

# 2-Pyrrolidinone

**Other names:** .alpha.-pyrrolidinone  
.alpha.-pyrrolidone  
.gamma.-aminobutyric acid lactam  
.gamma.-aminobutyric lactam  
.gamma.-aminobutyrolactam  
.gamma.-butyrolactam  
2-Oxopyrrolidine  
2-Pyrol  
2-Pyrol4-aminobutyric acid lactam  
2-Pyrrolidone  
2-Tetrahydropyrrolone  
4-AMINEBUTANOIC ACID  
4-Aminobutyric acid lactam  
ALPHA-PYRROLIDINONE  
Azacyclopentan-2-one  
BUTYROLACTAM  
Butanoic acid, 4-amino-  
Butanoic acid, 4-amino-, lactam  
LAM  
NSC 4593  
NSC 8413  
Pyrrolidon  
Pyrrolidone  
Pyrrolidone-2  
Pyrrolidone2-pyrrolidone  
Soluphor P  
a-Pyrrolidinone  
a-Pyrrolidone  
g-Aminobutyric acid lactam  
g-Aminobutyric lactam  
g-Aminobutyrolactam  
g-Butyrolactam  
«alpha»-Pyrrolidinone  
«alpha»-Pyrrolidone  
«gamma»-Aminobutyric acid lactam  
«gamma»-Aminobutyric lactam  
«gamma»-Aminobutyrolactam  
«gamma»-Butyrolactam  
Â«alphaÂ»-Pyrrolidinone  
Â«alphaÂ»-Pyrrolidone

Ä«gammaÄ»-Aminobutyric acid lactam  
 Ä«gammaÄ»-Aminobutyric lactam  
 Ä«gammaÄ»-Aminobutyrolactam  
 Ä«gammaÄ»-Butyrolactam  
**Inchi:** InChI=1S/C4H7NO/c6-4-2-1-3-5-4/h1-3H2,(H,5,6)  
**InchiKey:** HNJBEVLQSNELDL-UHFFFAOYSA-N  
**Formula:** C4H7NO  
**SMILES:** O=C1CCCN1  
**Mol. weight [g/mol]:** 85.10  
**CAS:** 616-45-5

## Physical Properties

Property code	Value	Unit	Source
chl	-2308.40 ± 0.34	kJ/mol	NIST Webbook
chl	-2288.20 ± 0.42	kJ/mol	NIST Webbook
gf	-7.82	kJ/mol	Joback Method
hf	-197.40 ± 3.10	kJ/mol	NIST Webbook
hfl	-266.04 ± 0.42	kJ/mol	NIST Webbook
hfus	8.08	kJ/mol	Joback Method
hvap	73.60 ± 1.30	kJ/mol	NIST Webbook
hvap	68.70 ± 1.50	kJ/mol	NIST Webbook
ie	9.45	eV	NIST Webbook
ie	9.32 ± 0.02	eV	NIST Webbook
ie	9.20	eV	NIST Webbook
ie	9.53	eV	NIST Webbook
log10ws	1.07		Aqueous Solubility Prediction Method
log10ws	1.07		Estimated Solubility Method
logp	-0.104		Crippen Method
mcvol	67.910	ml/mol	McGowan Method
nfpaf	%!d(float64=1)		KDB
nfpah	%!d(float64=2)		KDB
pc	5661.74	kPa	Joback Method
rinpol	1059.90		NIST Webbook
rinpol	1048.00		NIST Webbook
rinpol	1069.00		NIST Webbook
rinpol	1059.90		NIST Webbook
rinpol	1077.00		NIST Webbook
rinpol	1076.00		NIST Webbook
rinpol	1045.00		NIST Webbook

