1-Butanamine

Other names:	1-AMINOBUTANE
	1-Amino-butaan
	1-Aminobutan
	1-Butylamine
	BUTYLAMINE
	Butanamine
	Mono-n-butylamine
	Monobutilamina
	Monobutylamine
	N-Butylamin
	NORVALAMINE
	NSC 8029
	Norralamine
	UN 1125
	n-Butilamina
	n-Butylamine
	n-C4H9NH2
Inchi:	InChI=1S/C4H11N/c1-2-3-4-5/h2-5H2,1H3
InchiKey:	HQABUPZFAYXKJW-UHFFFAOYSA-N
Formula:	C4H11N
SMILES:	CCCCN
Mol. weight [g/mol]:	73.14
CAS:	109-73-9

Physical Properties

Property code	Value	Unit	Source
af	0.3290		KDB
affp	921.50	kJ/mol	NIST Webbook
aigt	585.37	K	KDB
basg	886.60	kJ/mol	NIST Webbook
chl	-2984.00	kJ/mol	NIST Webbook
chl	-3018.50 ± 1.10	kJ/mol	NIST Webbook
chs	-3018.00	kJ/mol	NIST Webbook
dm	1.30	debye	KDB

dvisc	0.0004760	Pa×s	A volumetric and viscosity study for the binary mixtures of 1-hexyl-3-methylimidazolium tetrafluoroborate with some molecular solvents
dvisc	0.0004930	Pa×s	Excess Molar Volumes and Viscosity Deviations of Binary Liquid Mixtures of 1,3-Dioxolane and 1,4-Dioxane with Butyl Acetate, Butyric Acid, Butylamine, and 2-Butanone at 298.15 K
fll	1.70	% in Air	KDB
flu	9.80	% in Air	KDB
fpc	272.04	K	KDB
fpo	260.93	K	KDB
gf	49.24	kJ/mol	KDB
hf	-92.11	kJ/mol	KDB
hf	-149.30	kJ/mol	NIST Webbook
hf	-95.00 ± 2.00	kJ/mol	NIST Webbook
hfl	-127.70 ± 1.20	kJ/mol	NIST Webbook
hfl	-182.00	kJ/mol	NIST Webbook
hfus	11.31	kJ/mol	Joback Method
hvap	35.14	kJ/mol	Joback Method
ie	9.40	eV	NIST Webbook
ie	8.79	eV	NIST Webbook
ie	8.70	eV	NIST Webbook
ie	8.73 ± 0.04	eV	NIST Webbook
ie	8.71 ± 0.03	eV	NIST Webbook
log10ws	-0.93		Crippen Method
logp	0.745		Crippen Method
mcvol	77.200	ml/mol	McGowan Method
nfpaf	%!d(float64=3)		KDB
nfpah	%!d(float64=2)		KDB
pc	4200.00 ± 41.96	kPa	NIST Webbook
pc	4250.00	kPa	KDB
pc	4154.33 ± 1.50	kPa	NIST Webbook
rinpol	627.00		NIST Webbook
rinpol	628.00		NIST Webbook
rinpol	628.00		NIST Webbook
rinpol	628.00		NIST Webbook
rinpol	626.00		NIST Webbook
rinpol	626.00		NIST Webbook
rinpol	614.00		NIST Webbook
rinpol	617.00		NIST Webbook
rinpol	621.00		NIST Webbook

