

Cyclohexylamine

Other names:	1-Aminocyclohexane
	1-Cyclohexylamine
	Aminocyclohexane
	Aminohexahydrobenzene
	Aniline, hexahydro-
	Benzenamine, hexahydro-
	CHA
	Cyclohexanamine
	Hexahydroaniline
	Hexahydrobenzenamine
	UN 2357
	cyclohexaneamine
Inchi:	InChI=1S/C6H13N/c7-6-4-2-1-3-5-6/h6H,1-5,7H2
InchiKey:	PAFZNILMFXTMIY-UHFFFAOYSA-N
Formula:	C6H13N
SMILES:	NC1CCCCC1
Mol. weight [g/mol]:	99.17
CAS:	108-91-8

Physical Properties

Property code	Value	Unit	Source
affp	934.40	kJ/mol	NIST Webbook
basg	899.60	kJ/mol	NIST Webbook
chl	-4071.30 ± 1.30	kJ/mol	NIST Webbook
chl	-4077.50 ± 1.60	kJ/mol	NIST Webbook
gf	90.54	kJ/mol	Joback Method
hf	-104.90 ± 1.30	kJ/mol	NIST Webbook
hf	-98.70	kJ/mol	NIST Webbook
hfl	-147.70 ± 1.30	kJ/mol	NIST Webbook
hfl	-141.50 ± 1.60	kJ/mol	NIST Webbook
hfus	8.33	kJ/mol	Joback Method
hvap	43.70	kJ/mol	NIST Webbook
hvap	42.80 ± 0.10	kJ/mol	NIST Webbook
hvap	42.80	kJ/mol	NIST Webbook
ie	8.86	eV	NIST Webbook
ie	8.40	eV	NIST Webbook
ie	8.40 ± 0.10	eV	NIST Webbook

log10ws	-1.77		Crippen Method
logp	1.278		Crippen Method
mcvol	94.520	ml/mol	McGowan Method
pc	4260.71	kPa	Joback Method
rinpol	862.00		NIST Webbook
rinpol	848.00		NIST Webbook
rinpol	870.00		NIST Webbook
rinpol	862.00		NIST Webbook
rinpol	855.00		NIST Webbook
rinpol	851.00		NIST Webbook
rinpol	863.00		NIST Webbook
rinpol	857.00		NIST Webbook
rinpol	857.00		NIST Webbook
rinpol	851.00		NIST Webbook
rinpol	857.00		NIST Webbook
ripol	1257.00		NIST Webbook
ripol	1257.00		NIST Webbook
ripol	1265.00		NIST Webbook
ripol	1267.00		NIST Webbook
ripol	1230.00		NIST Webbook
ripol	1222.00		NIST Webbook
ripol	1251.00		NIST Webbook
tb	407.70	K	NIST Webbook
tb	407.10	K	NIST Webbook
tb	405.15 ± 3.00	K	NIST Webbook
tb	408.15 ± 5.00	K	NIST Webbook
tb	407.40 ± 0.50	K	NIST Webbook
tb	407.00 ± 0.50	K	NIST Webbook
tc	626.80	K	Gas-Liquid Critical Temperatures of Some Alkenes, Amines, and Cyclic Hydrocarbons
tc	614.60	K	NIST Webbook
tf	252.00 ± 4.00	K	NIST Webbook
tf	255.40 ± 0.70	K	NIST Webbook
vc	0.334	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	206.73	J/molxK	465.57	Joback Method
cpg	221.50	J/molxK	502.39	Joback Method

