

Piperidine, 1-methyl-

Other names:	1-Methylpiperidine
	1-pipecoline
	N-Methylpiperidine
	UN 2399
	pipecoline
Inchi:	InChI=1S/C6H13N/c1-7-5-3-2-4-6-7/h2-6H2,1H3
InchiKey:	PAMIIKDUOTOBW-UHFFFAOYSA-N
Formula:	C6H13N
SMILES:	CN1CCCCC1
Mol. weight [g/mol]:	99.17
CAS:	626-67-5

Physical Properties

Property code	Value	Unit	Source
affp	971.10	kJ/mol	NIST Webbook
basg	940.10	kJ/mol	NIST Webbook
hvap	36.80 ± 0.60	kJ/mol	NIST Webbook
hvap	36.70 ± 0.10	kJ/mol	NIST Webbook
hvap	36.80 ± 0.60	kJ/mol	NIST Webbook
ie	7.80 ± 0.05	eV	NIST Webbook
ie	8.29 ± 0.02	eV	NIST Webbook
ie	7.74 ± 0.05	eV	NIST Webbook
ie	8.29	eV	NIST Webbook
ie	8.29 ± 0.05	eV	NIST Webbook
ie	8.29 ± 0.02	eV	NIST Webbook
ie	8.35	eV	NIST Webbook
log10ws	0.23		Aqueous Solubility Prediction Method
logp	1.102		Crippen Method
mcpvol	94.520	ml/mol	McGowan Method
rinpol	769.00		NIST Webbook
rinpol	749.00		NIST Webbook
rinpol	750.00		NIST Webbook
rinpol	769.00		NIST Webbook
rinpol	763.00		NIST Webbook
rinpol	763.00		NIST Webbook

rinpol	750.00		NIST Webbook
rinpol	779.00		NIST Webbook
rinpol	769.00		NIST Webbook
rinpol	766.00		NIST Webbook
rinpol	766.00		NIST Webbook
rinpol	760.00		NIST Webbook
ripol	981.00		NIST Webbook
ripol	1020.00		NIST Webbook
ripol	999.00		NIST Webbook
ripol	1003.00		NIST Webbook
ripol	928.00		NIST Webbook
ripol	934.00		NIST Webbook
ripol	957.00		NIST Webbook
ripol	959.00		NIST Webbook
ripol	986.00		NIST Webbook
ripol	967.00		NIST Webbook
tb	390.15 ± 3.00	K	NIST Webbook
tb	379.05 ± 0.50	K	NIST Webbook
tb	378.85 ± 0.20	K	NIST Webbook
tb	380.20	K	NIST Webbook
tb	379.65 ± 0.50	K	NIST Webbook

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpl	184.90	J/molxK	298.00	NIST Webbook
cpl	177.60	J/molxK	288.15	Excess Molar Enthalpies and Heat Capacities of {2-Methylpiperidine Water} and {N-Methylpiperidine Water} Systems of Low to Moderate Amine Compositions
cpl	194.60	J/molxK	333.15	Excess Molar Enthalpies and Heat Capacities of {2-Methylpiperidine Water} and {N-Methylpiperidine Water} Systems of Low to Moderate Amine Compositions

cpl	192.70	J/molxK	328.15	Excess Molar Enthalpies and Heat Capacities of {2-Methylpiperidine Water} and {N-Methylpiperidine Water} Systems of Low to Moderate Amine Compositions
cpl	191.20	J/molxK	323.15	Excess Molar Enthalpies and Heat Capacities of {2-Methylpiperidine Water} and {N-Methylpiperidine Water} Systems of Low to Moderate Amine Compositions
cpl	189.10	J/molxK	318.15	Excess Molar Enthalpies and Heat Capacities of {2-Methylpiperidine Water} and {N-Methylpiperidine Water} Systems of Low to Moderate Amine Compositions
cpl	187.50	J/molxK	313.16	Excess Molar Enthalpies and Heat Capacities of {2-Methylpiperidine Water} and {N-Methylpiperidine Water} Systems of Low to Moderate Amine Compositions
cpl	185.50	J/molxK	308.15	Excess Molar Enthalpies and Heat Capacities of {2-Methylpiperidine Water} and {N-Methylpiperidine Water} Systems of Low to Moderate Amine Compositions

cpl	183.50	J/molxK	303.16	Excess Molar Enthalpies and Heat Capacities of {2-Methylpiperidine Water} and {N-Methylpiperidine Water} Systems of Low to Moderate Amine Compositions
cpl	181.50	J/molxK	298.15	Excess Molar Enthalpies and Heat Capacities of {2-Methylpiperidine Water} and {N-Methylpiperidine Water} Systems of Low to Moderate Amine Compositions
cpl	179.50	J/molxK	293.15	Excess Molar Enthalpies and Heat Capacities of {2-Methylpiperidine Water} and {N-Methylpiperidine Water} Systems of Low to Moderate Amine Compositions
cpl	175.40	J/molxK	283.15	Excess Molar Enthalpies and Heat Capacities of {2-Methylpiperidine Water} and {N-Methylpiperidine Water} Systems of Low to Moderate Amine Compositions
hvapt	37.30	kJ/mol	326.50	NIST Webbook
hvapt	36.50	kJ/mol	320.50	NIST Webbook
pvap	9.86	kPa	313.47	Vapor Pressure and Its Temperature Dependence of 28 Organic Compounds: Cyclic Amines, Cyclic Ethers, and Cyclic and Open Chain Secondary Alcohols