rinpol	629.00		NIST Webbook
rinpol	629.00		NIST Webbook
rinpol	610.00		NIST Webbook
rinpol	609.40		NIST Webbook
rinpol	609.40		NIST Webbook
rinpol	608.00		NIST Webbook
rinpol	619.00		NIST Webbook
ripol	890.00		NIST Webbook
ripol	904.00		NIST Webbook
ripol	886.00		NIST Webbook
ripol	908.00		NIST Webbook
ripol	912.00		NIST Webbook
ripol	896.00		NIST Webbook
ripol	918.00		NIST Webbook
tb	350.00	K	Evolution of the Liquid Vapor Equilibrium Properties of Several Unsymmetrical Amines: Determination of Their Binary Isobaric Diagrams and Applications to the Distillation
tb	350.15	K	KDB
tc	524.15 ± 1.50	K	NIST Webbook
tc	531.90 ± 0.53	K	NIST Webbook
tc	524.00	K	NIST Webbook
tc	531.90	K	KDB
tf	224.05	K	KDB
tf	222.65 ± 0.50	K	NIST Webbook
tf	224.00 ± 0.10	K	NIST Webbook
tf	224.05	K	NIST Webbook
vc	0.277	m3/kmol	KDB
volm	9.99e-05	m3/mol	Thermodynamic study of (heptane + amine) mixtures. II. Excess and partial molar volumes at 298.15 K
zc	0.2661960		KDB

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	163.72	J/mol×K	454.29	Joback Method
cpg	138.68	J/mol×K	363.45	Joback Method
cpg	147.36	J/mol×K	393.73	Joback Method

cpg	155.70	J/mol×K	424.01	Joback Method
cpg	178.82	J/mol×K	514.85	Joback Method
cpg	185.91	J/mol×K	545.13	Joback Method
cpg	171.42	J/mol×K	484.57	Joback Method
cpl	188.00	J/mol×K	298.15	NIST Webbook
dvisc	0.0004000	Pa×s	313.15	Density and Viscosity Measurement of n-Butylamine with Hexyl Alcohol Isomer Binary Systems
dvisc	0.0004670	Pa×s	303.15	Relative Permittivity, Viscosity, and Speed of Sound for 2-Methoxyethanol + Butylamine Mixtures
dvisc	0.0004960	Pa×s	298.15	Relative Permittivity, Viscosity, and Speed of Sound for 2-Methoxyethanol + Butylamine Mixtures
dvisc	0.0005250	Pa×s	293.15	Relative Permittivity, Viscosity, and Speed of Sound for 2-Methoxyethanol + Butylamine Mixtures
dvisc	0.0004600	Pa×s	303.15	Density and Viscosity Measurement of n-Butylamine with Hexyl Alcohol Isomer Binary Systems
dvisc	0.0004440	Pa×s	303.15	Studies of viscosities of dilute solutions of alkylamine in non-electrolyte solvents. II. Haloalkanes and other polar solvents
dvisc	0.0003600	Pa×s	323.15	Density and Viscosity Measurement of n-Butylamine with Hexyl Alcohol Isomer Binary Systems

dvisc	0.0003930	Pa×s	313.15	Studies of viscosities of dilute solutions of alkylamine in non-electrolyte solvents. II. Haloalkanes and other polar solvents
hvapt	33.50 ± 0.10	kJ/mol	323.00	NIST Webbook
hvapt	35.50	kJ/mol	322.50	NIST Webbook
hvapt	34.70 ± 0.10	kJ/mol	313.00	NIST Webbook
hvapt	31.81	kJ/mol	350.20	NIST Webbook
hvapt	35.20	kJ/mol	320.50	NIST Webbook
hvapt	34.70	kJ/mol	331.50	NIST Webbook
hvapt	31.10 ± 0.10	kJ/mol	358.00	NIST Webbook
hvapt	32.40 ± 0.10	kJ/mol	343.00	NIST Webbook
hvapt	32.09	kJ/mol	350.10	KDB
pvap	66.66	kPa	337.90	Evolution of the Liquid Vapor Equilibrium Properties of Several Unsymmetrical Amines: Determination of Their Binary Isobaric Diagrams and Applications to the Distillation
pvap	86.66	kPa	345.10	Evolution of the Liquid Vapor Equilibrium Properties of Several Unsymmetrical Amines: Determination of Their Binary Isobaric Diagrams and Applications to the Distillation
pvap	101.33	kPa	350.00	Evolution of the Liquid Vapor Equilibrium Properties of Several Unsymmetrical Amines: Determination of Their Binary Isobaric Diagrams and Applications to the Distillation

