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

Â«gammaÂ»-Aminobutyric acid lactam
Â«gammaÂ»-Aminobutyric lactam
Â«gammaÂ»-Aminobutyrolactam
Â«gammaÂ»-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	-2288.20 ± 0.42	kJ/mol	NIST Webbook
chl	-2308.40 ± 0.34	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	9.53	eV	NIST Webbook
ie	9.32 ± 0.02	eV	NIST Webbook
ie	9.20	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	1048.00		NIST Webbook
rinpol	1076.00		NIST Webbook
rinpol	1077.00		NIST Webbook
rinpol	1059.90		NIST Webbook
rinpol	1069.00		NIST Webbook
rinpol	1045.00		NIST Webbook
rinpol	1078.00		NIST Webbook

rinpol	1059.90		NIST Webbook
ripol	2037.00		NIST Webbook
ripol	2002.00		NIST Webbook
ripol	2029.00		NIST Webbook
ripol	2048.00		NIST Webbook
ripol	1988.00		NIST Webbook
ripol	2017.00		NIST Webbook
ripol	2002.00		NIST Webbook
ripol	1988.00		NIST Webbook
ripol	2020.00		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	298.72 ± 0.10	K	NIST Webbook
tf	296.65	K	Aqueous Solubility Prediction Method
tf	298.65 ± 0.50	K	NIST Webbook
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	180.50	J/mol×K	659.52	Joback Method
cpg	172.11	J/mol×K	620.81	Joback Method
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
cpl	169.40	J/mol×K	300.00	NIST Webbook
cpl	168.36	J/mol×K	293.15	Excess heat capacities of (binary + ternary) mixtures containing [emim][BF4] and organic liquids

cpl	169.55	J/mol×K	298.15	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	172.37	J/mol×K	308.15	Excess heat capacities of (binary + ternary) mixtures containing [emim][BF4] and organic liquids
cpl	169.60	J/mol×K	300.00	NIST Webbook
cps	135.60	J/mol×K	290.00	NIST Webbook
dvisc	0.0133630	Pa×s	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	0.0034510	Pa×s	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	0.0046770	Pa×s	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	0.0106870	Pa×s	303.15	Densities, Viscosities, and Excess Molar Enthalpies of 2-Pyrrolidone + Butanol Isomers at T) (293.15, 298.15, and 303.15) K
dvisc	0.0130680	Pa×s	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	Pa×s	293.15	Densities, Viscosities, and Excess Molar Enthalpies of 2-Pyrrolidone + Butanol Isomers at T) (293.15, 298.15, and 303.15) K
dvisc	0.0062590	Pa×s	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	0.0088440	Pa×s	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
hfust	13.92	kJ/mol	299.08	NIST Webbook
hfust	13.92	kJ/mol	299.08	NIST Webbook
hfust	13.92	kJ/mol	299.00	NIST Webbook
hfust	13.92	kJ/mol	299.00	NIST Webbook
hvapt	60.00	kJ/mol	456.50	NIST Webbook
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	1098.90	kg/m3	308.15	Thermodynamic Properties of Ternary Mixtures Containing Ionic Liquids and Organic Solvents
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 Containing Ionic Liquids and Organic Solvents

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	1107.15	kg/m3	298.15	Excess Heat Capacities for Lactam + Chlorotoluene Binary Mixtures
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	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	1111.28	kg/m3	293.15	Excess Heat Capacities for Lactam + Chlorotoluene Binary Mixtures
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	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	1107.26	kg/m3	298.15	Topological investigations of the molecular species and molecular interactions that characterize pyrrolidin-2-one + lower alkanol 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	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	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	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 a,x-alkanediols in pyrrolidin-2-one: Thermophysical and spectroscopic measurements
rhol	1103.06	kg/m3	303.15	Excess Heat Capacities for Lactam + Chlorotoluene Binary Mixtures

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	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	1633.92	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	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	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
speedsl	1633.68	m/s	298.15	Isentropic compressibilities of (amide + water) mixtures: A comparative study

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(Pvp) = 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(Pvp) = 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

Densities, Viscosities, and Excess Molar Enthalpies of 2-Pyrrolidone + Butanol Isomers at T = (298.15, 298.15, and 303.15) K:	https://www.doi.org/10.1021/je801006q
Densities, Viscosities, Speeds of Sound, and Relative Permittivities for Water + Cyclic Amides	https://www.doi.org/10.1021/je0340809
Volumetric Properties of 1-Butyl-3-methylimidazolium Tetrafluoroborate and 2-pyrrolidone from T = (298.15 to 323.15) K at atmospheric pressure:	https://www.doi.org/10.1007/s10765-010-0861-2
Thermodynamic investigations of Excess Molar Volumes and Excess Isentropic Volumetric properties of Ternary Mixtures Containing 2-pyrrolidone and Cyclic Amides at 308.15 K	https://www.doi.org/10.1016/j.jct.2015.11.009
1-Pyrrolidone, 1-methyl-2-pyrrolidinone, and 2-pyrrolidinone at Different Temperatures	http://webbook.nist.gov/cgi/cbook.cgi?ID=C616455&Units=SI
Solubility of Acetylene in Alcohols and Ketones:	https://www.doi.org/10.1021/acs.jced.8b00126
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:	https://www.doi.org/10.1021/je049657g

