

Piperazine, 1-methyl-

Other names:	1-Methylpiperazine N-Methylpiperazine piperazine, N-methyl-
Inchi:	InChI=1S/C5H12N2/c1-7-4-2-6-3-5-7/h6H,2-5H2,1H3
InchiKey:	PVOAHINGSUIXLS-UHFFFAOYSA-N
Formula:	C5H12N2
SMILES:	CN1CCNCC1
Mol. weight [g/mol]:	100.16
CAS:	109-01-3

Physical Properties

Property code	Value	Unit	Source
log10ws	0.43		Crippen Method
logp	-0.479		Crippen Method
mcvol	90.410	ml/mol	McGowan Method
ripol	852.00		NIST Webbook
ripol	847.00		NIST Webbook
ripol	839.00		NIST Webbook
ripol	1262.00		NIST Webbook
ripol	1270.00		NIST Webbook
ripol	1282.00		NIST Webbook
ripol	1274.00		NIST Webbook
ripol	1266.00		NIST Webbook
ripol	1286.00		NIST Webbook
ripol	1262.00		NIST Webbook
ripol	1282.00		NIST Webbook
tb	411.20	K	NIST Webbook
tb	410.65 ± 0.30	K	NIST Webbook
tb	411.15	K	NIST Webbook
tf	267.82 ± 0.20	K	NIST Webbook
tf	266.75	K	NIST Webbook
tf	266.80 ± 0.60	K	NIST Webbook

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpl	218.00	J/molxK	353.15	Molar Heat Capacity (Cp) of Aqueous Cyclic Amine Solutions from (298.15 to 353.15) K
cpl	213.90	J/molxK	298.15	Molar Heat Capacity (Cp) of Aqueous Cyclic Amine Solutions from (298.15 to 353.15) K
cpl	215.70	J/molxK	313.15	Molar Heat Capacity (Cp) of Aqueous Cyclic Amine Solutions from (298.15 to 353.15) K
cpl	216.40	J/molxK	318.15	Molar Heat Capacity (Cp) of Aqueous Cyclic Amine Solutions from (298.15 to 353.15) K
cpl	215.00	J/molxK	308.15	Molar Heat Capacity (Cp) of Aqueous Cyclic Amine Solutions from (298.15 to 353.15) K
cpl	216.90	J/molxK	323.15	Molar Heat Capacity (Cp) of Aqueous Cyclic Amine Solutions from (298.15 to 353.15) K
cpl	217.30	J/molxK	328.15	Molar Heat Capacity (Cp) of Aqueous Cyclic Amine Solutions from (298.15 to 353.15) K
cpl	215.50	J/molxK	338.15	Molar Heat Capacity (Cp) of Aqueous Cyclic Amine Solutions from (298.15 to 353.15) K
cpl	216.20	J/molxK	343.15	Molar Heat Capacity (Cp) of Aqueous Cyclic Amine Solutions from (298.15 to 353.15) K

cpl	217.60	J/molxK	348.15	Molar Heat Capacity (Cp) of Aqueous Cyclic Amine Solutions from (298.15 to 353.15) K
cpl	217.20	J/molxK	333.15	Molar Heat Capacity (Cp) of Aqueous Cyclic Amine Solutions from (298.15 to 353.15) K
cpl	214.40	J/molxK	303.15	Molar Heat Capacity (Cp) of Aqueous Cyclic Amine Solutions from (298.15 to 353.15) K
dvisc	0.0021000	Paxs	293.15	Viscosities and densities for binary mixtures of N-methylpiperazine with methanol, ethanol, n-propanol, iso-propanol, n-butanol and iso-butanol at 293.15, 298.15 and 303.15K
dvisc	0.0016240	Paxs	303.15	Viscosities and densities for binary mixtures of N-methylpiperazine with methanol, ethanol, n-propanol, iso-propanol, n-butanol and iso-butanol at 293.15, 298.15 and 303.15K
dvisc	0.0018540	Paxs	298.15	Thermodynamic study of Binary Mixtures of Tricyclo [5.2.1.0(2.6)] Decane with N-Methylpiperazine or Triethylamine at T = (298.15 to 323.15) K
dvisc	0.0015830	Paxs	303.15	Thermodynamic study of Binary Mixtures of Tricyclo [5.2.1.0(2.6)] Decane with N-Methylpiperazine or Triethylamine at T = (298.15 to 323.15) K

