allo-L-isoleucine

Other names:	(2S,3S)-.alpha.-amino-.beta.-methyl-n-valeric acid
	(2S,3S)-.alpha.-amino-.beta.-methylvaleric acid
	(2S,3S)-2-amino-3-methylpentanoic acid
	(S)-isoleucine
	(S,S)-isoleucine
	.alpha.-amino-.beta.-methylvaleric acid
	2-amino-3-methylpentanoic acid
	2-amino-3-methylvaleric acid
	2S,3S-isoleucine
	L-(+)-isoleucine
	L-isoleucine
	L-norvaline, 3-methyl-, erythro-
	[S-(R*,R*)]-2-amino-3-methylpentanoic acid
	erythro-L-isoleucine
	isoleucine
	isoleucine, L-
	pentanoic acid, 2-amino-3-methyl-, [S-(R*,R*)]-
Inchi:	InChI=1S/C6H13NO2/c1-3-4(2)5(7)6(8)9/h4-5H,3,7H2,1-2H3,(H,8,9)
InchiKey:	AGPKZVBTJJNPAG-UHFFFAOYSA-N
Formula:	C6H13NO2
SMILES:	CCC(C)C(N)C(=O)O
Mol. weight [g/mol]:	131.17
CAS:	3107-04-8

Physical Properties

Property code	Value	Unit	Source
gf	-204.53	kJ/mol	Joback Method
hf	-408.75	kJ/mol	Joback Method
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	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	275.71	J/mol×K	554.38	Joback Method
cpg	285.39	J/mol×K	585.85	Joback Method
cpg	294.59	J/mol×K	617.32	Joback Method
cpg	303.34	J/mol×K	648.79	Joback Method
cpg	311.64	J/mol×K	680.26	Joback Method
cpg	319.50	J/mol×K	711.72	Joback Method
cpg	326.94	J/mol×K	743.19	Joback Method
hsubt	120.10 ± 0.80	kJ/mol	455.00	NIST Webbook

Sources

Joback Method: https://en.wikipedia.org/wiki/Joback_method

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KCl effect on the solubility of five different amino acids in water: https://www.doi.org/10.1016/j.fluid.2007.04.004

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

Densities and Speeds of Sound in L-Leucine/L-Isoleucine + Aqueous KCl/KNO3 Systems at 298.15 to 323.15 K: https://www.doi.org/10.1021/je200146j

Effect on the Solubility and Solvation Thermodynamics of l-Serine and l-Isoleucine in Aqueous Media: https://www.doi.org/10.1021/acs.jced.9b00363

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Molecular Method: http://link.springer.com/article/10.1007/BF02311772

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Studies on the Diffusion Coefficients of Amino Acids in Aqueous Solutions: https://www.doi.org/10.1021/je049582g

Solubility of l-serine, l-threonine and l-isoleucine in aqueous aliphatic alcohols at 101.3 kPa: https://www.doi.org/10.1016/j.fluid.2008.05.008

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Thermodynamics of proton dissociations from aqueous threonine and isoleucine in presence of aqueous electrolyte systems: 0.35 MPa: Apparent molar heat capacities and apparent molar volumes of zwitterionic, protonated cationic and deprotonated anionic forms: https://www.doi.org/10.1016/j.jct.2006.05.013

Intermolecular interactions in L-proline + L-threonine + L-isoleucine + L-valine + aqueous-D-xylose solutions at different temperatures by using physicochemical methods: https://www.doi.org/10.1016/j.jct.2006.03.009

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C3107048&Units=SI

Study of solute-solute and solute-solvent interactions of homologous series of some alpha-amino acids in (0.01 to 1.0) mol·kg-1, and at the pressure 0.35 MPa: https://www.doi.org/10.1016/j.jct.2016.06.030

Legend

cpg:	Ideal gas 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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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