pvap	26.66	kPa	314.70	Evolution of the Liquid Vapor Equilibrium Properties of Several Unsymmetrical Amines: Determination of Their Binary Isobaric Diagrams and Applications to the Distillation
pvap	19.99	kPa	308.30	Evolution of the Liquid Vapor Equilibrium Properties of Several Unsymmetrical Amines: Determination of Their Binary Isobaric Diagrams and Applications to the Distillation
pvap	46.66	kPa	328.20	Evolution of the Liquid Vapor Equilibrium Properties of Several Unsymmetrical Amines: Determination of Their Binary Isobaric Diagrams and Applications to the Distillation
pvap	59.99	kPa	334.80	Evolution of the Liquid Vapor Equilibrium Properties of Several Unsymmetrical Amines: Determination of Their Binary Isobaric Diagrams and Applications to the Distillation
pvap	33.33	kPa	319.90	Evolution of the Liquid Vapor Equilibrium Properties of Several Unsymmetrical Amines: Determination of Their Binary Isobaric Diagrams and Applications to the Distillation

rhol	714.00	kg/m3	318.15	Excess Molar Properties for Binary Systems of CnMIM-BF4 Ionic Liquids with Alkylamines in the Temperature Range (298.15 to 318.15) K. Experimental Results and Theoretical Model Calculations
rhol	723.67	kg/m3	308.15	Excess Molar Properties for Binary Systems of CnMIM-BF4 Ionic Liquids with Alkylamines in the Temperature Range (298.15 to 318.15) K. Experimental Results and Theoretical Model Calculations
rhol	733.33	kg/m3	298.15	Excess Molar Properties for Binary Systems of CnMIM-BF4 Ionic Liquids with Alkylamines in the Temperature Range (298.15 to 318.15) K. Experimental Results and Theoretical Model Calculations
rhol	732.23	kg/m3	298.15	Thermodynamics of amide + amine mixtures. 1. Volumetric, speed of sound, and refractive index data for N,Ndimethylformamide + N-propylpropan-1-amine, + N-butylbutan-1-amine, + butan-1-amine, or + hexan-1-amine systems at several temperatures

rhol	727.45	kg/m3	303.15	Thermodynamics of amide + amine mixtures. 1. Volumetric, speed of sound, and refractive index data for N,Ndimethylformamide + N-propylpropan-1-amine, + N-butylbutan-1-amine, + butan-1-amine, or + hexan-1-amine systems at several temperatures
rhol	737.05	kg/m3	293.15	Thermodynamics of amide + amine mixtures. 1. Volumetric, speed of sound, and refractive index data for N,Ndimethylformamide + N-propylpropan-1-amine, + N-butylbutan-1-amine, + butan-1-amine, or + hexan-1-amine systems at several temperatures
rhol	734.65	kg/m3	298.15	Volumetric properties for binary and ternary systems consist of 1-chlorobutane, n-butylamine and isobutanol at 298.15 K with application of the Prigogine-Flory-Patterson theory and ERAS-Model
rhol	728.65	kg/m3	303.15	Studies of viscosities of dilute solutions of alkylamines in non-electrolyte solvents III. Alkylamines in butanols 303.15K

rhol	719.17	kg/m3	313.15	Studies of partial molar volumes of alkylamine in non-electrolyte solvents I. Alkylamines in hydrocarbons at 303.15 and 313.15K	
rhol	728.65	kg/m3	303.15	Studies of partial molar volumes of alkylamine in non-electrolyte solvents I. Alkylamines in hydrocarbons at 303.15 and 313.15K	
rhol	709.21	kg/m3	323.15	Binary mixtures of ([C4mim][NTf2] + molecular organic solvents): Thermophysical, acoustic and transport properties at various compositions and temperatures	
rhol	714.10	kg/m3	318.15	Binary mixtures of ([C4mim][NTf2] + molecular organic solvents): Thermophysical, acoustic and transport properties at various compositions and temperatures	
rhol	718.66	kg/m3	313.15	Binary mixtures of ([C4mim][NTf2] + molecular organic solvents): Thermophysical, acoustic and transport properties at various compositions and temperatures	