rinpol	1078.00		NIST Webbook
ripol	2020.00		NIST Webbook
ripol	1988.00		NIST Webbook
ripol	1988.00		NIST Webbook
ripol	2017.00		NIST Webbook
ripol	2037.00		NIST Webbook
ripol	2048.00		NIST Webbook
ripol	2029.00		NIST Webbook
ripol	2002.00		NIST Webbook
ripol	2002.00		NIST Webbook
sl	189.70	J/mol×K	NIST Webbook
ss	136.80	J/mol×K	NIST Webbook
tb	518.20	K	NIST Webbook
tc	659.52	K	Joback Method
tf	298.65 ± 0.50	K	NIST Webbook
tf	298.72 ± 0.10	K	NIST Webbook
tf	296.65	K	Aqueous Solubility Prediction Method
tt	299.08 ± 0.01	K	NIST Webbook
vc	0.245	m3/kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	123.71	J/mol×K	427.24	Joback Method
cpg	134.20	J/mol×K	465.95	Joback Method
cpg	144.30	J/mol×K	504.67	Joback Method
cpg	153.99	J/mol×K	543.38	Joback Method
cpg	163.27	J/mol×K	582.09	Joback Method
cpg	172.11	J/mol×K	620.81	Joback Method
cpg	180.50	J/mol×K	659.52	Joback Method
cpl	172.37	J/mol×K	308.15	Excess heat capacities of (binary + ternary) mixtures containing [emim][BF4] and organic liquids
cpl	168.36	J/mol×K	293.15	Excess heat capacities of (binary + ternary) mixtures containing [emim][BF4] and organic liquids

cpl	171.18	J/mol×K	303.15	Excess heat capacities of (binary + ternary) mixtures containing [emim][BF4] and organic liquids
cpl	169.60	J/mol×K	300.00	NIST Webbook
cpl	169.55	J/mol×K	298.15	Excess heat capacities of (binary + ternary) mixtures containing [emim][BF4] and organic liquids
cpl	169.40	J/mol×K	300.00	NIST Webbook
cps	135.60	J/mol×K	290.00	NIST Webbook
dvisc	0.0034510	Paxs	338.15	Densities, Viscosities, Speeds of Sound, and Relative Permittivities for Water + Cyclic Amides (2-Pyrrolidinone, 1-Methyl-2-pyrrolidinone, and 1-Vinyl-2-pyrrolidinone) at Different Temperatures
dvisc	0.0088440	Paxs	308.15	Densities, Viscosities, Speeds of Sound, and Relative Permittivities for Water + Cyclic Amides (2-Pyrrolidinone, 1-Methyl-2-pyrrolidinone, and 1-Vinyl-2-pyrrolidinone) at Different Temperatures
dvisc	0.0130680	Paxs	298.15	Densities, Viscosities, and Excess Molar Enthalpies of 2-Pyrrolidone + Butanol Isomers at T ) (293.15, 298.15, and 303.15) K
dvisc	0.0158420	Paxs	293.15	Densities, Viscosities, and Excess Molar Enthalpies of 2-Pyrrolidone + Butanol Isomers at T ) (293.15, 298.15, and 303.15) K

dvisc	0.0133630	Paxs	298.15	Densities, Viscosities, Speeds of Sound, and Relative Permittivities for Water + Cyclic Amides (2-Pyrrolidinone, 1-Methyl-2-pyrrolidinone, and 1-Vinyl-2-pyrrolidinone) at Different Temperatures
dvisc	0.0046770	Paxs	328.15	Densities, Viscosities, Speeds of Sound, and Relative Permittivities for Water + Cyclic Amides (2-Pyrrolidinone, 1-Methyl-2-pyrrolidinone, and 1-Vinyl-2-pyrrolidinone) at Different Temperatures
dvisc	0.0062590	Paxs	318.15	Densities, Viscosities, Speeds of Sound, and Relative Permittivities for Water + Cyclic Amides (2-Pyrrolidinone, 1-Methyl-2-pyrrolidinone, and 1-Vinyl-2-pyrrolidinone) at Different Temperatures
dvisc	0.0106870	Paxs	303.15	Densities, Viscosities, and Excess Molar Enthalpies of 2-Pyrrolidone + Butanol Isomers at T ) (293.15, 298.15, and 303.15) K
hfust	13.92	kJ/mol	299.00	NIST Webbook
hfust	13.92	kJ/mol	299.00	NIST Webbook
hfust	13.92	kJ/mol	299.08	NIST Webbook
hfust	13.92	kJ/mol	299.08	NIST Webbook
hvapt	60.00	kJ/mol	456.50	NIST Webbook

