

# 1-Butanamine, N-butyl-

Other names:	(n-C <sub>4</sub> H <sub>9</sub> ) <sub>2</sub> NH Butylamine, di-n- DIBUTYLAMINE Di-n-butylamine Dibutilamina N-DIBUTYLAMINE N-butylbutanamine UN 2248 butanamine, N-butyl di-Normal-butylamine n-Butyl-1-butanamine
Inchi:	InChI=1S/C8H19N/c1-3-5-7-9-8-6-4-2/h9H,3-8H2,1-2H3
InchiKey:	JQVDAXLFBXTEQA-UHFFFAOYSA-N
Formula:	C <sub>8</sub> H <sub>19</sub> N
SMILES:	CCCCNCCCC
Mol. weight [g/mol]:	129.24
CAS:	111-92-2

## Physical Properties

Property code	Value	Unit	Source
af	0.5800		KDB
affp	968.50	kJ/mol	NIST Webbook
basg	935.30	kJ/mol	NIST Webbook
chl	-5657.44 ± 0.42	kJ/mol	NIST Webbook
chl	-5651.20 ± 2.20	kJ/mol	NIST Webbook
dm	1.10	debye	KDB
gf	105.87	kJ/mol	Joback Method
hf	-164.90	kJ/mol	NIST Webbook
hf	-171.10 ± 3.20	kJ/mol	NIST Webbook
hfl	-212.30 ± 2.50	kJ/mol	NIST Webbook
hfl	-206.10 ± 0.40	kJ/mol	NIST Webbook
hfus	21.57	kJ/mol	Joback Method
hvap	49.40 ± 0.10	kJ/mol	NIST Webbook
hvap	41.20 ± 2.00	kJ/mol	NIST Webbook
hvap	49.47	kJ/mol	NIST Webbook
hvap	45.70 ± 0.30	kJ/mol	NIST Webbook
hvap	49.44 ± 0.08	kJ/mol	NIST Webbook

hvap	48.10	kJ/mol	NIST Webbook
hvap	41.20	kJ/mol	NIST Webbook
ie	$7.69 \pm 0.03$	eV	NIST Webbook
log10ws	-1.44		Aqueous Solubility Prediction Method
logp	2.176		Crippen Method
mcvol	133.560	ml/mol	McGowan Method
pc	3110.00	kPa	KDB
pc	$3110.00 \pm 31.07$	kPa	NIST Webbook
rinpol	947.00		NIST Webbook
rinpol	943.00		NIST Webbook
rinpol	952.00		NIST Webbook
rinpol	943.00		NIST Webbook
rinpol	948.00		NIST Webbook
rinpol	947.00		NIST Webbook
rinpol	943.00		NIST Webbook
rinpol	951.00		NIST Webbook
rinpol	943.00		NIST Webbook
rinpol	952.00		NIST Webbook
rinpol	947.00		NIST Webbook
rinpol	951.00		NIST Webbook
rinpol	943.00		NIST Webbook
ripol	1103.00		NIST Webbook
ripol	1092.00		NIST Webbook
ripol	1095.00		NIST Webbook
ripol	1100.00		NIST Webbook
ripol	1106.00		NIST Webbook
ripol	1106.00		NIST Webbook
ripol	1090.00		NIST Webbook
tb	432.75	K	NIST Webbook
tb	$431.70 \pm 0.50$	K	NIST Webbook
tb	432.70	K	KDB
tb	$432.65 \pm 2.00$	K	NIST Webbook
tb	$433.15 \pm 3.00$	K	NIST Webbook
tb	$434.65 \pm 6.00$	K	NIST Webbook
tb	$431.65 \pm 5.00$	K	NIST Webbook
tb	$394.15 \pm 10.00$	K	NIST Webbook
tb	$433.15 \pm 4.00$	K	NIST Webbook
tb	432.20	K	NIST Webbook
tb	432.80	K	NIST Webbook
tc	$607.50 \pm 0.60$	K	NIST Webbook
tc	607.50	K	KDB
tc	607.50	K	Gas-Liquid Critical Temperatures of Some Alkenes, Amines, and Cyclic Hydrocarbons

