dl-2-Aminobutyric acid

Other names:	(.+-.)-.alpha.-aminobutyric acid
	(Â±)-2-aminobutyric acid
	2-Aminobutyric acid
	2-Aminobutyric acid, dl
	Aminobutyric acid,-2-
	Butanoic acid, 2-amino-
	Butanoic acid, 2-amino-, (.+/-.)-
	Butyric acid, 2-amino-, DL-
	Butyric acid, dl-2-amino-, beta-form
	Butyrine
	DL-.alpha.-amino-n-butyric acid
	DL-.alpha.-aminobutanoic acid
	DL-.alpha.-aminobutyric acid
	DL-2-amino-n-butyric acid
	DL-2-aminobutanoic acid
	NSC 3251
	butanoic acid, 2-amino-, (.+-.)-
	dl-Â«alphaÂ»-Amino-n-butyric acid
	Â«alphaÂ»-Aminobutyric acid
Inchi:	InChI=1S/C4H9NO2/c1-2-3(5)4(6)7/h3H,2,5H2,1H3,(H,6,7)
InchiKey:	QWCKQJZIFLGMSD-UHFFFAOYSA-N
Formula:	C4H9NO2
SMILES:	CCC([NH3+])C(=O)[O-]
Mol. weight [g/mol]:	103.12
CAS:	80-60-4

Physical Properties

Property code	Value	Unit	Source
ie	8.70	eV	NIST Webbook
log10ws	0.13		Crippen Method
logp	-2.243		Crippen Method
mcvol	84.640	ml/mol	McGowan Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cps	160.70	J/mol×K	323.00	NIST Webbook

Sources

Molecular interactions of some amino acids in aqueous 1-butyl-3-methylimidazolium bromide solutions at different temperatures: A volumetric approach:	https://www.doi.org/10.1016/j.jct.2018.05.008
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Binary Diffusion Coefficients of Aqueous Phenylalanine, Tyrosine Isomers, and Aminobutyric Acids at Infinitesimal Concentration and Temperatures from (293.2 to 333.2) K:	https://www.doi.org/10.1021/je3012698
Effect of sodium caproate on the volumetric and viscometric properties of glycine, DL-α-alanine, and DL-α-amino-n-butyric acid in aqueous solutions:	https://www.doi.org/10.1016/j.jct.2003.11.001
Solubility and Solvation Thermodynamics of a Series of Homologous α-Amino Acids in Nonaqueous Binary Mixtures of Ethylene Glycol and Dimethyl Sulfoxide:	https://www.doi.org/10.1021/je5007899
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C80604&Units=SI
Effect of glycine, DL-alanine and DL-2-aminobutyric acid on the temperature of maximum density of water:	https://www.doi.org/10.1016/j.jct.2015.04.024
Effect of temperature on the partial molar volume, isentropic compressibility and viscosity of DL-2-aminobutyric acid in water and in aqueous sodium chloride solutions:	https://www.doi.org/10.1016/j.jct.2016.09.040
Mode of action of betaine on some amino acids and globular proteins: Thermodynamic considerations:	https://www.doi.org/10.1016/j.jct.2017.03.025
Excess Volumes of Water in Hydrate Complexes of Some alpha-Amino Acids:	https://www.doi.org/10.1021/je400415r
Osmotic and activity coefficients of glycine, dl-a-alanine and dl-a-aminobutyric acid in aqueous solutions at temperatures between 288.15 and 303.15 K:	https://www.doi.org/10.1016/j.fluid.2006.10.012
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Partial Molar Volumes and Viscosities of Some r-Amino Acids in Micellar Solutions of Sodium Caprylate:	https://www.doi.org/10.1021/je049927v
Infinite Dilution Binary Diffusion Coefficients of Several r-Amino Acids in Water over a Temperature Range from (293.2 to 333.2) K with the Taylor Dispersion Technique:	https://www.doi.org/10.1021/je060149b
Thermodynamics of the interactions of a homologous series of some amino acids with trimethylamine N-oxide: Volumetric, compressibility, and calorimetric studies:	https://www.doi.org/10.1016/j.jct.2011.05.012
Study of Interactions between Amino Acids and Zinc Chloride in Aqueous Solutions through Volumetric Measurements at T = (288.15 to 318.15) K:	https://www.doi.org/10.1021/je8001464
Thermodynamics of the interactions of some amino acids and peptides with dodecyltrimethylammonium bromide and tetradecyltrimethylammonium bromide:	https://www.doi.org/10.1016/j.jct.2013.11.001
Surface Tension of Glycine, Alanine, Aminobutyric Acid, Norvaline, and Norleucine in Water and in Aqueous Solutions of Strong Electrolytes at Temperatures from (293.15 to 313.15) K:	https://www.doi.org/10.1021/acs.jced.7b00433
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Interaction of homologous series of amino acids with sarcosine in presence of denaturant: Volumetric and calorimetric approach:	https://www.doi.org/10.1016/j.jct.2013.09.009
Volumetric and Viscometric Studies of Some Amino Acids in Aqueous Solutions of Cadmium Chloride at T = (288.15 to 318.15) K and at Atmospheric Pressure:	https://www.doi.org/10.1021/je100909b
The vapour pressures over saturated aqueous solutions of the DL-2-aminobutyric acid:	https://www.doi.org/10.1016/j.jct.2007.12.005
Diffusion and structural behaviour of DL-2-aminobutyric acid, 4-aminobutyric acid, sodium D-gluconate, sodium hippurate, and potassium magnesium-L-aspartate:	https://www.doi.org/10.1016/j.jct.2019.03.009

Legend

cps:	Solid phase heat capacity
ie:	Ionization energy
log10ws:	Log10 of Water solubility in mol/l

logp: Octanol/Water partition coefficient

mcvol: McGowan's characteristic volume