rhol	723.67	kg/m3	308.15	Binary mixtures of ([C4mim][NTf2] + molecular organic solvents): Thermophysical, acoustic and transport properties at various compositions and temperatures	
rhol	728.50	kg/m3	303.15	Binary mixtures of ([C4mim][NTf2] + molecular organic solvents): Thermophysical, acoustic and transport properties at various compositions and temperatures	
rhol	733.33	kg/m3	298.15	Binary mixtures of ([C4mim][NTf2] + molecular organic solvents): Thermophysical, acoustic and transport properties at various compositions and temperatures	
rhol	722.66	kg/m3	308.15	Volumetric properties of binary mixtures of (acetonitrile + amines) at several temperatures with application of the ERAS model	
rhol	727.51	kg/m3	303.15	Volumetric properties of binary mixtures of (acetonitrile + amines) at several temperatures with application of the ERAS model	

rhol	732.33	kg/m3	298.15	Volumetric properties of binary mixtures of (acetonitrile + amines) at several temperatures with application of the ERAS model	
rhol	727.34	kg/m3	303.15	Volumetric behaviour of binary mixtures of (trichloromethane + amines) at temperatures between T = (288.15 and 303.15) K at p = 0.1 MPa	
rhol	732.15	kg/m3	298.15	Volumetric behaviour of binary mixtures of (trichloromethane + amines) at temperatures between T = (288.15 and 303.15) K at p = 0.1 MPa	
rhol	736.95	kg/m3	293.15	Volumetric behaviour of binary mixtures of (trichloromethane + amines) at temperatures between T = (288.15 and 303.15) K at p = 0.1 MPa	
rhol	741.72	kg/m3	288.15	Volumetric behaviour of binary mixtures of (trichloromethane + amines) at temperatures between T = (288.15 and 303.15) K at p = 0.1 MPa	

rhol	733.30	kg/m3	298.15	Volumetric, acoustic, viscometric, and spectroscopic properties for binary properties for binary mixtures of alkoxypropanol with mono, di-, and tri-alkylamines at a temperature of 298.15K
rhol	732.18	kg/m3	298.15	Thermodynamics of amide + amine mixtures. 5. Excess molar enthalpies of N,N-dimethylformamide or N,N-dimethylacetamide + N-propylpropan-1-amine, + N-butylbutan-1-amine, + butan-1-amine, or + hexan-1-amine systems at 298.15 K. Application of the ERAS model
rhol	737.12	kg/m3	293.15	Volumetric properties of binary mixtures of (acetonitrile + amines) at several temperatures with application of the ERAS model
rhol	739.00	kg/m3	293.00	KDB
speedsl	1228.92	m/s	303.15	Densities, Excess Molar Volumes, Speeds of Sound, and Isothermal Compressibilities for 2-(2-Hexyloxyethoxy)ethanol + n-Alkylamine at Temperatures Between 288.15 K and 308.15 K

speedsl	1228.92	m/s	303.15	Volumetric and Acoustic Properties for Binary Mixtures of Dipropylene Glycol Monopropyl Ether with Alkylamines at Temperatures Between 288.15 K and 308.15 K
speedsl	1205.72	m/s	308.15	Densities, Excess Molar Volumes, Speeds of Sound, and Isothermal Compressibilities for 2-(2-Hexyloxyethoxy)ethanol + n-Alkylamine at Temperatures Between 288.15 K and 308.15 K
speedsl	1249.96	m/s	298.15	Densities, Excess Molar Volumes, Speeds of Sound, and Isothermal Compressibilities for 2-(2-Hexyloxyethoxy)ethanol + n-Alkylamine at Temperatures Between 288.15 K and 308.15 K
speedsl	1273.56	m/s	293.15	Densities, Excess Molar Volumes, Speeds of Sound, and Isothermal Compressibilities for 2-(2-Hexyloxyethoxy)ethanol + n-Alkylamine at Temperatures Between 288.15 K and 308.15 K
speedsl	1296.08	m/s	288.15	Densities, Excess Molar Volumes, Speeds of Sound, and Isothermal Compressibilities for 2-(2-Hexyloxyethoxy)ethanol + n-Alkylamine at Temperatures Between 288.15 K and 308.15 K

