIST Webbook
hvapt	158.30	kJ/mol	418.15	Enthalpy of sublimation of natural aromatic amino acids determined by Knudsen's effusion mass spectrometric method

Correlations

Information	Value
Property code	cpg
Equation	$Y = A + B \cdot T + C \cdot T^2 + D \cdot T^3 + E \cdot T.$
Y unit	J/mol×K
Coeff. A	-2.97890e+01
Coeff. B	8.98500e-01
Coeff. C	-6.16200e-04
Coeff. D	1.59900e-07
Coeff. E	0.00000e+00
Basis	predicted
Temperature range (K), min.	273.00
Temperature range (K), max.	1000.00

Information	Value
Property code	pvap
Equation	$\ln(Y) = A + B/T + C \cdot \ln(T) + D \cdot T^2 + E/T^2$
Y unit	kPa
Coeff. A	4.12108e+01
Coeff. B	-1.81644e+04
Coeff. C	5.21569e-02
Coeff. D	-4.14026e-08
Coeff. E	0.00000e+00
Temperature range (K), min.	450.15
Temperature range (K), max.	468.15

Sources

Aqueous Solubility Prediction Method: http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa

Study of the 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

Chemeo Relay (1.0 beta):

Effect of 1-Ethyl-3-methylimidazolium Bromide Ionic Liquid on the Volumetric Behavior of Some Aqueous L-Amino Acids Solutions: https://www.doi.org/10.1021/je300953u

Effect of magnesium acetate on the volumetric and transport behavior of some amino acids in aqueous solutions: https://www.doi.org/10.1016/j.jct.2005.12.002

Enthalpy of sublimation of natural aromatic amino acids determined by Knudsen's effusion mass spectrometric method: https://www.doi.org/10.1016/j.jct.2014.02.003

KDB Vapor Pressure Data: https://www.cheric.org/research/kdb/hcprop/showprop.php?cmpid=1483

Tc, Pc, Vc at 298.15 K:

Temperature of Maximum Density for Binary Aqueous Solutions of Five Amino Acids:	https://www.doi.org/10.1021/acs.jced.9b00752
Thermodynamic Study of Some Amino Acids, 2-Aminopropanoic Acid, 2-Amino-3-methylbutanoic Acid, 2-Amino-4-methylpentanoic Acid, and 2-Amino-5-phenylpropanoic Acid in Aqueous Sodium Chloride Solutions at Different Temperatures: Volumetric and Ultrasonic Study:	https://www.doi.org/10.1021/je100857s
Effect of hydrophilic additives on volumetric and viscosity properties of aqueous solutions at T = (283.15 to 328.15) K	https://www.doi.org/10.1016/j.jct.2011.12.020
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
Chemeo Relay (1.0):	
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Solubility of the Proteinogenic a-Amino Acids in Water, Ethanol, and Ethanol–Water Mixtures:	https://www.doi.org/10.1021/acs.jced.7b00486
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C63912&Units=SI
Thermodynamics of the amino acid -ethylene glycol pair interaction:	https://www.doi.org/10.1016/j.tca.2014.03.044
Apparent Molar Volumes and Viscosities of Some Amino Acids in Aqueous Sodium Acetate Solutions at 298.15 K:	https://www.doi.org/10.1021/je034209e
KDB:	https://www.cheric.org/files/research/kdb/mol/mol1483.mol

Legend

af:	Acentric Factor
affp:	Proton affinity
basg:	Gas basicity
chs:	Standard solid enthalpy of combustion
cpg:	Ideal gas heat capacity
cps:	Solid phase heat capacity
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hsubt:	Enthalpy of sublimation at a given temperature
hvap:	Enthalpy of vaporization at standard conditions
hvapt:	Enthalpy of vaporization at a given temperature
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

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