Pyrrolidine

Other names:	AZACYCLOPENTANE AZOLIDINE BUTYLENIMINE NSC 62781 Perhydropyrrole Prolamine Pyrrole, tetrahydro- Pyrrolidine ring Tetrahydropyrrole Tetramethylenimine UN 1922 perhydroazole tetrahydroazole tetramethyleneimine
Inchi:	InChI=1S/C4H9N/c1-2-4-5-3-1/h5H,1-4H2
InchiKey:	RWRDLPDLKQPQOW-UHFFFAOYSA-N
Formula:	C4H9N
SMILES:	C1CCNC1
Mol. weight [g/mol]:	71.12
CAS:	123-75-1

Physical Properties

Property code	Value	Unit	Source
af	0.2740		KDB
affp	948.30	kJ/mol	NIST Webbook
basg	915.30	kJ/mol	NIST Webbook
chl	-2819.20 ± 0.75	kJ/mol	NIST Webbook
chl	-2819.30 ± 0.84	kJ/mol	NIST Webbook
dm	1.60	debye	KDB
gf	114.80	kJ/mol	KDB
hf	-3.40 ± 0.96	kJ/mol	NIST Webbook
hf	-3.60	kJ/mol	KDB
hf	-3.60 ± 0.92	kJ/mol	NIST Webbook
hfl	-41.20 ± 0.84	kJ/mol	NIST Webbook
hfl	-41.00 ± 0.84	kJ/mol	NIST Webbook
hfus	8.57	kJ/mol	Joback Method
hvap	37.52	kJ/mol	NIST Webbook

hvap	37.60	kJ/mol	NIST Webbook
hvap	37.60	kJ/mol	NIST Webbook
hvap	37.57 ± 0.06	kJ/mol	NIST Webbook
hvap	37.61 ± 0.10	kJ/mol	NIST Webbook
ie	8.41	eV	NIST Webbook
ie	8.82 ± 0.03	eV	NIST Webbook
ie	8.77 ± 0.02	eV	NIST Webbook
ie	8.77 ± 0.05	eV	NIST Webbook
ie	8.77 ± 0.02	eV	NIST Webbook
ie	8.82	eV	NIST Webbook
log10ws	1.15		Aqueous Solubility Prediction Method
logp	0.370		Crippen Method
mcvol	66.340	ml/mol	McGowan Method
pc	5700.00 ± 103.40	kPa	NIST Webbook
pc	5590.00	kPa	KDB
rinpol	686.00		NIST Webbook
rinpol	645.00		NIST Webbook
rinpol	695.00		NIST Webbook
rinpol	695.00		NIST Webbook
rinpol	695.00		NIST Webbook
rinpol	695.00		NIST Webbook
rinpol	688.00		NIST Webbook
rinpol	692.00		NIST Webbook
rinpol	674.90		NIST Webbook
rinpol	680.00		NIST Webbook
rinpol	690.00		NIST Webbook
rinpol	671.00		NIST Webbook
rinpol	671.00		NIST Webbook
rinpol	678.00		NIST Webbook
rinpol	695.00		NIST Webbook
rinpol	675.00		NIST Webbook
rinpol	660.00		NIST Webbook
ripol	999.00		NIST Webbook
ripol	1031.00		NIST Webbook
ripol	1020.00		NIST Webbook
ripol	1022.00		NIST Webbook
ripol	1032.00		NIST Webbook
ripol	1003.00		NIST Webbook
ripol	1006.00		NIST Webbook
ripol	1034.00		NIST Webbook
ripol	1047.00		NIST Webbook
ripol	1008.00		NIST Webbook
ripol	1038.00		NIST Webbook

ripol	995.00		NIST Webbook
ripol	994.00		NIST Webbook
ripol	1020.00		NIST Webbook
ripol	1040.00		NIST Webbook
sl	204.01	J/mol×K	NIST Webbook
sl	204.10	J/mol×K	NIST Webbook
tb	359.40	K	Evolution of the Liquid Vapor Equilibrium Properties of Several Unsymmetrical Amines: Determination of Their Binary Isobaric Diagrams and Applications to the Distillation
tb	359.71	K	KDB
tc	568.20	K	KDB
tc	568.60 ± 0.40	K	NIST Webbook
tc	570.00 ± 2.50	K	NIST Webbook
tc	568.60	K	NIST Webbook
tf	211.95 ± 0.50	K	NIST Webbook
tf	212.88	K	Aqueous Solubility Prediction Method
tf	215.31	K	KDB
tt	215.30	K	KDB
tt	215.24 ± 0.05	K	NIST Webbook
tt	215.31 ± 0.07	K	NIST Webbook
tt	215.30 ± 0.03	K	NIST Webbook
tt	215.31 ± 0.06	K	NIST Webbook
vc	0.249 ± 0.005	m3/kmol	NIST Webbook
vc	0.238	m3/kmol	KDB
zc	0.2816120		KDB