tc	595.80	K	NIST Webbook
tf	211.25 ± 0.50	K	NIST Webbook
tf	211.25	K	NIST Webbook
tf	211.65	K	Aqueous Solubility Prediction Method
tf	211.00	K	KDB
vc	0.518	m3/kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	353.63	J/mol×K	600.98	Joback Method
cpg	293.01	J/mol×K	460.67	Joback Method
cpg	306.12	J/mol×K	488.73	Joback Method
cpg	318.72	J/mol×K	516.80	Joback Method
cpg	330.83	J/mol×K	544.86	Joback Method
cpg	342.46	J/mol×K	572.92	Joback Method
cpg	279.38	J/mol×K	432.61	Joback Method
dvisc	0.0006650	Paxs	313.15	Studies of viscosities of dilute solutions of alkylamine in non-electrolyte solvents. II. Haloalkanes and other polar solvents
dvisc	0.0007580	Paxs	303.15	Studies of viscosities of dilute solutions of alkylamine in non-electrolyte solvents. II. Haloalkanes and other polar solvents
hvapt	50.80	kJ/mol	298.15	The vaporization enthalpy and vapor pressure of S (+)-methamphetamine at T = 298.15 K by correlation gas chromatography
hvapt	38.44	kJ/mol	432.80	NIST Webbook
hvapt	46.00	kJ/mol	411.00	NIST Webbook
hvapt	46.00 ± 0.10	kJ/mol	343.00	NIST Webbook
hvapt	44.80 ± 0.10	kJ/mol	358.00	NIST Webbook

hvapt	48.10	kJ/mol	291.00	NIST Webbook
rhol	751.46	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	755.53	kg/m3	298.15	Thermodynamics of ketone + amine mixtures. Part IX. Excess molar enthalpies at 298.15K for dipropylamine, or dibutylamine + 2-alkanone systems and modeling of linear or aromatic amine + 2-alkanone mixtures in terms of DISQUAC and ERAS
rhol	755.70	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	757.53	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	759.70	kg/m3	293.15	Volumetric properties of binary mixtures of (acetonitrile + amines) at several temperatures with application of the ERAS model
rhol	755.61	kg/m3	298.15	Volumetric properties of binary mixtures of (acetonitrile + amines) at several temperatures with application of the ERAS model
rhol	751.50	kg/m3	303.15	Volumetric properties of binary mixtures of (acetonitrile + amines) at several temperatures with application of the ERAS model
rhol	747.38	kg/m3	308.15	Volumetric properties of binary mixtures of (acetonitrile + amines) at several temperatures with application of the ERAS model
rhol	759.58	kg/m3	293.15	Acoustic, volumetric and spectral studies of binary liquid mixtures of aliphatic dialkylamine and 2-alkanols at different temperatures

rhol	767.00	kg/m3	293.00	KDB
rhol	751.37	kg/m3	303.15	Acoustic, volumetric and spectral studies of binary liquid mixtures of aliphatic dialkylamine and 2-alkanols at different temperatures
rhol	747.27	kg/m3	308.15	Acoustic, volumetric and spectral studies of binary liquid mixtures of aliphatic dialkylamine and 2-alkanols at different temperatures
rhol	752.28	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	743.44	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	752.28	kg/m3	303.15	Studies of viscosities of dilute solutions of alkylamines in non-electrolyte solvents III. Alkylamines in butanols 303.15K

rhol	759.70	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	755.52	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	755.48	kg/m3	298.15	Acoustic, volumetric and spectral studies of binary liquid mixtures of aliphatic dialkylamine and 2-alkanols at different temperatures
speedsl	1289.23	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