cpg	235.45	J/molxK	539.20	Joback Method
cpg	248.59	J/molxK	576.02	Joback Method
cpg	260.96	J/molxK	612.83	Joback Method
cpg	272.56	J/molxK	649.65	Joback Method
cpg	191.11	J/molxK	428.76	Joback Method
hfust	16.50	kJ/mol	255.10	NIST Webbook
hfust	14.92	kJ/mol	255.40	NIST Webbook
hvapt	36.14	kJ/mol	407.10	NIST Webbook
hvapt	40.60	kJ/mol	385.00	NIST Webbook
hvapt	40.80	kJ/mol	370.50	NIST Webbook
hvapt	42.70 ± 0.10	kJ/mol	313.00	NIST Webbook
hvapt	40.70 ± 0.10	kJ/mol	343.00	NIST Webbook
hvapt	40.80	kJ/mol	367.50	NIST Webbook
hvapt	39.60 ± 0.10	kJ/mol	358.00	NIST Webbook
pvap	4.57	kPa	323.15	Experimental determination of the isothermal (vapour + liquid) equilibria of binary aqueous solutions of sec-butylamine and cyclohexylamine at several temperatures
pvap	4.76	kPa	323.99	Experimental determination of the isothermal (vapour + liquid) equilibria of binary aqueous solutions of sec-butylamine and cyclohexylamine at several temperatures
pvap	4.76	kPa	323.99	Experimental determination of the isothermal (vapour + liquid) equilibria of binary aqueous solutions of sec-butylamine and cyclohexylamine at several temperatures

pvap	4.76	kPa	323.99	Experimental determination of the isothermal (vapour + liquid) equilibria of binary aqueous solutions of sec-butylamine and cyclohexylamine at several temperatures
pvap	7.56	kPa	334.00	Experimental determination of the isothermal (vapour + liquid) equilibria of binary aqueous solutions of sec-butylamine and cyclohexylamine at several temperatures
pvap	12.08	kPa	344.00	Experimental determination of the isothermal (vapour + liquid) equilibria of binary aqueous solutions of sec-butylamine and cyclohexylamine at several temperatures
pvap	17.65	kPa	354.06	Experimental determination of the isothermal (vapour + liquid) equilibria of binary aqueous solutions of sec-butylamine and cyclohexylamine at several temperatures
pvap	25.96	kPa	364.10	Experimental determination of the isothermal (vapour + liquid) equilibria of binary aqueous solutions of sec-butylamine and cyclohexylamine at several temperatures

pvap	25.96	kPa	364.10	Experimental determination of the isothermal (vapour + liquid) equilibria of binary aqueous solutions of sec-butylamine and cyclohexylamine at several temperatures
pvap	25.94	kPa	364.13	Experimental determination of the isothermal (vapour + liquid) equilibria of binary aqueous solutions of sec-butylamine and cyclohexylamine at several temperatures
pvap	25.96	kPa	364.13	Experimental determination of the isothermal (vapour + liquid) equilibria of binary aqueous solutions of sec-butylamine and cyclohexylamine at several temperatures
pvap	0.23	kPa	273.15	Experimental determination of the isothermal (vapour + liquid) equilibria of binary aqueous solutions of sec-butylamine and cyclohexylamine at several temperatures
pvap	0.46	kPa	283.15	Experimental determination of the isothermal (vapour + liquid) equilibria of binary aqueous solutions of sec-butylamine and cyclohexylamine at several temperatures

pvap	0.88	kPa	293.15	Experimental determination of the isothermal (vapour + liquid) equilibria of binary aqueous solutions of sec-butylamine and cyclohexylamine at several temperatures
pvap	1.60	kPa	303.15	Experimental determination of the isothermal (vapour + liquid) equilibria of binary aqueous solutions of sec-butylamine and cyclohexylamine at several temperatures
pvap	2.76	kPa	313.15	Experimental determination of the isothermal (vapour + liquid) equilibria of binary aqueous solutions of sec-butylamine and cyclohexylamine at several temperatures
pvap	4.76	kPa	323.97	Experimental determination of the isothermal (vapour + liquid) equilibria of binary aqueous solutions of sec-butylamine and cyclohexylamine at several temperatures
pvap	7.32	kPa	333.15	Experimental determination of the isothermal (vapour + liquid) equilibria of binary aqueous solutions of sec-butylamine and cyclohexylamine at several temperatures