dvisc	0.0012580	Paxs	313.15	Thermodynamic study of Binary Mixtures of Tricyclo [5.2.1.0(2.6)] Decane with N-Methylpiperazine or Triethylamine at T = (298.15 to 323.15) K
dvisc	0.0010640	Paxs	323.15	Thermodynamic study of Binary Mixtures of Tricyclo [5.2.1.0(2.6)] Decane with N-Methylpiperazine or Triethylamine at T = (298.15 to 323.15) K
dvisc	0.0018560	Paxs	298.15	Volumetric and Viscous Properties at Several Temperatures for Binary Mixtures of N-Methylpiperazine with Methylcyclohexane or n-Heptane
dvisc	0.0015440	Paxs	303.15	Volumetric and Viscous Properties at Several Temperatures for Binary Mixtures of N-Methylpiperazine with Methylcyclohexane or n-Heptane
dvisc	0.0012500	Paxs	313.15	Volumetric and Viscous Properties at Several Temperatures for Binary Mixtures of N-Methylpiperazine with Methylcyclohexane or n-Heptane
dvisc	0.0014090	Paxs	308.15	Thermodynamic study of Binary Mixtures of Tricyclo [5.2.1.0(2.6)] Decane with N-Methylpiperazine or Triethylamine at T = (298.15 to 323.15) K

dvisc	0.0018410	Paxs	298.15	Viscosities and densities for binary mixtures of N-methylpiperazine with methanol, ethanol, n-propanol, iso-propanol, n-butanol and iso-butanol at 293.15, 298.15 and 303.15K
hvapt	46.70	kJ/mol	296.50	NIST Webbook
pvap	3.12	kPa	319.47	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	313.21	Vapor Pressure and Its Temperature Dependence of 28 Organic Compounds: Cyclic Amines, Cyclic Ethers, and Cyclic and Open Chain Secondary Alcohols
pvap	1.65	kPa	307.83	Vapor Pressure and Its Temperature Dependence of 28 Organic Compounds: Cyclic Amines, Cyclic Ethers, and Cyclic and Open Chain Secondary Alcohols
pvap	2.50	kPa	315.32	Vapor Pressure and Its Temperature Dependence of 28 Organic Compounds: Cyclic Amines, Cyclic Ethers, and Cyclic and Open Chain Secondary Alcohols

pvap	1.65	kPa	307.75	Vapor Pressure and Its Temperature Dependence of 28 Organic Compounds: Cyclic Amines, Cyclic Ethers, and Cyclic and Open Chain Secondary Alcohols
pvap	1.34	kPa	304.25	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	302.86	Vapor Pressure and Its Temperature Dependence of 28 Organic Compounds: Cyclic Amines, Cyclic Ethers, and Cyclic and Open Chain Secondary Alcohols
pvap	1.00	kPa	299.32	Vapor Pressure and Its Temperature Dependence of 28 Organic Compounds: Cyclic Amines, Cyclic Ethers, and Cyclic and Open Chain Secondary Alcohols
pvap	0.93	kPa	298.20	Vapor Pressure and Its Temperature Dependence of 28 Organic Compounds: Cyclic Amines, Cyclic Ethers, and Cyclic and Open Chain Secondary Alcohols

pvap	2.88	kPa	317.91	Vapor Pressure and Its Temperature Dependence of 28 Organic Compounds: Cyclic Amines, Cyclic Ethers, and Cyclic and Open Chain Secondary Alcohols
pvap	0.93	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	0.68	kPa	293.21	Vapor Pressure and Its Temperature Dependence of 28 Organic Compounds: Cyclic Amines, Cyclic Ethers, and Cyclic and Open Chain Secondary Alcohols
pvap	0.58	kPa	290.75	Vapor Pressure and Its Temperature Dependence of 28 Organic Compounds: Cyclic Amines, Cyclic Ethers, and Cyclic and Open Chain Secondary Alcohols
pvap	0.46	kPa	287.23	Vapor Pressure and Its Temperature Dependence of 28 Organic Compounds: Cyclic Amines, Cyclic Ethers, and Cyclic and Open Chain Secondary Alcohols

