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
rinpol	847.00		NIST Webbook
rinpol	852.00		NIST Webbook
rinpol	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	1282.00		NIST Webbook
ripol	1266.00		NIST Webbook
ripol	1262.00		NIST Webbook
ripol	1286.00		NIST Webbook
tb	410.65 ± 0.30	K	NIST Webbook
tb	411.15	K	NIST Webbook
tb	411.20	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	217.60	J/mol×K	348.15	Molar Heat Capacity (Cp) of Aqueous Cyclic Amine Solutions from (298.15 to 353.15) K
cpl	214.40	J/mol×K	303.15	Molar Heat Capacity (Cp) of Aqueous Cyclic Amine Solutions from (298.15 to 353.15) K
cpl	215.00	J/mol×K	308.15	Molar Heat Capacity (Cp) of Aqueous Cyclic Amine Solutions from (298.15 to 353.15) K
cpl	215.70	J/mol×K	313.15	Molar Heat Capacity (Cp) of Aqueous Cyclic Amine Solutions from (298.15 to 353.15) K
cpl	216.40	J/mol×K	318.15	Molar Heat Capacity (Cp) of Aqueous Cyclic Amine Solutions from (298.15 to 353.15) K
cpl	216.90	J/mol×K	323.15	Molar Heat Capacity (Cp) of Aqueous Cyclic Amine Solutions from (298.15 to 353.15) K
cpl	217.30	J/mol×K	328.15	Molar Heat Capacity (Cp) of Aqueous Cyclic Amine Solutions from (298.15 to 353.15) K
cpl	217.20	J/mol×K	333.15	Molar Heat Capacity (Cp) of Aqueous Cyclic Amine Solutions from (298.15 to 353.15) K
cpl	215.50	J/mol×K	338.15	Molar Heat Capacity (Cp) of Aqueous Cyclic Amine Solutions from (298.15 to 353.15) K

cpl	216.20	J/mol×K	343.15	Molar Heat Capacity (Cp) of Aqueous Cyclic Amine Solutions from (298.15 to 353.15) K
cpl	218.00	J/mol×K	353.15	Molar Heat Capacity (Cp) of Aqueous Cyclic Amine Solutions from (298.15 to 353.15) K
cpl	213.90	J/mol×K	298.15	Molar Heat Capacity (Cp) of Aqueous Cyclic Amine Solutions from (298.15 to 353.15) K
dvisc	0.0012500	Pa×s	313.15	Volumetric and Viscous Properties at Several Temperatures for Binary Mixtures of N-Methylpiperazine with Methylcyclohexane or n-Heptane
dvisc	0.0015440	Pa×s	303.15	Volumetric and Viscous Properties at Several Temperatures for Binary Mixtures of N-Methylpiperazine with Methylcyclohexane or n-Heptane
dvisc	0.0018560	Pa×s	298.15	Volumetric and Viscous Properties at Several Temperatures for Binary Mixtures of N-Methylpiperazine with Methylcyclohexane or n-Heptane
dvisc	0.0010640	Pa×s	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	0.0014090	Pa×s	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	0.0015830	Pa×s	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	0.0018540	Pa×s	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	0.0016240	Pa×s	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	0.0018410	Pa×s	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	

dvisc	0.0012580	Pa×s	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	0.0021000	Pa×s	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
hvapt	46.70	kJ/mol	296.50	NIST Webbook
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	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	1.65	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	1.65	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	2.23	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	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	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	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	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	

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	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

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = 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
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:	https://www.doi.org/10.1016/j.tca.2012.06.011
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Volumetric and Viscous Properties at Several Temperatures for Binary Mixtures of N Methylpiperazine with Methylcyclohexane or n-Heptane:	https://www.doi.org/10.1021/je900969u
The Yaws Handbook of Vapor Pressure:	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure
Molar excess enthalpy (Hm E) for systems of aqueous piperazine derivatives:	https://www.doi.org/10.1016/j.jct.2015.06.006
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
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

High-Pressure Solubility of Carbon Dioxide (CO2) in Aqueous 1-Methyl Piperazine Solution:	https://www.doi.org/10.1021/je500526m
Grippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Physicochemical properties of {1-methyl piperazine (1) + water (2)} system at T = (298.15 to 343.15) K and atmospheric pressure:	https://www.doi.org/10.1016/j.jct.2011.06.020
Viscosities and densities for binary mixtures of N-methylpiperazine with methanol, ethanol, 1-propanol, 2-propanol, 1-butanol and 2-butanol at (293.15, 298.15 and 303.15) K:	https://www.doi.org/10.1016/j.fluid.2005.05.012
Molar Heat Capacity (Cp) of Aqueous Cyclic Amine Solutions from (298.15 to 363.15) K:	https://www.doi.org/10.1021/je400178k
CO2 solubility measurement and thermodynamic modeling for 1-methylpiperazine/water/CO2:	https://www.doi.org/10.1016/j.fluid.2015.03.021

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