speedsl	1205.72	m/s	308.15	Volumetric and Acoustic Properties for Binary Mixtures of Dipropylene Glycol Monopropyl Ether with Alkylamines at Temperatures Between 288.15 K and 308.15 K	
speedsl	1249.96	m/s	298.15	Volumetric and Acoustic Properties for Binary Mixtures of Dipropylene Glycol Monopropyl Ether with Alkylamines at Temperatures Between 288.15 K and 308.15 K	
speedsl	1273.56	m/s	293.15	Volumetric and Acoustic Properties for Binary Mixtures of Dipropylene Glycol Monopropyl Ether with Alkylamines at Temperatures Between 288.15 K and 308.15 K	
speedsl	1296.08	m/s	288.15	Volumetric and Acoustic Properties for Binary Mixtures of Dipropylene Glycol Monopropyl Ether with Alkylamines at Temperatures Between 288.15 K and 308.15 K	
srf	0.02	N/m	293.20	KDB	

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.45389e+01

Coeff. B	-3.02088e+03
Coeff. C	-4.64950e+01
Temperature range (K), min.	258.47
Temperature range (K), max.	373.87

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/T + C*ln(T) + D*T^2
Coeff. A	5.84534e+01
Coeff. B	-6.04187e+03
Coeff. C	-6.30480e+00
Coeff. D	2.90389e-06
Temperature range (K), min.	224.05
Temperature range (K), max.	531.90

Datasets

Viscosity, Pa*s

Temperature, K - Liquid	Pressure, kPa - Liquid	Viscosity, Pa*s - Liquid
303.15	101.33	0.0004442

Reference *https://www.doi.org/10.1016/j.tca.2009.07.008*

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

Studies of partial molar volumes of alkylamine in non-electrolyte solvents I. Alkylamines in hydrocarbons at 303.15 and 313.15K: https://www.doi.org/10.1016/j.tca.2005.08.012

KDB Pure (Korean Thermophysical Properties Databank): https://www.cheric.org/research/kdb/hcprop/showprop.php?cmpid=1262

Thermodynamic study of (heptane + amine) mixtures. II. Excess and partial molar volumes at 298.15 K: https://www.doi.org/10.1016/j.jct.2010.12.025

Excess Molar Volumes and Viscosity Deviations of Binary Liquid Mixtures of 1,3-Dioxolane and 1,4-Dioxane with Butyl Acetate, Butyric Acid, Butylamine, and 2-Butanone at 298.15 K: https://www.doi.org/10.1021/je0504109

Studies of viscosities of dilute solutions of alkylamine in non-electrolyte solvents. II. Haloalkanes and other polar solvents: https://www.doi.org/10.1016/j.tca.2004.08.013

Evolution of the Liquid Vapor Equilibrium Properties of Several Unsymmetrical Amines: Determination of Their Binary Isobaric Diagrams and Applications to the Distillation: https://www.doi.org/10.1021/je3009649

Studies of viscosities of dilute solutions of alkylamines in non-electrolyte solvents. III. Alkylamines in butanols 303.15K: https://www.doi.org/10.1016/j.tca.2009.02.005

Establishing benchmarks for the Second Industrial Fluids Simulation Challenge: https://www.doi.org/10.1016/j.fluid.2005.04.020

Thermodynamics of amide + amine mixtures. 1. Volumetric, speed of sound, and refractive index data for N,N-dimethylformamide + N-propylpropan-1-amine, + N-butylbutan-1-amine, + butan-1-amine, or + hexan-1-amine systems at several temperatures: https://www.doi.org/10.1021/acs.jced.5b00802

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Thermodynamic study of heptane + amine mixtures. V. Excess and solvation energies at 298.15 K with application of the Flory-Patterson theory and ERAS Model: https://www.doi.org/10.1016/j.fluid.2014.12.017