pvap	11.35	kPa	343.15	Experimental determination of the isothermal (vapour + liquid) equilibria of binary aqueous solutions of sec-butylamine and cyclohexylamine at several temperatures
pvap	17.98	kPa	353.15	Experimental determination of the isothermal (vapour + liquid) equilibria of binary aqueous solutions of sec-butylamine and cyclohexylamine at several temperatures
pvap	25.06	kPa	363.15	Experimental determination of the isothermal (vapour + liquid) equilibria of binary aqueous solutions of sec-butylamine and cyclohexylamine at several temperatures
pvap	0.46	kPa	283.20	Thermodynamic properties of cyclohexanamines: Experimental and theoretical study
pvap	0.56	kPa	286.20	Thermodynamic properties of cyclohexanamines: Experimental and theoretical study
pvap	0.72	kPa	290.10	Thermodynamic properties of cyclohexanamines: Experimental and theoretical study
pvap	0.91	kPa	293.30	Thermodynamic properties of cyclohexanamines: Experimental and theoretical study
pvap	1.06	kPa	296.20	Thermodynamic properties of cyclohexanamines: Experimental and theoretical study

pvap	1.18	kPa	298.10	Thermodynamic properties of cyclohexanamines: Experimental and theoretical study
pvap	1.28	kPa	299.30	Thermodynamic properties of cyclohexanamines: Experimental and theoretical study
pvap	1.54	kPa	302.30	Thermodynamic properties of cyclohexanamines: Experimental and theoretical study
pvap	1.79	kPa	305.30	Thermodynamic properties of cyclohexanamines: Experimental and theoretical study
pvap	2.11	kPa	308.30	Thermodynamic properties of cyclohexanamines: Experimental and theoretical study
pvap	7.51	kPa	333.15	Activity Coefficients at Infinite Dilution of Cyclohexylamine + Octane, Toluene, Ethylbenzene, or Aniline and Excess Molar Volumes in Binary Mixtures of Cyclohexylamine + Heptane, Octane, Nonane, Decane, Undecane, Aniline, or Water
pvap	25.59	kPa	363.15	Activity Coefficients at Infinite Dilution of Cyclohexylamine + Octane, Toluene, Ethylbenzene, or Aniline and Excess Molar Volumes in Binary Mixtures of Cyclohexylamine + Heptane, Octane, Nonane, Decane, Undecane, Aniline, or Water

pvap	4.76	kPa	323.92	Experimental determination of the isothermal (vapour + liquid) equilibria of binary aqueous solutions of sec-butylamine and cyclohexylamine at several temperatures
pvap	2.85	kPa	313.81	Experimental determination of the isothermal (vapour + liquid) equilibria of binary aqueous solutions of sec-butylamine and cyclohexylamine at several temperatures
pvap	2.85	kPa	313.79	Experimental determination of the isothermal (vapour + liquid) equilibria of binary aqueous solutions of sec-butylamine and cyclohexylamine at several temperatures
pvap	1.66	kPa	303.84	Experimental determination of the isothermal (vapour + liquid) equilibria of binary aqueous solutions of sec-butylamine and cyclohexylamine at several temperatures
pvap	1.66	kPa	303.82	Experimental determination of the isothermal (vapour + liquid) equilibria of binary aqueous solutions of sec-butylamine and cyclohexylamine at several temperatures

pvap	1.66	kPa	303.79	Experimental determination of the isothermal (vapour + liquid) equilibria of binary aqueous solutions of sec-butylamine and cyclohexylamine at several temperatures
pvap	0.92	kPa	293.88	Experimental determination of the isothermal (vapour + liquid) equilibria of binary aqueous solutions of sec-butylamine and cyclohexylamine at several temperatures
pvap	0.92	kPa	293.86	Experimental determination of the isothermal (vapour + liquid) equilibria of binary aqueous solutions of sec-butylamine and cyclohexylamine at several temperatures
pvap	0.92	kPa	293.83	Experimental determination of the isothermal (vapour + liquid) equilibria of binary aqueous solutions of sec-butylamine and cyclohexylamine at several temperatures
pvap	0.49	kPa	283.86	Experimental determination of the isothermal (vapour + liquid) equilibria of binary aqueous solutions of sec-butylamine and cyclohexylamine at several temperatures

