Piperazine, 1,4-dimethyl-

Other names:	1,4-Dimethylpiperazine
	Lupetazine
	N,N'-Dimethyipiperazine
	N,N'-Dimethylpiperazine
	Texacat DMP
	piperazine, N,N'-dimethyl-
Inchi:	InChI=1S/C6H14N2/c1-7-3-5-8(2)6-4-7/h3-6H2,1-2H3
InchiKey:	RXYPXQSKLGGKOL-UHFFFAOYSA-N
Formula:	C6H14N2
SMILES:	CN1CCN(C)CC1
Mol. weight [g/mol]:	114.19
CAS:	106-58-1

Physical Properties

Property code	Value	Unit	Source
hvap	43.80 ± 0.30	kJ/mol	NIST Webbook
hvap	41.20 ± 0.40	kJ/mol	NIST Webbook
ie	8.77	eV	NIST Webbook
log10ws	0.63		Crippen Method
logp	-0.136		Crippen Method
mcvol	104.500	ml/mol	McGowan Method
tb	404.15 ± 0.30	K	NIST Webbook
tb	403.65 ± 1.50	K	NIST Webbook
tc	606.00	K	Critical temperatures and pressures of caprolactam, dimethyl sulfoxide, 1,4-dimethylpiperazine, and 2,6-dimethylpiperazine
tf	272.15 ± 0.20	K	NIST Webbook

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source

cpl	216.50	J/mol×K	298.15	Molar Heat Capacity (Cp) of Aqueous Cyclic Amine Solutions from (298.15 to 353.15) K
cpl	221.70	J/mol×K	303.15	Molar Heat Capacity (Cp) of Aqueous Cyclic Amine Solutions from (298.15 to 353.15) K
cpl	222.10	J/mol×K	308.15	Molar Heat Capacity (Cp) of Aqueous Cyclic Amine Solutions from (298.15 to 353.15) K
cpl	223.40	J/mol×K	313.15	Molar Heat Capacity (Cp) of Aqueous Cyclic Amine Solutions from (298.15 to 353.15) K
cpl	224.60	J/mol×K	318.15	Molar Heat Capacity (Cp) of Aqueous Cyclic Amine Solutions from (298.15 to 353.15) K
cpl	225.30	J/mol×K	323.15	Molar Heat Capacity (Cp) of Aqueous Cyclic Amine Solutions from (298.15 to 353.15) K
cpl	225.70	J/mol×K	328.15	Molar Heat Capacity (Cp) of Aqueous Cyclic Amine Solutions from (298.15 to 353.15) K
cpl	227.50	J/mol×K	333.15	Molar Heat Capacity (Cp) of Aqueous Cyclic Amine Solutions from (298.15 to 353.15) K
cpl	228.50	J/mol×K	338.15	Molar Heat Capacity (Cp) of Aqueous Cyclic Amine Solutions from (298.15 to 353.15) K
cpl	229.60	J/mol×K	343.15	Molar Heat Capacity (Cp) of Aqueous Cyclic Amine Solutions from (298.15 to 353.15) K

cpl	231.70	J/mol×K	348.15	Molar Heat Capacity (Cp) of Aqueous Cyclic Amine Solutions from (298.15 to 353.15) K
cpl	235.90	J/mol×K	353.15	Molar Heat Capacity (Cp) of Aqueous Cyclic Amine Solutions from (298.15 to 353.15) K
hvapt	41.20	kJ/mol	298.15	Vapour pressure and enthalpy of vaporization of aliphatic poly-amines
hvapt	44.30 ± 0.30	kJ/mol	289.50	NIST Webbook
hvapt	41.60	kJ/mol	297.50	NIST Webbook
pvap	0.42	kPa	276.29	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	281.23	Vapor Pressure and Its Temperature Dependence of 28 Organic Compounds: Cyclic Amines, Cyclic Ethers, and Cyclic and Open Chain Secondary Alcohols
pvap	0.79	kPa	286.01	Vapor Pressure and Its Temperature Dependence of 28 Organic Compounds: Cyclic Amines, Cyclic Ethers, and Cyclic and Open Chain Secondary Alcohols

