

D-Leucine

Other names:	(R)-(-)-Leucine (S)-(+)-leucine (S)-2-amino-4-methylpentanoic acid (S)-2-amino-4-methylvaleric acid (S)-leucine .alpha.-amino-.gamma.-methylvaleric acid .alpha.-aminoisocaproic acid 4-methyl-L-norvaline L-(+)-leucine L.alpha.-aminoisocaproic acid L-leucine Leucine, D-
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)CC(N)C(=O)O
Mol. weight [g/mol]:	131.17
CAS:	328-38-1

Physical Properties

Property code	Value	Unit	Source
chs	-3581.40 ± 0.84	kJ/mol	NIST Webbook
gf	-204.53	kJ/mol	Joback Method
hf	-408.75	kJ/mol	Joback Method
hfs	-637.56 ± 0.84	kJ/mol	NIST Webbook
hfus	15.13	kJ/mol	Joback Method
hvap	62.24	kJ/mol	Joback Method
log10ws	-0.74		Crippen Method
logp	0.444		Crippen Method
mcvol	112.820	ml/mol	McGowan Method
pc	4077.71	kPa	Joback Method
tb	554.38	K	Joback Method
tc	743.19	K	Joback Method
tf	321.39	K	Joback Method
vc	0.413	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	275.71	J/molxK	554.38	Joback Method
cpg	285.39	J/molxK	585.85	Joback Method
cpg	294.59	J/molxK	617.32	Joback Method
cpg	303.34	J/molxK	648.79	Joback Method
cpg	311.64	J/molxK	680.26	Joback Method
cpg	319.50	J/molxK	711.72	Joback Method
cpg	326.94	J/molxK	743.19	Joback Method
psub	9.00e-04	kPa	420.70	Sublimation and vapour pressure estimation of I-leucine using thermogravimetric analysis
psub	2.90e-03	kPa	440.30	Sublimation and vapour pressure estimation of I-leucine using thermogravimetric analysis
psub	0.04	kPa	469.90	Sublimation and vapour pressure estimation of I-leucine using thermogravimetric analysis
psub	0.53	kPa	499.20	Sublimation and vapour pressure estimation of I-leucine using thermogravimetric analysis
psub	2.16	kPa	517.50	Sublimation and vapour pressure estimation of I-leucine using thermogravimetric analysis

Sources

Viscosities of L-Phenylalanine, L-Leucine, L-Glutamic Acid, or L-Proline
 Partial molar volume and partial molar
 compressibility of quaternary ammonium
 cations in aqueous solutions at
 different temperatures and pressures
 and the group contributions in
 the partial molar volumes of solutes
 and their (water-solvent) interactions of
 homologous series of amino acids with
 thiamine hydrochloride in aqueous
 medium at T = (305.15, 310.15, 315.15)
 K: A volumetric and acoustic approach:

<https://www.doi.org/10.1021/je1000878>

<https://www.doi.org/10.1016/j.jct.2011.01.004>

<https://www.doi.org/10.1016/j.jct.2010.08.004>

<https://www.doi.org/10.1016/j.jct.2016.06.026>

Volumetric and Viscometric Studies of Some Amino Acids in Aqueous Solutions at Different Temperatures: Thermodynamic and Atmospheric Partial Molar Volumes and Compressibilities of Some Saccharides in Aqueous Solutions of Leucine at Different Temperatures: Conductivity and fluorescence studies on the micellization properties of Sodium cholate between Amino Acids and Zinc Chloride in Aqueous Solution at Different Temperatures (Molecular Interactions between Amino Acids and Zinc Chloride in Aqueous Solution at Different Temperatures) in Water over a Temperature Range estimated from 293.15 K using the Taylor Dispersion Method and analysis: <https://www.doi.org/10.1021/je100909b>

Solvation behaviour of biologically active compounds in aqueous solutions of amino acids: bactericidal drug amoxicillin at different temperatures: Mode of action of betaine on some amino acids and globular proteins: Thermodynamics of the interactions of a homologous series of some amino acids with KCl and KNO₃ on Partial Molal Volumes and Partial Molar Heat Capacities of some amino acids in aqueous solutions at T = (283.15 to 333.15) K: Joback Method: <https://www.doi.org/10.1016/j.tca.2006.04.004>
<https://www.doi.org/10.1021/je400977r>
<http://pubs.acs.org/doi/abs/10.1021/ci9903071>
<https://www.doi.org/10.1016/j.jct.2014.10.014>
<https://www.doi.org/10.1021/je8001464>
<https://www.doi.org/10.1021/je060149b>
<https://www.doi.org/10.1016/j.tca.2008.10.009>
https://www.chemeo.com/doc/models/crippen_log10ws
<https://www.doi.org/10.1016/j.jct.2014.03.015>
<http://link.springer.com/article/10.1007/BF02311772>
<https://www.doi.org/10.1016/j.jct.2017.03.025>
<https://www.doi.org/10.1016/j.jct.2011.05.012>
<https://www.doi.org/10.1007/s10765-008-0514-x>
<https://www.doi.org/10.1016/j.jct.2011.12.020>
<http://webbook.nist.gov/cgi/cbook.cgi?ID=C328381&Units=SI>
https://en.wikipedia.org/wiki/Joback_method
<https://www.doi.org/10.1016/j.jct.2013.10.022>
<https://www.doi.org/10.1016/j.jct.2016.06.018>
<https://www.doi.org/10.1016/j.jct.2003.09.010>
<https://www.doi.org/10.1021/acs.jced.6b00168>
<https://www.doi.org/10.1021/acs.jced.7b00486>
<https://www.doi.org/10.1016/j.tca.2008.10.023>
<https://www.doi.org/10.1021/je900909s>
<https://www.doi.org/10.1021/je200146j>
<https://www.doi.org/10.1016/j.jct.2013.09.009>
<https://www.doi.org/10.1021/je500647a>
<https://www.doi.org/10.1016/j.tca.2015.02.014>
<https://www.doi.org/10.1021/je100857s>
<https://www.doi.org/10.1016/j.jct.2013.11.001>
<https://www.doi.org/10.1021/je034168m>
<https://www.doi.org/10.1016/j.jct.2008.07.019>
<https://www.doi.org/10.1016/j.fluid.2015.03.012>
<https://www.doi.org/10.1016/j.jct.2010.11.015>
<https://www.doi.org/10.1016/j.jct.2019.06.002>

Legend

- chs: Standard solid enthalpy of combustion
- cpg: Ideal gas heat capacity
- gfg: 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
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
psub:	Sublimation pressure
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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