pvap	0.25	kPa	274.30	Experimental determination of the isothermal (vapour + liquid) equilibria of binary aqueous solutions of sec-butylamine and cyclohexylamine at several temperatures
pvap	25.59	kPa	363.15	An equipment for dynamic measurements of vapour liquid equilibria and results in binary systems containing cyclohexylamine
pvap	17.53	kPa	353.15	An equipment for dynamic measurements of vapour liquid equilibria and results in binary systems containing cyclohexylamine
pvap	11.67	kPa	343.15	An equipment for dynamic measurements of vapour liquid equilibria and results in binary systems containing cyclohexylamine
pvap	0.92	kPa	293.88	Experimental determination of the isothermal (vapour + liquid) equilibria of binary aqueous solutions of sec-butylamine and cyclohexylamine at several temperatures
pvap	7.52	kPa	333.15	An equipment for dynamic measurements of vapour liquid equilibria and results in binary systems containing cyclohexylamine

rfi	1.46240	288.15	Vapor liquid equilibria in ternary systems of associating components (water, aniline, cyclohexylamine) and hydrocarbons (octane or toluene)
rfi	1.46240	288.15	Liquid-Liquid(-Liquid) Equilibria in Ternary Systems of Water + Cyclohexylamine + Aromatic Hydrocarbon (Toluene or Propylbenzene) or Aliphatic Hydrocarbon (Heptane or Octane)
rfi	1.44336	323.15	Experimental Determination of Densities and Refractive Indices of the Ternary Mixture 2-Methyl-2-propanol + Cyclohexylamine + n-Heptane at T = (303.15 to 323.15) K
rfi	1.44599	318.15	Experimental Determination of Densities and Refractive Indices of the Ternary Mixture 2-Methyl-2-propanol + Cyclohexylamine + n-Heptane at T = (303.15 to 323.15) K
rfi	1.44856	313.15	Experimental Determination of Densities and Refractive Indices of the Ternary Mixture 2-Methyl-2-propanol + Cyclohexylamine + n-Heptane at T = (303.15 to 323.15) K

rfi	1.45114		308.15	Experimental Determination of Densities and Refractive Indices of the Ternary Mixture 2-Methyl-2-propanol + Cyclohexylamine + n-Heptane at T = (303.15 to 323.15) K
rfi	1.45375		303.15	Experimental Determination of Densities and Refractive Indices of the Ternary Mixture 2-Methyl-2-propanol + Cyclohexylamine + n-Heptane at T = (303.15 to 323.15) K
rfi	1.46240		288.15	Ternary Liquid-Liquid(-Liquid) Equilibria of Aniline + Cyclohexylamine + Water, Aniline + Cyclohexylamine + Octane, Aniline + Water + Toluene, and Aniline + Water + Octane
rhoI	871.29	kg/m3	288.15	Experimental determination and modelling of densities and excess molar volumes of ternary system (1-butanol + cyclohexylamine + n-heptane) and corresponding binaries from 288.15 to 323.15K
rhoI	848.71	kg/m3	313.15	Experimental and Computational Studies of Binary Mixtures of Isobutanol + Cyclohexylamine
rhoI	853.24	kg/m3	308.15	Experimental and Computational Studies of Binary Mixtures of Isobutanol + Cyclohexylamine

