Piperazine

Other names:	1,4-Diazacyclohexane
	1,4-Diethylenediamine
	1,4-Piperazine
	Antiren
	Asca-Trol No. 3
	Diethylenediamine
	Diethyleneimine
	Dispermine
	Eraverm
	Hexahydro-1,4-diazine
	Hexahydropyrazine
	Lumbrical
	NSC 474
	Piperazidine
	Piperazin
	Piperazine, anhydrous
	Pipersol
	Pyrazine hexahydride
	Pyrazine, hexahydro-
	UN 2579
	Upixon
	Uvilon
	Vermex
	Worm-A-Ton
	Wurmirazin
Inchi:	InChI=1S/C4H10N2/c1-2-6-4-3-5-1/h5-6H,1-4H2
InchiKey:	GLUUGHFHXGJENI-UHFFFAOYSA-N
Formula:	C4H10N2
SMILES:	C1CNCCN1
Mol. weight [g/mol]:	86.14
CAS:	110-85-0

Physical Properties

Property code	Value	Unit	Source
affp	943.70	kJ/mol	NIST Webbook
basg	914.70	kJ/mol	NIST Webbook

chs	-2957.60 ± 1.60	kJ/mol	NIST Webbook
chs	-2961.40 ± 1.10	kJ/mol	NIST Webbook
gf	190.38	kJ/mol	Joback Method
hf	25.00 ± 6.30	kJ/mol	NIST Webbook
hf	21.20	kJ/mol	NIST Webbook
hfs	-45.60 ± 1.60	kJ/mol	NIST Webbook
hfs	-41.80 ± 1.10	kJ/mol	NIST Webbook
hfus	16.06	kJ/mol	Joback Method
hsub	67.00 ± 6.30	kJ/mol	NIST Webbook
hsub	66.80	kJ/mol	NIST Webbook
hvap	38.75	kJ/mol	Joback Method
ie	8.98	eV	NIST Webbook
ie	8.72	eV	NIST Webbook
log10ws	1.07		Aqueous Solubility Prediction Method
logp	-0.821		Crippen Method
mcvol	76.320	ml/mol	McGowan Method
pc	5800.00 ± 200.00	kPa	NIST Webbook
pc	5420.00	kPa	Critical Point and Vapor Pressure Measurements for Four Compounds by a Low Residence Time Flow Method
rhoc	321.97 ± 24.98	kg/m3	NIST Webbook
rinpol	852.00		NIST Webbook
rinpol	813.00		NIST Webbook
rinpol	813.00		NIST Webbook
rinpol	870.00		NIST Webbook
rinpol	840.00		NIST Webbook
rinpol	852.00		NIST Webbook
rinpol	852.00		NIST Webbook
ripol	1391.00		NIST Webbook
ripol	1415.00		NIST Webbook
ripol	1440.00		NIST Webbook
ripol	1386.00		NIST Webbook
ripol	1410.00		NIST Webbook
ripol	1440.00		NIST Webbook
ripol	1390.00		NIST Webbook
ripol	1405.00		NIST Webbook
ripol	1386.00		NIST Webbook
tb	415.15 ± 1.50	K	NIST Webbook
tb	418.15 ± 2.00	K	NIST Webbook
tb	419.20	K	NIST Webbook
tc	661.00 ± 2.00	K	NIST Webbook
tf	380.48	K	Aqueous Solubility Prediction Method