speedsl	1269.47	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	1246.69	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	1226.70	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	1206.97	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	1261.23	m/s	293.15	Thermodynamics of (ketone + amine) mixtures. Part VI. Volumetric and speed of sound data at (293.15, 298.15, and 303.15) K for (2-heptanone + dipropylamine, +dibutylamine, or +triethylamine) systems

speedsl	1241.38	m/s	298.15	Thermodynamics of (ketone + amine) mixtures. Part VI. Volumetric and speed of sound data at (293.15, 298.15, and 303.15) K for (2-heptanone + dipropylamine, +dibutylamine, or +triethylamine) systems
speedsl	1222.21	m/s	303.15	Thermodynamics of (ketone + amine) mixtures. Part VI. Volumetric and speed of sound data at (293.15, 298.15, and 303.15) K for (2-heptanone + dipropylamine, +dibutylamine, or +triethylamine) systems
speedsl	1261.20	m/s	293.15	Thermodynamics of ketone + amine mixtures Part IV. Volumetric and speed of sound data at (293.15; 298.15 and 303.15 K) for 2-butanone +dipropylamine, +dibutylamine or +triethylamine systems
speedsl	1241.30	m/s	298.15	Thermodynamics of ketone + amine mixtures Part IV. Volumetric and speed of sound data at (293.15; 298.15 and 303.15 K) for 2-butanone +dipropylamine, +dibutylamine or +triethylamine systems

speedsl	1222.50	m/s	303.15	Thermodynamics of ketone + amine mixtures Part IV. Volumetric and speed of sound data at (293.15; 298.15 and 303.15 K) for 2-butanone +dipropylamine, +dibutylamine or +triethylamine systems
speedsl	1289.23	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	1269.47	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	1246.69	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	1226.70	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	1206.97	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
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## Correlations

Information	Value
Property code	pvap
Equation	$\ln(P_{vp}) = A + B/(T + C)$
Coeff. A	1.58831e+01
Coeff. B	-4.15391e+03
Coeff. C	-6.12460e+01
Temperature range (K), min.	327.60
Temperature range (K), max.	454.18

Information	Value
Property code	pvap
Equation	$\ln(P_{vp}) = A + B/T + C*\ln(T) + D*T^2$
Coeff. A	2.10868e+02
Coeff. B	-1.39301e+04
Coeff. C	-2.93550e+01
Coeff. D	2.24570e-05
Temperature range (K), min.	211.15
Temperature range (K), max.	607.50

## Datasets

### Viscosity, Pa\*s

Temperature, K - Liquid

Pressure, kPa - Liquid

Viscosity, Pa\*s - Liquid

## Sources

### KDB Vapor Pressure Data:

**Thermodynamics of ketone + amine mixtures. Part IX. Excess molar volumes at 298.15 K for Properties for Binary Mixtures of Propylene Glycol + Ketones and Aldehydes at Temperatures of 298.15 K and Partial pressures of 1000 pascals dilute binary mixtures of diisopropylacetone (DIQUAC) and propionitrile + amine mixtures 1. Volumetric properties of Joback Method and refractive index data for N,N-dimethylformamide + N,N-dimethylpropyl-amine, speeds of sound and isothermal compressibilities for binary amine + butan-1-amine, g/g hexanol-1-amine systems at several temperatures, partial molar volumes of alkylamines in non-electrolyte solvents I. Alkylamine mixtures of dioxane and 303.15 K at 298.15 K. Part IV. Volumetric and speed of propagation (298.15 K and 303.15 K) of S2 + butan-1-naphthamine at 298.15 K in polar and non-polar or nitrogen containing solvents (ketonitrile + amines) at several temperatures with application amine ERKS model. II: Excess and partial molar volumes in mixtures with Peasol's handbook of vapor pressure, tertiary, and cyclic amines KDB at 298.15 K:**

**Thermodynamic study of heptane + amine mixtures. V. Excess and covariation of critical temperatures of Some Alkenes, Amines, and Cyclic Molecules. Method:**

