

# D-Valine

<b>Other names:</b>	(R)-Valine (S)-(+)-valine (S)-3-amino-2-methylbutanoic acid (S)-Valine 2-Amino-3-methylbutanoic acid(D) L-2-amino-3-methylbutanoic acid L-2-amino-3-methylbutyric acid L-2-aminoisovaleric acid L-valine NSC 20654 Valine, D- butanoic acid, 2-amino-3-methyl-, (S)-
<b>Inchi:</b>	InChI=1S/C5H11NO2/c1-3(2)4(6)5(7)8/h3-4H,6H2,1-2H3,(H,7,8)/t4-/m0/s1
<b>InchiKey:</b>	KZSNJWFQEVHDMF-BYPYZUCNSA-N
<b>Formula:</b>	C5H11NO2
<b>SMILES:</b>	CC(C)C(N)C(=O)O
<b>Mol. weight [g/mol]:</b>	117.15
<b>CAS:</b>	640-68-6

## Physical Properties

Property code	Value	Unit	Source
gf	-212.95	kJ/mol	Joback Method
hf	-388.11	kJ/mol	Joback Method
hfus	12.54	kJ/mol	Joback Method
hvap	60.01	kJ/mol	Joback Method
log10ws	-0.32		Crippen Method
logp	0.054		Crippen Method
mcvol	98.730	ml/mol	McGowan Method
pc	4627.70	kPa	Joback Method
tb	531.50	K	Joback Method
tc	722.61	K	Joback Method
tf	310.12	K	Joback Method
vc	0.357	m <sup>3</sup> /kmol	Joback Method

# Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	232.36	J/molxK	531.50	Joback Method
cpg	241.05	J/molxK	563.35	Joback Method
cpg	249.30	J/molxK	595.20	Joback Method
cpg	257.14	J/molxK	627.06	Joback Method
cpg	264.58	J/molxK	658.91	Joback Method
cpg	271.63	J/molxK	690.76	Joback Method
cpg	278.30	J/molxK	722.61	Joback Method
cps	158.00	J/molxK	298.00	NIST Webbook
cps	158.20	J/molxK	298.00	NIST Webbook

## Sources

- Intermolecular interactions of <https://www.doi.org/10.1016/j.jct.2016.06.018>  
.alpha.-amino acids and glycol  
The thermodynamic interactions of <https://www.doi.org/10.1016/j.jct.2013.11.001>  
serine and glycine with water  
Density and electrical conductances of <https://www.doi.org/10.1021/je500975a>  
amino acids + ionic liquid ([HmIm]Br)  
Viscosity studies of L-phenyl-, <https://www.doi.org/10.1016/j.jct.2010.08.004>  
L-proline, L-valine, L-leucine + aqueous  
solutions at different <http://link.springer.com/article/10.1007/BF02311772>  
temperatures:  
Densities and electrical conductances <https://www.doi.org/10.1016/j.fluid.2010.04.002>  
of amino acids + ionic liquid ([HmIm]Br)  
Viscosity studies of L-phenyl-, <https://www.doi.org/10.1016/j.jct.2008.07.019>  
L-proline, L-valine, L-leucine + aqueous  
solutions at different [https://www.chemeo.com/doc/models/crippen\\_log10ws](https://www.chemeo.com/doc/models/crippen_log10ws)  
temperatures:  
Density and Viscosity Study of <https://www.doi.org/10.1021/acs.jced.5b01031>  
Interactions of Some Amino Acids in  
Aqueous Solutions between some <https://www.doi.org/10.1016/j.tca.2006.07.009>  
amino acids and cyclohexanone in  
aqueous solutions of biologically <https://www.doi.org/10.1016/j.jct.2014.03.015>  
active compounds in aqueous  
solutions: Interactions of glycine, <https://www.doi.org/10.1016/j.tca.2014.06.028>  
alanine and proline in aqueous  
solutions of some amino acids <https://www.doi.org/10.1016/j.jct.2010.11.015>  
with the type of some amino acids  
lipid bilayers and protein with <https://www.doi.org/10.1021/je500255d>  
Molecular Dynamics Simulation of  
Solubility of Alanine in Biological <https://www.doi.org/10.1021/je500035r>  
Media: N,N-Dimethylformamide,  
N-methyl-2-pyrrolidone, Water, Ethanol, <https://www.doi.org/10.1016/j.jct.2015.11.015>  
N,N-Dimethylacetamide, Acetone, and  
Ethyl Propyl Carbazate between liquid and <https://www.doi.org/10.1021/je501178z>  
solid states: Thermodynamic studies of  
Amino Acids in Mannitol Aqueous <https://www.doi.org/10.1016/j.jct.2017.03.025>  
solutions at different temperatures by  
amino acids and globular proteins:  
Thermodynamic considerations <https://www.doi.org/10.1021/je7001418>  
B-Coefficients of Some Amino Acids in  
Aqueous Solution Behavior of some amino <https://www.doi.org/10.1016/j.jct.2016.03.016>  
acids in aqueous solutions of  
poly(ethylene glycol) PEG <https://www.doi.org/10.1016/j.jct.2016.06.030>  
solutions: Thermodynamic studies of  
interactions of amino acids and <https://www.doi.org/10.1016/j.jct.2012.05.009>  
lipid bilayers and protein with  
Molecular Dynamics Simulation of <https://www.doi.org/10.1016/j.jct.2019.06.002>  
Solubility of Alanine in Biological  
Media: N,N-Dimethylformamide,  
N-methyl-2-pyrrolidone, Water, Ethanol, <https://www.doi.org/10.1016/j.jct.2015.11.015>  
N,N-Dimethylacetamide, Acetone, and  
Ethyl Propyl Carbazate between liquid and  
solid states: Thermodynamic studies of  
Amino Acids in Mannitol Aqueous  
solutions at different temperatures by  
amino acids and globular proteins:  
Thermodynamic considerations  
B-Coefficients of Some Amino Acids in  
Aqueous Solution Behavior of some amino  
acids in aqueous solutions of  
poly(ethylene glycol) PEG  
solutions: Thermodynamic studies of  
interactions of amino acids and  
lipid bilayers and protein with  
Molecular Dynamics Simulation of  
Solubility of Alanine in Biological  
Media: N,N-Dimethylformamide,  
N-methyl-2-pyrrolidone, Water, Ethanol,  
N,N-Dimethylacetamide, Acetone, and  
Ethyl Propyl Carbazate between liquid and  
solid states: Thermodynamic studies of  
Amino Acids in Mannitol Aqueous  
solutions at different temperatures by  
amino acids and globular proteins:  
Thermodynamic considerations  
DL-mandelic acid in aqueous medium  
at temperatures from 293.15 K to 313.15  
K:



Temperature and concentration dependence towards physicochemical interactions in the enantiomers L-proline, L-valine and L-franconine with NO<sub>2</sub> and NO<sub>3</sub> radicals: An effect of concentration and temperatures: An experimental and theoretical study: Properties of the novel cyclic alpha-amino acids in aqueous solution: Physicochemical and thermodynamic properties of the novel cyclic alpha-amino acids: Volumetric and calorimetric studies: Acoustic Properties of Procainamide Hydrochloride in Aqueous Solution and in Aqueous Air: Ternary Mixtures of Procainamide Hydrochloride with Water and Ethanol: Volumetric, compressibility, and calorimetric studies:

<https://www.doi.org/10.1016/j.jct.2018.09.026>  
<https://www.doi.org/10.1016/j.tca.2008.10.023>  
<https://www.doi.org/10.1016/j.jct.2019.03.011>  
<https://www.doi.org/10.1007/s10765-015-2006-0>  
<https://www.doi.org/10.1016/j.jct.2013.08.018>  
<https://www.doi.org/10.1021/acs.jced.7b00452>  
<https://www.doi.org/10.1016/j.jct.2011.05.012>

## Legend

<b>cp<sub>g</sub>:</b>	Ideal gas heat capacity
<b>cp<sub>s</sub>:</b>	Solid phase heat capacity
<b>g<sub>f</sub>:</b>	Standard Gibbs free energy of formation
<b>h<sub>f</sub>:</b>	Enthalpy of formation at standard conditions
<b>h<sub>fus</sub>:</b>	Enthalpy of fusion at standard conditions
<b>h<sub>vap</sub>:</b>	Enthalpy of vaporization at standard conditions
<b>log<sub>10</sub>w<sub>s</sub>:</b>	Log <sub>10</sub> of Water solubility in mol/l
<b>log<sub>p</sub>:</b>	Octanol/Water partition coefficient
<b>mc<sub>vol</sub>:</b>	McGowan's characteristic volume
<b>pc:</b>	Critical Pressure
<b>tb:</b>	Normal Boiling Point Temperature
<b>tc:</b>	Critical Temperature
<b>tf:</b>	Normal melting (fusion) point
<b>vc:</b>	Critical Volume

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