4-Aminobutanoic acid

Other names:	.gamma.-aminobutyric acid
	.omega.-aminobutyric acid
	3-carboxypropylamine
	4-Amino-n-butyric acid
	4-aminobutanoic acid [GABA]
	4-aminobutyric acid
	Aminalon
	Aminobutyric acid,-4-
	Butanoic acid, 4-amino-
	Butyric acid, 4-amino-
	DF 468
	GABA
	Gaballon
	Gamarex
	Gamastan
	Gammagee
	Gammalon
	Gammalone
	Gammar
	Gammasol
	Gamulin
	Globulin, immune human serum
	Immu-G
	Immuglobin
	Mielogen
	Mielomade
	NSC 27418
	Reanal
	piperidic acid
	piperidinic acid
	«gamma»-Amino-n-butyric acid
	«gamma»-Aminobutanoic acid
	«gamma»-Aminobutyric acid
	«omega»-Aminobutyric acid
Inchi:	InChI=1S/C4H9NO2/c5-3-1-2-4(6)7/h1-3,5H2,(H,6,7)
InchiKey:	BTCSSZJGUNDROE-UHFFFAOYSA-N
Formula:	C4H9NO2
SMILES:	NCCCC(=O)O
Mol. weight [g/mol]:	103.12
CAS:	56-12-2

Physical Properties

Property code	Value	Unit	Source
chs	-2282.40 ± 0.84	kJ/mol	NIST Webbook
chs	-2279.23 ± 0.11	kJ/mol	NIST Webbook
chs	-2280.00 ± 4.70	kJ/mol	NIST Webbook
gf	-216.49	kJ/mol	Joback Method
hf	-441.00 ± 2.00	kJ/mol	NIST Webbook
hfs	-561.00 ± 4.70	kJ/mol	NIST Webbook
hfs	-581.10 ± 0.30	kJ/mol	NIST Webbook
hfus	17.00	kJ/mol	Joback Method
hsub	140.00 ± 2.00	kJ/mol	NIST Webbook
hvap	58.56	kJ/mol	Joback Method
ie	8.70	eV	NIST Webbook
ie	9.60	eV	NIST Webbook
log10ws	-0.03		Crippen Method
logp	-0.190		Crippen Method
mcvol	84.640	ml/mol	McGowan Method
pc	5175.72	kPa	Joback Method
tb	509.50	K	Joback Method
tc	695.04	K	Joback Method
tf	328.85	K	Joback Method
vc	0.314	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	190.29	J/mol×K	509.50	Joback Method
cpg	222.70	J/mol×K	664.11	Joback Method
cpg	216.84	J/mol×K	633.19	Joback Method
cpg	210.68	J/mol×K	602.27	Joback Method
cpg	204.20	J/mol×K	571.35	Joback Method
cpg	197.41	J/mol×K	540.42	Joback Method
cpg	228.27	J/mol×K	695.04	Joback Method
cps	146.40	J/mol×K	298.15	NIST Webbook
cps	133.60	J/mol×K	298.00	NIST Webbook
hsubt	140.00 ± 2.00	kJ/mol	395.00	NIST Webbook

hsubt	138.90 ± 0.60	kJ/mol	395.50	NIST Webbook
hsubt	139.00 ± 4.00	kJ/mol	467.50	NIST Webbook
hvapt	87.00 ± 2.00	kJ/mol	496.50	NIST Webbook

Sources

Measurement and Correlation of Solubility of -Aminobutyric Acid in Different Binary Solvents:	https://www.doi.org/10.1021/acs.jced.5b00829
Studies on molecular interactions of some neurotransmitters in water using Crippen Method:	https://www.doi.org/10.1016/j.jct.2015.09.020
Volumetric and compressibility measurements at T = (278.15, 288.15 and 298.15) K:	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 (278.2 to 333.2) K:	https://www.doi.org/10.1021/je3012698
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
Volumetric Properties of Some a,w-Aminocarboxylic Acids in Aqueous Sodium Acetate and Magnesium Acetate Solutions at T = 288.15 to 328.15 K:	https://www.doi.org/10.1021/je100476h
Osmotic and activity coefficients of alpha, omega-amino acids in aqueous solutions at 298.15 K:	https://www.doi.org/10.1016/j.fluid.2014.02.004
Determination and correlation of solubility and thermodynamics of mixing of 4-aminobutyric acid in mono-solvents and binary solvent mixtures:	https://www.doi.org/10.1016/j.jct.2016.07.014
Enthalpic interactions between some amino acids and cyclohexanone in aqueous solutions at 298.15K:	https://www.doi.org/10.1016/j.tca.2006.07.009
Ultrasonic Studies of 4-Aminobutyric Acid in Aqueous Metformin Hydrochloride Solutions at Different Temperatures:	https://www.doi.org/10.1007/s10765-010-0862-1
Binary Diffusion Coefficients of Aqueous Straight-Chain Amino Acids at Infinitesimal Concentration and Temperatures from (278.2 to 333.2) K:	https://www.doi.org/10.1021/je301370s
Partial Molar Volumes, Partial Molar Compressibilities, and Viscosities of Glycine, DL-Alanine, and DL-2-Aminobutyric Acid in Aqueous Solutions from 278.15 to 308.15 K:	https://www.doi.org/10.1021/acs.jced.8b00236
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C56122&Units=SI
alpha,w-Amino Acids in Water and in Aqueous Solutions of Sodium Chloride over a Temperature Range of 278.2-318.2 K:	https://www.doi.org/10.1016/j.jct.2016.09.014
The structure and diffusion behaviour of the neurotransmitter gamma-aminobutyric acid (GABA) in neutral aqueous solutions:	https://www.chemeo.com/doc/models/crippen_log10ws
The vapour pressures over saturated aqueous solutions of DL-2-aminobutyric acid, 4-aminobutyric acid, sodium propionate, sodium nitrate, and potassium nitrate:	https://www.doi.org/10.1016/j.jct.2007.12.005
Effect of temperature on the partial molar volumes, partial molar adiabatic compressibilities, and viscosity B-coefficients of DL-4-aminobutyric acid in water and in aqueous sodium chloride solutions:	https://www.doi.org/10.1016/j.jct.2017.07.037
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Effect of temperature on the partial molar volumes, partial molar adiabatic compressibilities, and viscosity B-coefficients of DL-4-aminobutyric acid in water and in aqueous sodium chloride solutions:	https://www.doi.org/10.1021/acs.jced.9b00327
Physicochemical Properties of Neurotransmitter GABA:	https://www.doi.org/10.1016/j.jct.2011.04.019
Thermodynamic and Theoretical Approach:	

Legend

chs:	Standard solid enthalpy of combustion
cpg:	Ideal gas heat capacity
cps:	Solid phase heat capacity
gf:	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
hsub:	Enthalpy of sublimation at standard conditions
hsubt:	Enthalpy of sublimation at a given temperature

hvap:	Enthalpy of vaporization at standard conditions
hvapt:	Enthalpy of vaporization at a given temperature
ie:	Ionization energy
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