pvap	1.13	kPa	292.03	Vapor Pressure and Its Temperature Dependence of 28 Organic Compounds: Cyclic Amines, Cyclic Ethers, and Cyclic and Open Chain Secondary Alcohols	
pvap	1.23	kPa	293.52	Vapor Pressure and Its Temperature Dependence of 28 Organic Compounds: Cyclic Amines, Cyclic Ethers, and Cyclic and Open Chain Secondary Alcohols	
pvap	1.60	kPa	298.16	Vapor Pressure and Its Temperature Dependence of 28 Organic Compounds: Cyclic Amines, Cyclic Ethers, and Cyclic and Open Chain Secondary Alcohols	
pvap	1.79	kPa	300.21	Vapor Pressure and Its Temperature Dependence of 28 Organic Compounds: Cyclic Amines, Cyclic Ethers, and Cyclic and Open Chain Secondary Alcohols	
pvap	2.02	kPa	302.54	Vapor Pressure and Its Temperature Dependence of 28 Organic Compounds: Cyclic Amines, Cyclic Ethers, and Cyclic and Open Chain Secondary Alcohols	

pvap	2.18	kPa	303.82	Vapor Pressure and Its Temperature Dependence of 28 Organic Compounds: Cyclic Amines, Cyclic Ethers, and Cyclic and Open Chain Secondary Alcohols	
pvap	2.24	kPa	304.32	Vapor Pressure and Its Temperature Dependence of 28 Organic Compounds: Cyclic Amines, Cyclic Ethers, and Cyclic and Open Chain Secondary Alcohols	
pvap	2.70	kPa	308.08	Vapor Pressure and Its Temperature Dependence of 28 Organic Compounds: Cyclic Amines, Cyclic Ethers, and Cyclic and Open Chain Secondary Alcohols	
pvap	3.06	kPa	310.37	Vapor Pressure and Its Temperature Dependence of 28 Organic Compounds: Cyclic Amines, Cyclic Ethers, and Cyclic and Open Chain Secondary Alcohols	
pvap	3.60	kPa	313.79	Vapor Pressure and Its Temperature Dependence of 28 Organic Compounds: Cyclic Amines, Cyclic Ethers, and Cyclic and Open Chain Secondary Alcohols	

pvap	4.75	kPa	319.53	Vapor Pressure and Its Temperature Dependence of 28 Organic Compounds: Cyclic Amines, Cyclic Ethers, and Cyclic and Open Chain Secondary Alcohols

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	404.70	K	100.00	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.55296e+01
Coeff. B	-3.82598e+03
Coeff. C	-5.35040e+01
Temperature range (K), min.	272.56
Temperature range (K), max.	427.94

Sources

Vapour pressure and enthalpy of vaporization of aliphatic poly-amines:	https://www.doi.org/10.1016/j.jct.2009.09.003
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
The Yaws Handbook of Vapor Pressure:	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure
Critical temperatures and pressures of caprolactam, dimethyl sulfoxide, 1,4-dimethylpiperazine, and 2,6-dimethylpiperazine:	https://www.doi.org/10.1016/j.fluid.2018.05.029
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
Molar Heat Capacity (Cp) of Aqueous Cyclic Amine Solutions from (298.15 to 373.15) K:	https://www.doi.org/10.1021/je400178k
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C106581&Units=SI

Molar excess enthalpy (Hm E) for systems of aqueous piperazine derivatives. https://www.doi.org/10.1016/j.jct.2015.06.006

McGowan Method: http://link.springer.com/article/10.1007/BF02311772

Legend

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
tb:	Normal Boiling Point Temperature
tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature
tf:	Normal melting (fusion) point