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	161.19	J/mol×K	568.40	Joback Method
cpg	113.40	J/mol×K	394.25	Joback Method
cpg	124.01	J/mol×K	429.08	Joback Method
cpg	134.07	J/mol×K	463.91	Joback Method
cpg	143.61	J/mol×K	498.74	Joback Method
cpg	152.65	J/mol×K	533.57	Joback Method
cpg	102.22	J/mol×K	359.42	Joback Method
cpl	156.57	J/mol×K	298.15	NIST Webbook
cpl	156.57	J/mol×K	298.15	NIST Webbook

cpl	160.20	J/mol×K	298.00	NIST Webbook
hfust	8.58	kJ/mol	215.30	NIST Webbook
hfust	0.54	kJ/mol	207.10	NIST Webbook
hfust	8.58	kJ/mol	215.30	NIST Webbook
hvapt	35.80	kJ/mol	355.00	NIST Webbook
hvapt	38.40	kJ/mol	293.00	NIST Webbook
hvapt	33.01	kJ/mol	359.70	NIST Webbook
hvapt	33.09	kJ/mol	359.00	KDB
hvapt	37.30	kJ/mol	327.00	NIST Webbook
hvapt	35.80 ± 0.10	kJ/mol	322.00	NIST Webbook
hvapt	34.50 ± 0.10	kJ/mol	340.00	NIST Webbook
hvapt	33.00 ± 0.10	kJ/mol	360.00	NIST Webbook
kvisc	0.0000010	m2/s	293.15	Densities and Viscosities of Aqueous Solutions of Pyrrolidine and Piperidine from (20 to 50) deg C
kvisc	0.0000007	m2/s	313.15	Densities and Viscosities of Aqueous Solutions of Pyrrolidine and Piperidine from (20 to 50) deg C
kvisc	0.0000006	m2/s	323.15	Densities and Viscosities of Aqueous Solutions of Pyrrolidine and Piperidine from (20 to 50) deg C
kvisc	0.0000008	m2/s	303.15	Densities and Viscosities of Aqueous Solutions of Pyrrolidine and Piperidine from (20 to 50) deg C
pvap	86.66	kPa	354.90	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	337.60	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	329.00	Evolution of the Liquid Vapor Equilibrium Properties of Several Unsymmetrical Amines: Determination of Their Binary Isobaric Diagrams and Applications to the Distillation
pvap	66.66	kPa	347.50	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	323.40	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	316.90	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	359.40	Evolution of the Liquid Vapor Equilibrium Properties of Several Unsymmetrical Amines: Determination of Their Binary Isobaric Diagrams and Applications to the Distillation	
pvap	17.54	kPa	313.46	Vapor Pressure and Its Temperature Dependence of 28 Organic Compounds: Cyclic Amines, Cyclic Ethers, and Cyclic and Open Chain Secondary Alcohols	
pvap	2.04	kPa	273.16	Vapor Pressure and Its Temperature Dependence of 28 Organic Compounds: Cyclic Amines, Cyclic Ethers, and Cyclic and Open Chain Secondary Alcohols	
pvap	3.86	kPa	283.73	Vapor Pressure and Its Temperature Dependence of 28 Organic Compounds: Cyclic Amines, Cyclic Ethers, and Cyclic and Open Chain Secondary Alcohols	
pvap	13.59	kPa	307.93	Vapor Pressure and Its Temperature Dependence of 28 Organic Compounds: Cyclic Amines, Cyclic Ethers, and Cyclic and Open Chain Secondary Alcohols	

pvap	6.50	kPa	293.10	Vapor Pressure and Its Temperature Dependence of 28 Organic Compounds: Cyclic Amines, Cyclic Ethers, and Cyclic and Open Chain Secondary Alcohols	
pvap	6.52	kPa	293.25	Vapor Pressure and Its Temperature Dependence of 28 Organic Compounds: Cyclic Amines, Cyclic Ethers, and Cyclic and Open Chain Secondary Alcohols	
pvap	8.46	kPa	298.15	Vapor Pressure and Its Temperature Dependence of 28 Organic Compounds: Cyclic Amines, Cyclic Ethers, and Cyclic and Open Chain Secondary Alcohols	
pvap	10.87	kPa	303.25	Vapor Pressure and Its Temperature Dependence of 28 Organic Compounds: Cyclic Amines, Cyclic Ethers, and Cyclic and Open Chain Secondary Alcohols	
pvap	4.98	kPa	288.23	Vapor Pressure and Its Temperature Dependence of 28 Organic Compounds: Cyclic Amines, Cyclic Ethers, and Cyclic and Open Chain Secondary Alcohols	