pvap	1.24	kPa	273.18	Vapor Pressure and Its Temperature Dependence of 28 Organic Compounds: Cyclic Amines, Cyclic Ethers, and Cyclic and Open Chain Secondary Alcohols
pvap	2.23	kPa	282.90	Vapor Pressure and Its Temperature Dependence of 28 Organic Compounds: Cyclic Amines, Cyclic Ethers, and Cyclic and Open Chain Secondary Alcohols
pvap	2.90	kPa	287.85	Vapor Pressure and Its Temperature Dependence of 28 Organic Compounds: Cyclic Amines, Cyclic Ethers, and Cyclic and Open Chain Secondary Alcohols
pvap	3.75	kPa	292.70	Vapor Pressure and Its Temperature Dependence of 28 Organic Compounds: Cyclic Amines, Cyclic Ethers, and Cyclic and Open Chain Secondary Alcohols
pvap	3.92	kPa	293.51	Vapor Pressure and Its Temperature Dependence of 28 Organic Compounds: Cyclic Amines, Cyclic Ethers, and Cyclic and Open Chain Secondary Alcohols

pvap	4.96	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	5.49	kPa	300.35	Vapor Pressure and Its Temperature Dependence of 28 Organic Compounds: Cyclic Amines, Cyclic Ethers, and Cyclic and Open Chain Secondary Alcohols
pvap	6.16	kPa	302.86	Vapor Pressure and Its Temperature Dependence of 28 Organic Compounds: Cyclic Amines, Cyclic Ethers, and Cyclic and Open Chain Secondary Alcohols
pvap	7.95	kPa	308.47	Vapor Pressure and Its Temperature Dependence of 28 Organic Compounds: Cyclic Amines, Cyclic Ethers, and Cyclic and Open Chain Secondary Alcohols
rhoI	803.85	kg/m3	308.15	Temperatures of liquid-liquid separation and excess molar volumes of {N-methylpiperidine-water} and {2-methylpiperidine-water} systems

rhoI	822.24	kg/m3	288.15	Temperatures of liquid-liquid separation and excess molar volumes of {N-methylpiperidine-water} and {2-methylpiperidine-water} systems
rhoI	803.61	kg/m3	308.15	Determination of Infinite Dilution Partial Molar Excess Enthalpies and Volumes for Some Ionic Liquid Precursors in Water and Methanol Using Tandem Flow Mixing Calorimetry and Vibrating-Tube Densimetry
rhoI	808.16	kg/m3	303.15	Determination of Infinite Dilution Partial Molar Excess Enthalpies and Volumes for Some Ionic Liquid Precursors in Water and Methanol Using Tandem Flow Mixing Calorimetry and Vibrating-Tube Densimetry
rhoI	812.62	kg/m3	298.15	Determination of Infinite Dilution Partial Molar Excess Enthalpies and Volumes for Some Ionic Liquid Precursors in Water and Methanol Using Tandem Flow Mixing Calorimetry and Vibrating-Tube Densimetry

rhoI	817.22	kg/m3	293.15	Determination of Infinite Dilution Partial Molar Excess Enthalpies and Volumes for Some Ionic Liquid Precursors in Water and Methanol Using Tandem Flow Mixing Calorimetry and Vibrating-Tube Densimetry
rhoI	821.53	kg/m3	288.15	Determination of Infinite Dilution Partial Molar Excess Enthalpies and Volumes for Some Ionic Liquid Precursors in Water and Methanol Using Tandem Flow Mixing Calorimetry and Vibrating-Tube Densimetry
rhoI	810.89	kg/m3	298.15	Temperatures of liquid-liquid separation and excess molar volumes of {N-methylpiperidine-water} and {2-methylpiperidine-water} systems
rhoI	785.64	kg/m3	328.15	Temperatures of liquid-liquid separation and excess molar volumes of {N-methylpiperidine-water} and {2-methylpiperidine-water} systems
rhoI	796.93	kg/m3	318.15	Temperatures of liquid-liquid separation and excess molar volumes of {N-methylpiperidine-water} and {2-methylpiperidine-water} systems

rhoI	781.62	kg/m3	338.15	Temperatures of liquid-liquid separation and excess molar volumes of {N-methylpiperidine-water} and {2-methylpiperidine-water} systems
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Correlations

Information	Value
Property code	pvap
Equation	$\ln(P_{vp}) = A + B/(T + C)$
Coeff. A	1.42259e+01
Coeff. B	-3.20286e+03
Coeff. C	-4.68320e+01
Temperature range (K), min.	276.62
Temperature range (K), max.	406.12

Sources

Temperatures of liquid-liquid separation and excess molar volumes of {N-methylpiperidine-water} and {2-methylpiperidine-water} systems	https://www.doi.org/10.1016/j.fluid.2010.05.001
Determination of infinite dilution partial molar excess enthalpies and volumes for some low molecular weight organic compounds in water and {N-methylpiperidine-water} and {2-methylpiperidine-water} systems	https://www.doi.org/10.1021/je200093f
Excess molar enthalpies and volumes for {N-methylpiperidine-water} and {2-methylpiperidine-water} systems	https://www.doi.org/10.1016/j.fluid.2016.10.010
Excess molar enthalpies and heat capacities of {2-methylpiperidine-water} and {N-methylpiperidine-water} systems	https://www.doi.org/10.1021/je5008444
Excess molar enthalpies and heat capacities of {N-methylpiperidine-water} and {2-methylpiperidine-water} systems	http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDataset002.xlsx
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C626675&Units=SI

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
The Yaws Handbook of Vapor Pressure:	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure
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

Legend

affp:	Proton affinity
basg:	Gas basicity

cpl:	Liquid phase heat capacity
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
pvap:	Vapor pressure
rho:	Liquid Density
rinpol:	Non-polar retention indices
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature

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