rhoI	857.79	kg/m3	303.15	Experimental and Computational Studies of Binary Mixtures of Isobutanol + Cyclohexylamine
rhoI	862.31	kg/m3	298.15	Experimental and Computational Studies of Binary Mixtures of Isobutanol + Cyclohexylamine
rhoI	866.85	kg/m3	293.15	Experimental and Computational Studies of Binary Mixtures of Isobutanol + Cyclohexylamine
rhoI	839.55	kg/m3	323.15	Experimental determination and modelling of densities and excess molar volumes of ternary system (1-butanol + cyclohexylamine + n-heptane) and corresponding binaries from 288.15 to 323.15K
rhoI	867.20	kg/m3	293.15	Thermodynamics of mixtures with strongly negative deviations from Raoult s law. XII. Densities, viscosities and refractive indices at T = (293.15 to 303.15) K for (1-heptanol, or 1-decanol + cyclohexylamine) systems. Application of the ERAS model to (1-alkanol + cyclohexylamine) mixtures

rhoI	862.69	kg/m3	298.15	<p>Thermodynamics of mixtures with strongly negative deviations from Raoult s law. XII.</p> <p>Densities, viscosities and refractive indices at T = (293.15 to 303.15) K for (1-heptanol, or 1-decanol + cyclohexylamine) systems.</p> <p>Application of the ERAS model to (1-alkanol + cyclohexylamine) mixtures</p>
rhoI	844.07	kg/m3	318.15	<p>Experimental determination and modelling of densities and excess molar volumes of ternary system (1-butanol + cyclohexylamine + n-heptane) and corresponding binaries from 288.15 to 323.15K</p>
rhoI	858.12	kg/m3	303.15	<p>Thermodynamics of mixtures with strongly negative deviations from Raoult s law. XII.</p> <p>Densities, viscosities and refractive indices at T = (293.15 to 303.15) K for (1-heptanol, or 1-decanol + cyclohexylamine) systems.</p> <p>Application of the ERAS model to (1-alkanol + cyclohexylamine) mixtures</p>

rhoI	853.14	kg/m3	308.15	Experimental determination and modelling of densities and excess molar volumes of ternary system (1-butanol + cyclohexylamine + n-heptane) and corresponding binaries from 288.15 to 323.15K
rhoI	857.67	kg/m3	303.15	Experimental determination and modelling of densities and excess molar volumes of ternary system (1-butanol + cyclohexylamine + n-heptane) and corresponding binaries from 288.15 to 323.15K
rhoI	862.21	kg/m3	298.15	Experimental determination and modelling of densities and excess molar volumes of ternary system (1-butanol + cyclohexylamine + n-heptane) and corresponding binaries from 288.15 to 323.15K
rhoI	866.75	kg/m3	293.15	Experimental determination and modelling of densities and excess molar volumes of ternary system (1-butanol + cyclohexylamine + n-heptane) and corresponding binaries from 288.15 to 323.15K

rhoI	848.61	kg/m ³	313.15	Experimental determination and modelling of densities and excess molar volumes of ternary system (1-butanol + cyclohexylamine + n-heptane) and corresponding binaries from 288.15 to 323.15K
speedsl	1342.00	m/s	318.15	Densities, Viscosities, Sound Speed, and IR Studies of N-methyl-2-pyrrolidone with Cyclohexylamine, Cyclohexanol, and Cyclohexene at different Temperatures.
speedsl	1379.20	m/s	308.15	Densities, Viscosities, Sound Speed, and IR Studies of N-methyl-2-pyrrolidone with Cyclohexylamine, Cyclohexanol, and Cyclohexene at different Temperatures.
speedsl	1397.80	m/s	303.15	Densities, Viscosities, Sound Speed, and IR Studies of N-methyl-2-pyrrolidone with Cyclohexylamine, Cyclohexanol, and Cyclohexene at different Temperatures.
speedsl	1301.80	m/s	323.15	Temperature dependence of densities, speeds of sound, and derived properties of cyclohexylamine + cyclohexane or benzene in the range (293.15 to 323.15) K