tf	383.20 ± 0.60	K	NIST Webbook
tf	384.55 ± 0.20	K	NIST Webbook
tf	383.46 ± 0.30	K	NIST Webbook
tt	384.60 ± 0.30	K	NIST Webbook
vc	0.268	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	201.92	J/mol×K	640.79	Joback Method
cpg	181.90	J/mol×K	564.60	Joback Method
cpg	171.04	J/mol×K	526.51	Joback Method
cpg	159.62	J/mol×K	488.42	Joback Method
cpg	147.62	J/mol×K	450.33	Joback Method
cpg	135.05	J/mol×K	412.24	Joback Method
cpg	192.19	J/mol×K	602.70	Joback Method
cpl	218.70	J/mol×K	398.20	Liquid heat capacity of the solvent system (piperazine + n-methyldiethanolamine + water)
cpl	220.50	J/mol×K	403.20	Liquid heat capacity of the solvent system (piperazine + n-methyldiethanolamine + water)
cpl	222.80	J/mol×K	408.20	Liquid heat capacity of the solvent system (piperazine + n-methyldiethanolamine + water)
cpl	225.00	J/mol×K	413.20	Liquid heat capacity of the solvent system (piperazine + n-methyldiethanolamine + water)
cpl	237.00	J/mol×K	413.00	NIST Webbook
cpl	216.30	J/mol×K	393.20	Liquid heat capacity of the solvent system (piperazine + n-methyldiethanolamine + water)

psub	0.20	kPa	313.57	Vapor Pressure and Its Temperature Dependence of 28 Organic Compounds: Cyclic Amines, Cyclic Ethers, and Cyclic and Open Chain Secondary Alcohols	
psub	0.30	kPa	318.25	Vapor Pressure and Its Temperature Dependence of 28 Organic Compounds: Cyclic Amines, Cyclic Ethers, and Cyclic and Open Chain Secondary Alcohols	
psub	0.31	kPa	318.69	Vapor Pressure and Its Temperature Dependence of 28 Organic Compounds: Cyclic Amines, Cyclic Ethers, and Cyclic and Open Chain Secondary Alcohols	
psub	0.37	kPa	321.12	Vapor Pressure and Its Temperature Dependence of 28 Organic Compounds: Cyclic Amines, Cyclic Ethers, and Cyclic and Open Chain Secondary Alcohols	
psub	0.08	kPa	304.27	Vapor Pressure and Its Temperature Dependence of 28 Organic Compounds: Cyclic Amines, Cyclic Ethers, and Cyclic and Open Chain Secondary Alcohols	

psub	0.05	kPa	299.16	Vapor Pressure and Its Temperature Dependence of 28 Organic Compounds: Cyclic Amines, Cyclic Ethers, and Cyclic and Open Chain Secondary Alcohols	
psub	0.03	kPa	292.58	Vapor Pressure and Its Temperature Dependence of 28 Organic Compounds: Cyclic Amines, Cyclic Ethers, and Cyclic and Open Chain Secondary Alcohols	
psub	0.01	kPa	286.85	Vapor Pressure and Its Temperature Dependence of 28 Organic Compounds: Cyclic Amines, Cyclic Ethers, and Cyclic and Open Chain Secondary Alcohols	
psub	0.01	kPa	286.78	Vapor Pressure and Its Temperature Dependence of 28 Organic Compounds: Cyclic Amines, Cyclic Ethers, and Cyclic and Open Chain Secondary Alcohols	
psub	6.50e-03	kPa	279.48	Vapor Pressure and Its Temperature Dependence of 28 Organic Compounds: Cyclic Amines, Cyclic Ethers, and Cyclic and Open Chain Secondary Alcohols	

psub	0.12	kPa	308.37	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	1.49629e+01
Coeff. B	-3.59933e+03
Coeff. C	-7.12570e+01
Temperature range (K), min.	316.52
Temperature range (K), max.	444.19