pvap	0.37	kPa	284.39	Vapor Pressure and Its Temperature Dependence of 28 Organic Compounds: Cyclic Amines, Cyclic Ethers, and Cyclic and Open Chain Secondary Alcohols
pvap	0.30	kPa	281.27	Vapor Pressure and Its Temperature Dependence of 28 Organic Compounds: Cyclic Amines, Cyclic Ethers, and Cyclic and Open Chain Secondary Alcohols
pvap	0.25	kPa	278.91	Vapor Pressure and Its Temperature Dependence of 28 Organic Compounds: Cyclic Amines, Cyclic Ethers, and Cyclic and Open Chain Secondary Alcohols
pvap	0.21	kPa	276.72	Vapor Pressure and Its Temperature Dependence of 28 Organic Compounds: Cyclic Amines, Cyclic Ethers, and Cyclic and Open Chain Secondary Alcohols
pvap	0.19	kPa	274.99	Vapor Pressure and Its Temperature Dependence of 28 Organic Compounds: Cyclic Amines, Cyclic Ethers, and Cyclic and Open Chain Secondary Alcohols

pvap	0.18	kPa	274.39	Vapor Pressure and Its Temperature Dependence of 28 Organic Compounds: Cyclic Amines, Cyclic Ethers, and Cyclic and Open Chain Secondary Alcohols
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Correlations

Information	Value
Property code	pvap
Equation	$\ln(P_{vp}) = A + B/(T + C)$
Coeff. A	1.55432e+01
Coeff. B	-3.88545e+03
Coeff. C	-5.54500e+01
Temperature range (K), min.	310.14
Temperature range (K), max.	435.19

Sources

NIST Webbook:

<http://webbook.nist.gov/cgi/cbook.cgi?ID=C109013&Units=SI>

High-Pressure Solubility of Carbon Dioxide (CO₂) in Aqueous 1-Methylpiperazine Solutions for binary mixtures of N-methylpiperazine with Methanol, Ethanol, n-Propanol, Isobutanol, n-butanol and iso-butanol at 298.15, 308.15 and 318.15 K for systems of aqueous piperazine and its derivatives
 Vapor Pressure and Its Temperature Dependence of 28 Organic Compounds: Cyclic Amines, Cyclic Ethers, and Cyclic and Open Chain Secondary Alcohols:
 Crippen Method

<https://www.doi.org/10.1021/je500526m>

<https://www.doi.org/10.1016/j.fluid.2005.05.012>

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

<https://www.doi.org/10.1016/j.jct.2015.06.006>

<https://www.doi.org/10.1021/acs.jced.6b00576>

https://www.chemeo.com/doc/models/crippen_log10ws

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

Molar Heat Capacity (Cp) of Aqueous Cyclic Amine Solutions from (298.15 to 343.15) K
 Solubility measurement and thermodynamic modeling for the ternary system of binary mixtures of Tricyclo [5.2.1.0(2.6)] deltamethrin and Methylpiperazine at several temperatures (298.15, 313.15) K
 Vapor Pressure and Its Temperature Dependence of 28 Organic Compounds: Cyclic Amines, Cyclic Ethers, and Cyclic and Open Chain Secondary Alcohols:
 Crippen Method

<https://www.doi.org/10.1021/je400178k>

<https://www.doi.org/10.1016/j.fluid.2015.03.021>

<https://www.doi.org/10.1016/j.tca.2012.06.011>

<https://www.doi.org/10.1021/je900969u>

<https://www.doi.org/10.1016/j.jct.2011.06.020>

<http://pubs.acs.org/doi/abs/10.1021/ci9903071>

Legend

cpl:	Liquid phase heat capacity
dvisc:	Dynamic viscosity
hvapt:	Enthalpy of vaporization at a given temperature
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pvap:	Vapor pressure
rinpol:	Non-polar retention indices
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tf:	Normal melting (fusion) point

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