speedsl	1323.10	m/s	318.15	Temperature dependence of densities, speeds of sound, and derived properties of cyclohexylamine + cyclohexane or benzene in the range (293.15 to 323.15) K
speedsl	1344.50	m/s	313.15	Temperature dependence of densities, speeds of sound, and derived properties of cyclohexylamine + cyclohexane or benzene in the range (293.15 to 323.15) K
speedsl	1366.00	m/s	308.15	Temperature dependence of densities, speeds of sound, and derived properties of cyclohexylamine + cyclohexane or benzene in the range (293.15 to 323.15) K
speedsl	1387.30	m/s	303.15	Temperature dependence of densities, speeds of sound, and derived properties of cyclohexylamine + cyclohexane or benzene in the range (293.15 to 323.15) K
speedsl	1408.80	m/s	298.15	Temperature dependence of densities, speeds of sound, and derived properties of cyclohexylamine + cyclohexane or benzene in the range (293.15 to 323.15) K

speedsl	1430.50	m/s	293.15	Temperature dependence of densities, speeds of sound, and derived properties of cyclohexylamine + cyclohexane or benzene in the range (293.15 to 323.15) K
speedsl	1360.60	m/s	313.15	Densities, Viscosities, Sound Speed, and IR Studies of N-methyl-2-pyrrolidone with Cyclohexylamine, Cyclohexanol, and Cyclohexene at different Temperatures.

Correlations

Information	Value
Property code	pvap
Equation	$\ln(P_{vp}) = A + B/T + C \cdot \ln(T) + D \cdot T^2$
Coeff. A	8.66698e+01
Coeff. B	-7.88954e+03
Coeff. C	-1.06327e+01
Coeff. D	7.33244e-06
Temperature range (K), min.	255.45
Temperature range (K), max.	615.00

Sources

Experimental and Computational Studies of Binary Mixtures of Measurement and Prediction of Vapor Liquid(-Liquid) Equilibria in Ternary Systems Containing Water and Organic Compounds. A review of some Alkanes, Alkenes, and Cyclic Hydrocarbons. Determination and modelling of densities and excess measurements and Prediction of Vapor-Liquid Equilibria in Ternary Systems. Crippen Method for Estimating and Corresponding Components, Cyclohexylamine, and Cyclohexanol. Experimental determination of the isothermal vapor-liquid equilibria of binary aqueous solutions of sec-butylamine and cyclohexylamine at several temperatures:

- <https://www.doi.org/10.1021/acs.jced.6b00158>
- <https://www.doi.org/10.1021/acs.jced.7b00100>
- <https://www.doi.org/10.1021/je0341357>
- <https://www.doi.org/10.1016/j.tca.2009.07.002>
- <https://www.doi.org/10.1021/acs.jced.7b00721>
- https://www.chemeo.com/doc/models/crippen_log10ws
- <https://www.doi.org/10.1016/j.fluid.2005.05.003>
- <https://www.doi.org/10.1016/j.jct.2011.08.009>

Ternary Liquid-Liquid(-Liquid)
Equilibria of Aniline + Cyclohexylamine
+ Water, Methanol + Cyclohexylamine +
Octane, Aniline + Water + Toluene, and
Aniline + Water-Liquid-Liquid Equilibria in
Ternary Systems of Water +
Cyclohexylamine, Properties of
Equilibrium Ternary Experimental and
Predicted Phase Diagrams with
Strongly Negative Deviations from
Raoult's Law, Krichevskii, and Scatchard
and Hildebrand Studies of Systems 1,2-293.15 to
298.15 K, with Cyclohexylamine, Cyclohexanol,
Cyclohexylamine, and Cyclohexene at
Different Temperatures
Legend
(Aniline + Cyclohexylamine)
mixtures

Legend

affp:	Proton affinity
basg:	Gas basicity
chl:	Standard liquid enthalpy of combustion
cpg:	Ideal gas heat capacity
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
hfust:	Enthalpy of fusion 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
pvap:	Vapor pressure
rfi:	Refractive Index
rhoL:	Liquid Density
rinpol:	Non-polar retention indices
ripol:	Polar retention indices
speedsl:	Speed of sound in fluid
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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