rhol	854.60	kg/m3	298.15	Densities and Excess and Partial Molar Volumes of Aqueous Pyrrolidine at 25 and 50 C and Aqueous Morpholine at 25 and 60 C
rhol	852.00	kg/m3	295.00	KDB
rhol	833.70	kg/m3	323.15	Densities and Excess and Partial Molar Volumes of Aqueous Pyrrolidine at 25 and 50 C and Aqueous Morpholine at 25 and 60 C
sfust	39.84	J/mol×K	215.30	NIST Webbook
sfust	2.61	J/mol×K	207.10	NIST Webbook
speedsl	1263.00	m/s	323.00	Speed of sound and isentropic compressibility of aqueous solutions of pyrrolidine and piperidine
speedsl	1389.40	m/s	293.00	Speed of sound and isentropic compressibility of aqueous solutions of pyrrolidine and piperidine
speedsl	1348.00	m/s	303.00	Speed of sound and isentropic compressibility of aqueous solutions of pyrrolidine and piperidine
speedsl	1305.80	m/s	313.00	Speed of sound and isentropic compressibility of aqueous solutions of pyrrolidine and piperidine
srf	0.03	N/m	303.15	Surface Behavior of Aqueous Solutions of Pyrrolidine and Piperidine
srf	0.03	N/m	313.15	Surface Behavior of Aqueous Solutions of Pyrrolidine and Piperidine

srf	0.03	N/m	323.15	Surface Behavior of Aqueous Solutions of Pyrrolidine and Piperidine
srf	0.03	N/m	298.15	Densities, Viscosities, Surface Tensions, and Speeds of Sound of Aqueous Solutions of Piperidine + Pyrrolidine + Water
srf	0.03	N/m	293.15	Surface Behavior of Aqueous Solutions of Pyrrolidine and Piperidine
srf	0.03	N/m	293.20	KDB
srf	0.03	N/m	298.15	Surface Behavior of Aqueous Solutions of Pyrrolidine and Piperidine

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.44189e+01
Coeff. B	-2.96769e+03
Coeff. C	-5.71920e+01
Temperature range (K), min.	267.20
Temperature range (K), max.	383.05

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/T + C*ln(T) + D*T^2
Coeff. A	1.08983e+02
Coeff. B	-8.21427e+03
Coeff. C	-1.40875e+01
Coeff. D	1.06991e-05
Temperature range (K), min.	215.31
Temperature range (K), max.	568.55

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
KDB Vapor Pressure Data:	https://www.cheric.org/research/kdb/hcprop/showprop.php?cmpid=1340
Speed of sound and isentropic compressibility of aqueous solutions of pyrrolidine and piperidine:	https://www.doi.org/10.1021/je050483s
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
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
Densities, Viscosities, Surface Tensions, and Speeds of Sound of Aqueous Solutions of Piperidine + Pyrrolidine + Water:	https://www.doi.org/10.1021/je700290j
Experimental solid-liquid-liquid equilibrium data for the H2O + NaOH + pyrrolidine ternary system. Application to the extraction of N-aminopyrrolidine:	https://www.doi.org/10.1016/j.fluid.2014.07.019
KDB Pure (Korean Thermophysical Properties Databank):	https://www.cheric.org/research/kdb/hcprop/showprop.php?cmpid=1340
Densities and Viscosities of Aqueous Solutions of Pyrrolidine and Piperidine from (20 to 50) deg C:	https://www.doi.org/10.1021/je050005h
Thermodynamic study of (heptane + amine) mixtures. III: Excess and partial molar volumes in mixtures with secondary, tertiary, and cyclic amines at 298.15 K:	https://www.doi.org/10.1016/j.jct.2011.04.017
Densities and Excess and Partial Molar Volumes of Aqueous Pyrrolidine at 25 and 60 C and Aqueous Morpholine at 25 and 60 C:	https://www.doi.org/10.1021/je020191g
The Yaws Handbook of Vapor Pressure:	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C123751&Units=SI
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
KDB:	https://www.cheric.org/files/research/kdb/mol/mol1340.mol
Surface Behavior of Aqueous Solutions of Pyrrolidine and Piperidine:	https://www.doi.org/10.1021/je049888n
Vapor Pressure and Its Temperature Dependence of 28 Organic Compounds: Cyclic Amines, Cyclic Ethers, and Cyclic and Open Chain Secondary Alcohols:	https://www.doi.org/10.1021/acs.jced.6b00576
Aqueous Solubility Prediction Method:	http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa

Legend

af:	Acentric Factor
affp:	Proton affinity
basg:	Gas basicity
chl:	Standard liquid enthalpy of combustion
cpg:	Ideal gas heat capacity
cpl:	Liquid phase heat capacity
dm:	Dipole Moment
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
kvisc:	Kinematic viscosity
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
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
srf:	Surface Tension
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
tt:	Triple Point Temperature
vc:	Critical Volume
zc:	Critical Compressibility