Piperazine, 1,4-dimethyl-

Other names: 1,4-Dimethylpiperazine

Lupetazine

N,N'-Dimethylpiperazine 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	41.20 ± 0.40	kJ/mol	NIST Webbook
hvap	43.80 ± 0.30	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

срІ	235.90	J/mol×K	353.15	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	
срІ	231.70	J/mol×K	348.15	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	228.50	J/mol×K	338.15	Molar Heat Capacity (Cp) of Aqueous Cyclic Amine Solutions from (298.15 to 353.15) K	
срІ	227.50	J/mol×K	333.15	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	
срІ	225.30	J/mol×K	323.15	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	223.40	J/mol×K	313.15	Molar Heat Capacity (Cp) of Aqueous Cyclic Amine Solutions from (298.15 to 353.15) K	
cpl	216.50	J/mol×K	298.15	Molar Heat Capacity (Cp) of Aqueous Cyclic Amine Solutions from (298.15 to 353.15) K	
hvapt	41.60	kJ/mol	297.50	NIST Webbook	
hvapt	44.30 ± 0.30	kJ/mol	289.50	NIST Webbook	
hvapt	41.20	kJ/mol	298.15	Vapour pressure and enthalpy of vaporization of aliphatic poly-amines	
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	
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	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	2.18	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	2.02	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	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	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	1.23	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	1.13	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	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	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	0.42	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	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	

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

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C106581&Units=SI

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

Molar Heat Capacity (Cp) of Aqueous Cyclic Amine Solutions from (298.15 to Yapony pressure and enthalpy of vaporization of aliphatic poly-amines: Critical temperatures and pressures of caprolactam, dimethyl sulfoxide, Yaponicensalise and pressure permitensalise and pressure permitensalise and pressure permitensalise of Compoundes of Ciclic Amines, Cyclic Ethers, and Cyclic and Open Chain Secondary Alcohols: of Vapor Pressure: https://www.doi.org/10.1021/je400178k https://www.doi.org/10.1016/j.jct.2009.09.003 https://www.doi.org/10.1016/j.fluid.2018.05.029 https://www.doi.org/10.1021/acs.jced.6b00576

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

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

Crippen Method:

http://pubs.acs.org/doi/abs/10.1021/ci990307l

Molar excess enthalpy (Hm E) for systems of aqueous piperazine derivatives:

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

Legend

cpl: Liquid phase heat capacity

hvap: Enthalpy of vaporization at standard conditionshvapt: Enthalpy of vaporization at a given temperature

ie: Ionization energy

log10ws:Log10 of Water solubility in mol/llogp:Octanol/Water partition coefficientmcvol:McGowan's characteristic volume

pvap: Vapor pressure

tb: Normal Boiling Point Temperaturetbrp: Boiling point at reduced pressure

tc: Critical Temperature

tf: Normal melting (fusion) point

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