Surface Tension of Aqueous Solutions of Short N-Alkyl-2-pyrrolidinones:	https://www.doi.org/10.1021/je800589e
Excess molar volumes and excess isentropic compressibilities of 2-pyrrolidinone at 308.15K:	https://www.doi.org/10.1016/j.tca.2009.07.017
KDB Vapor Pressure Data:	https://www.cheric.org/research/kdb/hcprop/showprop.php?cmpid=1339
Thermodynamic Properties of Ternary Liquid Mixtures of 2-Pyrrolidinone with Alcohols + Hydrocarbons:	https://www.doi.org/10.1007/s10765-010-0717-9
Densities, Ultrasonic speeds, excess and partial molar properties of binary mixtures of 2-pyrrolidone with isomeric propanediols at temperatures from 303.15 K to 323.15 K:	https://www.doi.org/10.1016/j.jct.2017.03.022
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
Effect of placement of hydroxyl groups in isomeric butanediol on the behaviour of thermophysical and spectroscopic properties of pyrrolidin-2-one:	https://www.doi.org/10.1016/j.jct.2004.11.020
The Yaws Handbook of Vapor Pressure:	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure
Isentropic compressibilities of (amide + water) mixtures: A comparative study:	https://www.doi.org/10.1016/j.jct.2007.05.015
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Excess Molar Enthalpies of Dibromomethane with Benzene, Methanol, Dimethylsulfoxide, and Pyrrolidin-2-one at 303.15 K:	https://www.doi.org/10.1021/je9005882
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Thermodynamic and Topological Studies of 1-Ethyl-3-methylimidazolium Tetrafluoroborate + Pyrrolidin-2-one and 1-Methyl-pyrrolidin-2-one Mixtures:	https://www.doi.org/10.1021/je300542s
KDB:	https://www.cheric.org/files/research/kdb/mol/mol1339.mol
Topological investigations of the molecular species and molecular interactions that characterize pyrrolidin-2-one + lower alkanol mixtures:	https://www.doi.org/10.1016/j.tca.2009.03.014
Aqueous Solubility Prediction Method:	http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa
Estimated Solubility Method:	http://pubs.acs.org/doi/suppl/10.1021/ci034243x/suppl_file/ci034243xsi20040112_053635.txt
Excess Heat Capacities for Lactam + Chlorotoluene Binary Mixtures:	https://www.doi.org/10.1021/je400408w
Excess heat capacities of (binary + ternary) mixtures containing [emim][BF4] and organic liquids:	https://www.doi.org/10.1016/j.jct.2014.07.014
Effect of β-cyclodextrin on the behaviour of thermophysical and spectroscopic properties of binary aqueous solutions of pyrrolidin-2-one:	https://www.doi.org/10.1016/j.jct.2012.08.026
Molecular interactions of 1,x-alkanediols in pyrrolidin-2-one: Thermodynamic and spectroscopic investigations:	https://www.doi.org/10.1016/j.jct.2007.08.005
Thermodynamic Properties of Ternary Mixtures Containing Ionic Liquids and Organic Solvents:	https://www.doi.org/10.1021/je301353z
Excess molar enthalpies for [emim][BF4] + pyrrolidin-2-one or 1-methyl-2-pyrrolidin-4-one + pyridine or water mixtures:	https://www.doi.org/10.1016/j.jct.2013.09.015
Thermodynamic properties of ternary mixtures of 1-ethyl-3-methylimidazolium tetrafluoroborate with 1-methyl pyrrolidin-2-one or pyrrolidin-2-one + water:	https://www.doi.org/10.1016/j.tca.2013.04.011
Thermodynamic properties of ternary mixtures containing 1-ethyl-3-methylimidazolium tetrafluoroborate with cyclic amides and cyclopentanone or cyclohexanone at T = (293.15, 298.15, 303.15 and 308.15)K:	https://www.doi.org/10.1016/j.jct.2015.02.018

Legend

chl:	Standard liquid enthalpy of combustion
cpg:	Ideal gas heat capacity
cpl:	Liquid phase heat capacity
cps:	Solid phase heat capacity
dvisc:	Dynamic viscosity
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
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
sfust:	Entropy of fusion at a given temperature
sl:	Liquid phase molar entropy at standard conditions
speedsl:	Speed of sound in fluid
ss:	Solid phase molar entropy at standard conditions
tb:	Normal Boiling Point Temperature
tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature
tf:	Normal melting (fusion) point
tt:	Triple Point Temperature
vc:	Critical Volume