L-Leucine

Other names:	(S)-(+)-leucine (S)-2-amino-4-methylpentanoic acid (S)-2-amino-4-methylvaleric acid (S)-leucine .alpha.-amino-.gamma.-methylvaleric acid .alpha.-aminoisocaproic acid 2-Amino-4-methylpentanoic acid, (L)- 2-Amino-4-methylvaleric acid, (L)- 4-methyl-L-norvaline L-(+)-leucine L-(-)-2-Amino-4-methylpentanoic acid L-.alpha.-aminoisocaproic acid L-Norvaline, 4-methyl- L-«alpha»-Aminoisocaproic acid Leu Leucin Leucine, L- NSC 46709 Norvaline, 4-methyl-, (L)- Pentanoic acid, 2-amino-4-methyl-, (S)- Valeric acid, 2-amino-4-methyl-, (S)- iso-C4H9CH(NH2)COOH «alpha»-Amino-«gamma»-methylvaleric acid Leucine
Inchi:	InChI=1S/C6H13NO2/c1-4(2)3-5(7)6(8)9/h4-5H,3,7H2,1-2H3,(H,8,9)/t5-/m0/s1
InchiKey:	ROHFNLRQFUQHCH-YFKPBYRVSA-N
Formula:	C6H13NO2
SMILES:	CC(C)C[C@H](N)C(=O)O
Mol. weight [g/mol]:	131.17
CAS:	61-90-5

Physical Properties

Property code	Value	Unit	Source
af	0.6587		Cheméo Relay (1.0)
affp	914.60	kJ/mol	NIST Webbook
basg	880.60	kJ/mol	NIST Webbook

chg	-3570.00 ± 1.90	kJ/mol	NIST Webbook
chs	-3572.00 ± 0.30	kJ/mol	NIST Webbook
chs	-3581.50 ± 0.84	kJ/mol	NIST Webbook
chs	-3596.00	kJ/mol	NIST Webbook
chs	-3600.40	kJ/mol	NIST Webbook
hf	-497.07	kJ/mol	Cheméo Relay (1.0)
hfl	-648.90 ± 2.00	kJ/mol	NIST Webbook
hfs	-637.39 ± 0.92	kJ/mol	NIST Webbook
hfs	-646.80	kJ/mol	NIST Webbook
hfus	19.59	kJ/mol	Joback Method
hvap	64.70	kJ/mol	Cheméo Relay (1.0)
ie	8.51	eV	NIST Webbook
log10ws	-1.30		Cheméo Relay (1.0)
logp	0.444		Crippen Method
mcvol	112.820	ml/mol	McGowan Method
pc	3754.57	kPa	Joback Method
ss	211.79	J/mol×K	NIST Webbook
tb	497.04	K	Cheméo Relay (1.0)
tc	667.18	K	Cheméo Relay (1.0)
tf	563.15	K	Jean-Claude Bradley Open Melting Point Dataset (2014, CC0)
vc	0.397	m3/kmol	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cps	191.00	J/mol×K	298.00	NIST Webbook
cps	200.96	J/mol×K	298.15	NIST Webbook
cps	201.40	J/mol×K	298.15	NIST Webbook
cps	190.60	J/mol×K	298.00	NIST Webbook
hsubt	150.60 ± 0.80	kJ/mol	455.00	NIST Webbook
hsubt	148.70 ± 6.50	kJ/mol	459.00	NIST Webbook
hsubt	150.60 ± 0.80	kJ/mol	455.00	NIST Webbook
hsubt	151.00 ± 0.80	kJ/mol	455.00	NIST Webbook
psub	9.00e-04	kPa	420.70	Sublimation and vapour pressure estimation of l-leucine using thermogravimetric analysis

psub	2.90e-03	kPa	440.30	Sublimation and vapour pressure estimation of l-leucine using thermogravimetric analysis
psub	0.04	kPa	469.90	Sublimation and vapour pressure estimation of l-leucine using thermogravimetric analysis
psub	0.53	kPa	499.20	Sublimation and vapour pressure estimation of l-leucine using thermogravimetric analysis
psub	2.16	kPa	517.50	Sublimation and vapour pressure estimation of l-leucine using thermogravimetric analysis

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	5.16100e+00
Coeff. B	6.98340e-01
Coeff. C	-4.25000e-04
Coeff. D	9.82000e-08
Coeff. E	0.00000e+00
Basis	predicted
Temperature range (K), min.	273.00
Temperature range (K), max.	1000.00

Sources

Joback Method:	https://en.wikipedia.org/wiki/Joback_method
Conductivity and fluorescence studies on the micellization properties of sodium cholate and sodium deoxycholate in aqueous medium at different temperatures: Effect of selected amino acids:	https://www.doi.org/10.1016/j.jct.2014.10.014
Interaction of some hydrophobic amino acids, peptides, and protein with aqueous 3-chloro-1,2-propanediol and 2-chloro-1-propanol: Biophysical studies:	https://www.doi.org/10.1016/j.jct.2010.11.015

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
Jean-Claude Bradley Open Melting Point Dataset (2014-12-10)	https://figshare.com/articles/Jean_Claude_Bradley_Open_Melting_Point_Datset/1031637
Mode of action of betaine on some amino acids and globular proteins:	https://www.doi.org/10.1016/j.jct.2017.03.025
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Interactions of Saccharides in Aqueous Glycine and Leucine Solutions at Different Temperatures:	https://www.doi.org/10.1021/je500647a
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Solubility of the Proteinogenic α-Amino Acids in Water, Ethanol, and Ethanol–Water Mixtures:	https://www.doi.org/10.1021/acs.jced.7b00486
Partial molar volumes and partial molar compressibility of four homologous alpha-amino acids in aqueous sodium chloride at different temperatures:	https://www.doi.org/10.1016/j.jct.2011.01.004
Thermodynamic Study of Some Amino Acids: 2-Aminoisobutyric Acid, 2-Amino-n-butyric Acid, 2-Amino-3-methylbutanoic Acid, and 2-Amino-2-methylpropanoic Acid in Aqueous Solutions at Different Temperatures: Volumetric and Viscometric Studies:	https://www.doi.org/10.1021/je100857s
Partial Molar Volumes and Isentropic Compressibilities of Some Saccharides in Water at 298.15 K	https://www.doi.org/10.1021/je400977r
Effect of hydrophilic additives on volumetric and viscosity properties of amino acids in aqueous solutions at different temperatures: Volumetric and viscometric studies:	https://www.doi.org/10.1016/j.jct.2011.12.020
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Chemeo Relay (1.0, beta):	https://www.chemeo.com/doc/models/crippen_log10ws
Interactions of some amino acids and glycine peptideswith aqueous sodium dodecyl sulfate and cetyltrimethylammonium bromide at T = (288.15 to 318.15) K:	https://www.doi.org/10.1016/j.jct.2003.09.010
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Ultrasonic Velocities and Densities of Phenylalanine, Leucine, Glutamic Acid, and Proline in Aqueous Solutions of Sodium Chloride at 298.15 K	https://www.doi.org/10.1021/je900909s
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Legend

af:	Acentric Factor
affp:	Proton affinity
basg:	Gas basicity
chg:	Standard gas enthalpy of combustion
chs:	Standard solid enthalpy of combustion
cpg:	Ideal gas heat capacity
cps:	Solid phase heat capacity
hf:	Enthalpy of formation at standard conditions
hfl:	Liquid phase enthalpy of formation at standard conditions
hfs:	Solid phase 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
ie:	Ionization energy
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
psub:	Sublimation 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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