rhol	1107.15	kg/m3	298.15	Thermodynamic properties of ternary mixtures of 1-ethyl-3-methylimidazolium tetrafluoroborate with 1-methyl pyrrolidin-2-one or pyrrolidin-2-one + water
rhol	1098.90	kg/m3	308.15	Thermodynamic Properties of Ternary Mixtures Containing Ionic Liquids and Organic Solvents
rhol	1107.26	kg/m3	298.15	Topological investigations of the molecular species and molecular interactions that characterize pyrrolidin-2-one + lower alkanol mixtures
rhol	1107.15	kg/m3	298.15	Excess Heat Capacities for Lactam + Chlorotoluene Binary Mixtures
rhol	1103.06	kg/m3	303.15	Excess Heat Capacities for Lactam + Chlorotoluene Binary Mixtures
rhol	1086.75	kg/m3	323.15	Volumetric properties of 1-butyl-3-methylimidazolium tetrafluoroborate and 2-pyrrolidone from T = (298.15 to 323.15) K at atmospheric pressure
rhol	1090.82	kg/m3	318.15	Volumetric properties of 1-butyl-3-methylimidazolium tetrafluoroborate and 2-pyrrolidone from T = (298.15 to 323.15) K at atmospheric pressure

rhol	1094.90	kg/m3	313.15	Volumetric properties of 1-butyl-3-methylimidazolium tetrafluoroborate and 2-pyrrolidone from T = (298.15 to 323.15) K at atmospheric pressure
rhol	1098.99	kg/m3	308.15	Volumetric properties of 1-butyl-3-methylimidazolium tetrafluoroborate and 2-pyrrolidone from T = (298.15 to 323.15) K at atmospheric pressure
rhol	1111.28	kg/m3	293.15	Excess Heat Capacities for Lactam + Chlorotoluene Binary Mixtures
rhol	1103.07	kg/m3	303.15	Volumetric properties of 1-butyl-3-methylimidazolium tetrafluoroborate and 2-pyrrolidone from T = (298.15 to 323.15) K at atmospheric pressure
rhol	1103.02	kg/m3	303.15	Thermodynamic Properties of Ternary Mixtures Containing Ionic Liquids and Organic Solvents
rhol	1107.15	kg/m3	298.15	Thermodynamic Properties of Ternary Mixtures Containing Ionic Liquids and Organic Solvents
rhol	1111.28	kg/m3	293.15	Thermodynamic properties of ternary mixtures of 1-ethyl-3-methylimidazolium tetrafluoroborate with 1-methyl pyrrolidin-2-one or pyrrolidin-2-one + water

rhol	1106.82	kg/m3	298.15	Excess Molar Volumes and Kinematic Viscosities for Binary Mixtures of Dipropylene Glycol Monobutyl Ether and Dipropylene Glycol tert-Butyl Ether with 2-Pyrrolidinone, N-Methyl-2-pyrrolidinone, N,N-Dimethylformamide, and N,N-Dimethylacetamide at 298.15 K
rhol	1098.90	kg/m3	308.15	Thermodynamic properties of ternary mixtures of 1-ethyl-3-methylimidazolium tetrafluoroborate with 1-methyl pyrrolidin-2-one or pyrrolidin-2-one + water
rhol	1107.16	kg/m3	298.15	Volumetric properties of 1-butyl-3-methylimidazolium tetrafluoroborate and 2-pyrrolidone from T = (298.15 to 323.15) K at atmospheric pressure
rhol	1107.15	kg/m3	298.15	Excess molar enthalpies for [emim][BF4] + pyrrolidin-2-one or 1-methyl pyrrolidin-2-one + pyridine or water mixtures
rhol	1097.14	kg/m3	308.15	Effect of B-cyclodextrin on the behaviour of thermophysical and spectroscopic properties of binary mixtures of (isomeric butanediol + pyrrolidin-2-one)
rhol	1097.14	kg/m3	308.15	Molecular interactions of $\alpha,\omega$ -alkanediols in pyrrolidin-2-one: Thermophysical and spectroscopic measurements

rhol	1097.14	kg/m3	308.15	Effect of placement of hydroxyl groups in isomeric butanediol on the behaviour of thermophysical and spectroscopic properties of pyrrolidin-2-one
rhol	1107.26	kg/m3	298.15	Topological Investigations of Excess Molar Volumes and Excess Isentropic Compressibilities of Ternary Mixtures Containing Pyrrolidin-2-one at 308.15 K
rhol	1111.28	kg/m3	293.15	Thermodynamic Properties of Ternary Mixtures Containing Ionic Liquids and Organic Solvents
rhol	1103.02	kg/m3	303.15	Thermodynamic properties of ternary mixtures of 1-ethyl-3-methylimidazolium tetrafluoroborate with 1-methyl pyrrolidin-2-one or pyrrolidin-2-one + water
rhol	994.28	kg/m3	298.15	Thermodynamic Properties of Ternary Liquid Mixtures of 2-Pyrrolidinone with Aromatic Hydrocarbons
sfust	46.50	J/mol×K	299.08	NIST Webbook
sfust	46.50	J/mol×K	299.08	NIST Webbook
speedsl	1617.14	m/s	303.15	Thermodynamic and Topological Studies of 1-Ethyl-3-methylimidazolium Tetrafluoroborate + Pyrrolidin-2-one and 1-Methyl-pyrrolidin-2-one Mixtures

