Phenylalanine

Other names:

(-)-Phenylalanine
(-)-«beta»-Phenylalanine
(-)-Â«betaÂ»-Phenylalanine
(S)-2-Amino-3-phenylpropanoic acid
(S)-2-Amino-3-phenylpropionic acid
(S)-Phenylalanine
(S)-«alpha»-Aminobenzenepropanoic acid
(S)-Â«alphaÂ»-Aminobenzenepropanoic acid
3-Phenyl-L-alanine
3-Phenylalanine
Alanine, 3-phenyl-
Alanine, phenyl-
Alanine, phenyl-, L-
Antibiotic FN 1636
Benzenepropanoic acid, «alpha»-amino-, (S)-
Benzenepropanoic acid, Â«alphaÂ»-amino-, (S)-
DL-3-PHENYLALANINE
DL-PHENYLALANINE
Hydrocinnamic acid, «alpha»-amino-
Hydrocinnamic acid, Â«alphaÂ»-amino-
L-Alanine, 3-phenyl-
L-Alanine, phenyl-
L-Antibiotic FN 1636
L-Phenylalanine
L-«beta»-Phenylalanine
L-Â«betaÂ»-Phenylalanine
NSC 79477
PAL
Phenyl-«alpha»-alanine
Phenyl-Â«alphaÂ»-alanine
«alpha»-Amino-«beta»-phenylpropionic acid
«alpha»-Aminohydrocinnamic acid
«beta»-Phenyl-L-alanine
«beta»-Phenyl-«alpha»-alanine
«beta»-Phenyl-«alpha»-alanine, L-
«beta»-Phenylalanine
Â«alphaÂ»-Amino-Â«betaÂ»-phenylpropionic acid
Â«alphaÂ»-Aminohydrocinnamic acid
Â«betaÂ»-Phenyl-L-alanine
Â«betaÂ»-Phenyl-Â«alphaÂ»-alanine

	Â«betaÂ»-Phenyl-Â«alphaÂ»-alanine, L-
	Â«betaÂ»-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-/m1/s1
InchiKey:	COLNVLDHVKWLRT-MRVPVSSYSA-N
Formula:	C9H11NO2
SMILES:	NC(Cc1ccccc1)C(=O)O
Mol. weight [g/mol]:	165.19
CAS:	63-91-2

Physical Properties

Property code	Value	Unit	Source
affp	922.90	kJ/mol	NIST Webbook
basg	888.90	kJ/mol	NIST Webbook
chs	-4646.30 ± 0.80	kJ/mol	NIST Webbook
chs	-4667.40	kJ/mol	NIST Webbook
gf	-64.42	kJ/mol	Joback Method
hf	-228.86	kJ/mol	Joback Method
hfus	20.47	kJ/mol	Joback Method
hvap	71.58	kJ/mol	Joback Method
log10ws	-0.92		Aqueous Solubility Prediction Method
logp	0.641		Crippen Method
mcvol	131.330	ml/mol	McGowan Method
pc	4266.28	kPa	Joback Method
ss	213.64	J/mol×K	NIST Webbook
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	372.30	J/mol×K	793.44	Joback Method
cpg	379.99	J/mol×K	829.27	Joback Method
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	387.10	J/mol×K	865.09	Joback Method
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

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/T + C*ln(T) + D*T^2
Coeff. A	4.12108e+01
Coeff. B	-1.81644e+04
Coeff. C	5.21569e-02
Coeff. D	-4.14026e-08
Temperature range (K), min.	450.15
Temperature range (K), max.	468.15

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C63912&Units=SI
KDB Vapor Pressure Data: https://www.cheric.org/research/kdb/hcprop/showprop.php?cmpid=1483
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Joback Method: https://en.wikipedia.org/wiki/Joback_method
KDB: https://www.cheric.org/research/kdb/hcprop/showprop.php?cmpid=1483
Aqueous Solubility Prediction Method: http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa

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
hfus:	Enthalpy of fusion at standard conditions
hsubt:	Enthalpy of sublimation at a given temperature
hvap:	Enthalpy of vaporization at standard conditions
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