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Density and Viscosity Measurement of n-Butylamine with Hexyl Alcohol Isomer Binary Systems: https://www.doi.org/10.1021/je0498053

Binary mixtures of ([C4mim][NTf2] + molecular organic solvents): Thermophysical, acoustic and transport properties at various compositions and temperatures: https://www.doi.org/10.1016/j.jct.2015.09.022

Densities, Excess Molar Volumes, Speeds of Sound, and Isothermal Compressibilities for 2-(2-Hexyloxyethoxy)ethanol + n-Alkylamine at Temperatures Between T = 288.15 K and 308.15 K: https://www.doi.org/10.1021/je800026p

Volumetric behaviour of binary mixtures of (trichloromethane + amines) at temperatures between T = (288.15 and 303.15) K at p = 0.1 MPa: https://www.doi.org/10.1016/j.jct.2008.05.003

Studies of viscosities of dilute solutions of alkylamines in non-electrolyte solvents: IV. Alkylamines in 1,4-dioxane and oxolane at 303.15K: https://www.doi.org/10.1016/j.tca.2009.07.008

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C109739&Units=SI

Volumetric and Acoustic Properties for Binary Mixtures of Dipropylene Glycol Monopropyl Ether with Alkylamines at Temperatures Between 288.15 K and 308.15 K: https://www.doi.org/10.1007/s10765-009-0593-3

A volumetric and viscosity study for the binary mixtures of 1-hexyl-3-methylimidazolium tetrafluoroborate with some molecular solvents: https://www.doi.org/10.1016/j.jct.2010.12.027

Thermodynamics of amide + amine mixtures. 5. Excess molar enthalpies of N,N-dimethylformamide or N,N-dimethylacetamide + N-propylpropan-1-amine, + N-butylbutan-1-amine, + butan-1-amine, or + hexan-1-amine systems at 298.15 K. Application of the ERAS model: https://www.doi.org/10.1016/j.fluid.2019.112283

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

KDB: https://www.cheric.org/files/research/kdb/mol/mol1262.mol

Excess Molar Properties for Binary Systems of CnMIM-BF4 Ionic Liquids with Alkylamines in the Temperature Range (298.15 to 318.15) K. Experimental Results and Theoretical Model Calculations: https://www.doi.org/10.1021/je301167q

Thermodynamic Parameters of Anionic Surfactant-Additive Systems at the Cloud Point: https://www.doi.org/10.1021/je100502b

KDB Vapor Pressure Data: https://www.cheric.org/research/kdb/hcprop/showprop.php?cmpid=1262

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

Volumetric, acoustic, viscometric, and spectroscopic properties for binary mixtures of alkoxypropanol with mono-, di-, and tri-alkylamines at a temperature of 298.15K: https://www.doi.org/10.1016/j.jct.2005.12.007

Relative Permittivity, Viscosity, and Speed of Sound for 2-Methoxyethanol + Butylamine Mixtures: https://www.doi.org/10.1021/je030127e

Legend

af:	Acentric Factor
affp:	Proton affinity
aigt:	Autoignition Temperature
basg:	Gas basicity
chl:	Standard liquid enthalpy of combustion
chs:	Standard solid enthalpy of combustion
cpg:	Ideal gas heat capacity
cpl:	Liquid phase heat capacity
dm:	Dipole Moment
dvisc:	Dynamic viscosity
fll:	Lower Flammability Limit
flu:	Upper Flammability Limit
fpc:	Flash Point (Closed Cup Method)
fpo:	Flash Point (Open Cup Method)
gf:	Standard Gibbs free energy of formation

hf:	Enthalpy of formation at standard conditions
hfl:	Liquid phase enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
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
nfpaf:	NFPA Fire Rating
nfpah:	NFPA Health Rating
pc:	Critical Pressure
pvap:	Vapor pressure
rhol:	Liquid Density
rinpol:	Non-polar retention indices
ripol:	Polar retention indices
speedsl:	Speed of sound in fluid
srf:	Surface Tension
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume
volm:	Molar Volume
zc:	Critical Compressibility