speedsl	1633.92	m/s	298.15	Thermodynamic and Topological Studies of 1-Ethyl-3-methylimidazolium Tetrafluoroborate + Pyrrolidin-2-one and 1-Methyl-pyrrolidin-2-one Mixtures
speedsl	1650.13	m/s	293.15	Thermodynamic and Topological Studies of 1-Ethyl-3-methylimidazolium Tetrafluoroborate + Pyrrolidin-2-one and 1-Methyl-pyrrolidin-2-one Mixtures
speedsl	1633.68	m/s	298.15	Isentropic compressibilities of (amide + water) mixtures: A comparative study
speedsl	1601.85	m/s	308.15	Thermodynamic and Topological Studies of 1-Ethyl-3-methylimidazolium Tetrafluoroborate + Pyrrolidin-2-one and 1-Methyl-pyrrolidin-2-one Mixtures

## Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	406.20	K	1.60	NIST Webbook

## Correlations

Information	Value
Property code	pvap
Equation	$\ln(P_{vp}) = A + B/(T + C)$
Coeff. A	1.54130e+01
Coeff. B	-4.81100e+03

Coeff. C	-7.25160e+01
Temperature range (K), min.	390.59
Temperature range (K), max.	548.78

Information	Value
Property code	pvap
Equation	$\ln(P_{\text{vap}}) = A + B/T + C*\ln(T) + D*T^2$
Coeff. A	8.41872e+01
Coeff. B	-1.06834e+04
Coeff. C	-9.56959e+00
Coeff. D	3.04035e-06
Temperature range (K), min.	298.15
Temperature range (K), max.	792.00

## Sources

### Crippen Method:

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

**Effect of B-cyclodextrin on the behaviour of thermophysical and spectroscopic properties of binary mixtures of (isomeric butanediol + 5-hydroxy-1,3-naphthalanes for [emim][BF<sub>4</sub>] + pyrrolidin-2-one or MeOH + pyrrolidin-2-one + pyridine or water mixtures:**

<https://www.doi.org/10.1016/j.jct.2012.08.026>

**Estimated Solubility Method: Studies of the hydrodynamic and topological properties of binary mixtures of 4-pyridylbenzene and 4-phenylbenzene in various solvents: Molar volumes and excess entropies: Corresponding pressures and excess entropic compressibilities at 308.15 K for 1-methylimidazolium vapor Pressure:**

<https://www.doi.org/10.1016/j.jct.2013.09.015>

**KDB:**  
**Excess Heat Capacities for Lactam + Chlorotoluene Binary Mixtures:**  
**Excess Molar Enthalpies of Dibromomethane with Benzene, Methane, Dimethylsulfoxide, and Pyrrolidin-2-one at 303.15 K:**  
**Aqueous Solubility Prediction Method:**

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

**Surface Tension of Aqueous Solutions of Short N-Alkyl-2-pyrrolidinones:**  
**Thermodynamic Properties of Ternary Mixtures Containing Ionic Liquids and Organic Solvents:**  
**Densities, Viscosities, Speeds of Sound, and Relative Permittivities for Isentropic Compressibilities of (amide + water) mixtures: A comparative study:**  
**Molecular interactions of and a xylkanediol with pyrrolidin-2-one: Thermodynamic analysis spectroscopic measurements of 2-Pyrrolidinone with Aromatic hydrocarbons:**  
**Properties of ternary mixtures of Topological investigations of the reactivities and molar properties and molar hyperconjugations characterizing 2-one + pyrrolidin-2-one + lower alkanol mixtures:**

<https://www.doi.org/10.1016/j.jct.2004.11.020>

**Topological investigations of the reactivities and molar properties and molar hyperconjugations characterizing 2-one + pyrrolidin-2-one + lower alkanol mixtures:**