**Thermodynamics of (ketone + amine) mixtures. Part VI. Volumetric and speed Acoustic, volumetric (298.15 and 293.15), and studies of primary, secondary mixtures of aliphatic ketones and aliphatic amines at different temperatures, molar enthalpies of N,N-dimethylformamide or N,N-dimethylacetamide + N,N-dimethylacetamide + N,N-dimethylformamide, and spectroscopic properties for binary amine, propylene, and propionaldehyde Method, 298.15 K in polar solvents at 298.15 K, alkoxypropano with benzene, di- and tri-alkylamines at a temperature of 298.15 K, solutions of alkylamines in non-electrolyte solvents: IV.**

**Alkylamines in 1,4-dioxane and oxolane at 303.15K:**

<https://www.cheric.org/research/kdb/hcprop/showprop.php?cmpid=1274>

<https://www.doi.org/10.1016/j.fluid.2013.01.011>

<https://www.doi.org/10.1007/s10765-009-0593-3>

<https://www.doi.org/10.1016/j.tca.2004.08.013>

<https://www.doi.org/10.1016/j.tca.2009.02.005>

<https://www.doi.org/10.1021/acs.jced.5b00802>

[https://en.wikipedia.org/wiki/Joback\\_method](https://en.wikipedia.org/wiki/Joback_method)

<https://www.doi.org/10.1021/je800026p>

<http://pubs.acs.org/doi/abs/10.1021/ci990307l>

<https://www.doi.org/10.1016/j.tca.2005.08.012>

<https://www.doi.org/10.1016/j.tca.2010.09.004>

<https://www.doi.org/10.1016/j.jct.2013.08.005>

<https://www.doi.org/10.1016/j.jct.2015.09.002>

<https://www.doi.org/10.1016/j.jct.2011.04.017>

<https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure>

<https://www.cheric.org/files/research/kdb/mol/mol1274.mol>

<https://www.doi.org/10.1016/j.fluid.2014.12.017>

<https://www.doi.org/10.1021/je0341357>

<http://link.springer.com/article/10.1007/BF02311772>

<https://www.doi.org/10.1016/j.jct.2011.05.003>

<https://www.doi.org/10.1016/j.jct.2018.12.012>

<https://www.doi.org/10.1016/j.fluid.2019.112283>

<http://webbook.nist.gov/cgi/cbook.cgi?ID=C111922&Units=SI>

<https://www.doi.org/10.1016/j.jct.2005.12.007>

<http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDataset002.xlsx>

<https://www.doi.org/10.1016/j.tca.2009.07.008>

## Legend

<b>af:</b>	Acentric Factor
<b>affp:</b>	Proton affinity
<b>basg:</b>	Gas basicity

<b>chl:</b>	Standard liquid enthalpy of combustion
<b>cpg:</b>	Ideal gas heat capacity
<b>dm:</b>	Dipole Moment
<b>dvisc:</b>	Dynamic viscosity
<b>gf:</b>	Standard Gibbs free energy of formation
<b>hf:</b>	Enthalpy of formation at standard conditions
<b>hfl:</b>	Liquid phase enthalpy of formation at standard conditions
<b>hfus:</b>	Enthalpy of fusion at standard conditions
<b>hvap:</b>	Enthalpy of vaporization at standard conditions
<b>hvapt:</b>	Enthalpy of vaporization at a given temperature
<b>ie:</b>	Ionization energy
<b>log10ws:</b>	Log10 of Water solubility in mol/l
<b>logp:</b>	Octanol/Water partition coefficient
<b>mcvol:</b>	McGowan's characteristic volume
<b>pc:</b>	Critical Pressure
<b>pvap:</b>	Vapor pressure
<b>rhol:</b>	Liquid Density
<b>rinpol:</b>	Non-polar retention indices
<b>ripol:</b>	Polar retention indices
<b>speedsl:</b>	Speed of sound in fluid
<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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<https://www.chemeo.com/cid/37-921-8/1-Butanamine-N-butyl.pdf>

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