<https://www.doi.org/10.1007/s10765-010-0861-2>

<https://www.doi.org/10.1016/j.tca.2009.07.017>

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

<https://www.cheric.org/files/research/kdb/mol/mol1339.mol>

<https://www.doi.org/10.1021/je400408w>

<https://www.doi.org/10.1021/je9005882>

<http://webbook.nist.gov/cgi/cbook.cgi?ID=C616455&Units=SI>

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

<https://www.doi.org/10.1021/je800589e>

<https://www.doi.org/10.1021/je301353z>

<https://www.doi.org/10.1016/j.jct.2014.07.014>

<https://www.doi.org/10.1021/je0340809>

<https://www.doi.org/10.1016/j.jct.2007.05.015>

<https://www.doi.org/10.1016/j.jct.2007.08.005>

<https://www.doi.org/10.1007/s10765-010-0717-9>

<https://www.doi.org/10.1016/j.tca.2013.04.011>

<https://www.doi.org/10.1016/j.tca.2009.03.014>

<b>Joback Method:</b>	<a href="https://en.wikipedia.org/wiki/Joback_method">https://en.wikipedia.org/wiki/Joback_method</a>
<b>Excess Molar Volumes and Kinematic Viscosities for Binary Mixtures of Thermodynamically Inert Binary Aromatic Compounds with tert-Butyl Ether Densities of 1,2-Dimethylazobium Excess Molar Entropies of Formation of 2-Pyridinolanes and 2-Pyridinethiones at 298.15 K, and Solubility of Acetylene in Alcohols and Ketones:</b>	<a href="https://www.doi.org/10.1021/je049657g">https://www.doi.org/10.1021/je049657g</a>
<b>Volumetric properties of 1-butyl-3-methylimidazolium Densities, ultrasonic speeds, excess enthalpies of solvation, and binary enthalpies of miscibility with isomeric propanediols at temperatures from 303.15 K to 323.15 K:</b>	<a href="https://www.doi.org/10.1016/j.jct.2015.02.018">https://www.doi.org/10.1016/j.jct.2015.02.018</a>
<b>Water-solubility of 1,2-dimethylhexanone at 298.15 K, 293.15 K, and 288.15 K:</b>	<a href="https://www.doi.org/10.1021/je801006q">https://www.doi.org/10.1021/je801006q</a>
<b>Water-solubility of 1,2-dimethylhexanone at 298.15 K, 293.15 K, and 288.15 K:</b>	<a href="https://www.cheric.org/research/kdb/hcprop/showprop.php?cmpid=1339">https://www.cheric.org/research/kdb/hcprop/showprop.php?cmpid=1339</a>
<b>Ketones:</b>	<a href="https://www.doi.org/10.1021/acs.jced.8b00126">https://www.doi.org/10.1021/acs.jced.8b00126</a>
<b>Volumetric properties of 1-butyl-3-methylimidazolium Densities, ultrasonic speeds, excess enthalpies of solvation, and binary enthalpies of miscibility with isomeric propanediols at temperatures from 303.15 K to 323.15 K:</b>	<a href="https://www.doi.org/10.1016/j.jct.2015.11.009">https://www.doi.org/10.1016/j.jct.2015.11.009</a>
<b>Densities, ultrasonic speeds, excess enthalpies of solvation, and binary enthalpies of miscibility with isomeric propanediols at temperatures from 303.15 K to 323.15 K:</b>	<a href="https://www.doi.org/10.1016/j.jct.2017.03.022">https://www.doi.org/10.1016/j.jct.2017.03.022</a>

## Legend

<b>chl:</b>	Standard liquid enthalpy of combustion
<b>cpg:</b>	Ideal gas heat capacity
<b>cpl:</b>	Liquid phase heat capacity
<b>cps:</b>	Solid phase heat capacity
<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>hfust:</b>	Enthalpy of fusion at a given temperature
<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>nfpaf:</b>	NFPA Fire Rating
<b>nfpah:</b>	NFPA Health Rating
<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>sfust:</b>	Entropy of fusion at a given temperature
<b>sl:</b>	Liquid phase molar entropy at standard conditions
<b>speedsl:</b>	Speed of sound in fluid
<b>ss:</b>	Solid phase molar entropy at standard conditions
<b>tb:</b>	Normal Boiling Point Temperature
<b>tbrp:</b>	Boiling point at reduced pressure
<b>tc:</b>	Critical Temperature

**tf:** Normal melting (fusion) point

**tt:** Triple Point Temperature

**vc:** Critical Volume

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