Sources

Density and Viscosity of Partially Carbonated Aqueous Solutions Containing a Tertiary Alkanolamine and Piperazine at Temperatures between 298.15 and 353.15 K:	https://www.doi.org/10.1021/acs.jced.7b00144
The Yaws Handbook of Vapor Pressure:	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure
Physical Properties of a Complex Solution of (Potassium Citrate + Piperazine) as a CO2 Capture Agent:	https://www.doi.org/10.1021/je3003354
Experiment and modeling solubility of CO2 in aqueous solutions of Diisopropanolamine + 2-amino-2-methyl-1-propanol + piperazine at high pressures:	https://www.doi.org/10.1016/j.jct.2013.11.025
Liquid heat capacity of the solvent system (piperazine + n-methyldiethanolamine + water):	https://www.doi.org/10.1016/j.jct.2009.07.005
Solubility of Hydrogen Sulfide in Aqueous Solutions of Piperazine in the Low Gas-Loading Region:	https://www.doi.org/10.1021/je900721q
Density and Viscosity of Aqueous Solutions of (2-Piperidineethanol + Piperazine) from (288 to 333) K and Surface Tension of Aqueous Solutions of (N-Methyldiethanolamine + Piperazine), (2-Amino-2-methyl-1-propanol + Piperazine), and (2-Piperidineethanol + Piperazine) from (293 to 323) K:	https://www.doi.org/10.1021/je0603271
Densities, Viscosities, and Liquid Diffusivities in Aqueous Piperazine and Aqueous (Piperazine + N-Methyldiethanolamine) Solutions:	https://www.doi.org/10.1021/je800031p
Solid Solubility in the Aqueous 2-Amino-2-methyl propanol (AMP) Plus Piperazine (PZ) System:	https://www.doi.org/10.1021/acs.jced.8b01220
Solubility of N2O in and Density and Viscosity of Aqueous Solutions of Piperazine, Ammonia, and Their Mixtures from (283.15 to 323.15) K:	https://www.doi.org/10.1021/je300102d
Viscosity Measurement and Correlation of Unloaded and CO2-Loaded Aqueous Solutions of N-Methyldiethanolamine-Piperazine:	https://www.doi.org/10.1021/acs.jced.9b00021
Molar heat capacities of diethylenetriamine and 3-(methylamino)propylamine, their aqueous binaries, and aqueous ternaries with piperazine:	https://www.doi.org/10.1016/j.tca.2013.10.016
Heat capacities of aqueous binary and ternary mixtures (with piperazine) of N-(2-aminoethyl)piperazine and N,N,N'-trimethylethylenediamine at temperatures (308.2-353.2) K:	https://www.doi.org/10.1016/j.jct.2016.08.006
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
Surface thermodynamics of DMA2P, DMA2P-MEA and DMA2P-PZ aqueous solutions:	https://www.doi.org/10.1016/j.jct.2016.12.022
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

Solubility of Carbon Dioxide in Aqueous Solutions of Piperazine in the Low Gas Loading Region:	https://www.doi.org/10.1021/je0601917
Density and Viscosity of Aqueous Solutions of (N-Methyldiethanolamine + Piperazine) and	https://www.doi.org/10.1021/je060195b
Aqueous Solubility Prediction Method:	http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa
(2-Amino-2-methyl-1-propanol + Piperazine) from (288 to 338) K:	https://www.doi.org/10.1016/j.fluid.2010.11.004
Vapour-liquid equilibria of carbon dioxide in dilute and concentrated aqueous solutions of piperazine at low to high pressure:	https://www.doi.org/10.1021/acs.jced.8b01174
Physicochemical Properties of the System N,N-Dimethyl-dipropylene-diamino-triacetonediamine	https://www.doi.org/10.1021/je050378i
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Solubilities of CO2 in and Densities and Viscosities of the Piperazine + 1-Ethyl-3-methylimidazolium Acetate + H2O System:	https://www.doi.org/10.1016/j.jct.2016.10.007
Equilibrium and Physicochemical Properties of Novel Aqueous Blends of	https://www.doi.org/10.1021/je200124h
Liquid heat capacity of the solvent system (piperazine	https://www.doi.org/10.1016/j.jct.2009.11.006
2-amino-2-methyl-1-propanol + water):	https://www.doi.org/10.1016/j.fluid.2011.08.017
Critical Point and Vapor Pressure Measurements for Four Compounds by a Low Residence Time Flow Method:	https://www.doi.org/10.1021/je0602465
Physical Properties of Piperazine (PZ) Activated Aqueous Solutions of 2-Amino-2-Hydroxymethyl-1,	https://www.doi.org/10.1021/je2008523
3-Propanediol (AHPD + PZ):	https://www.doi.org/10.1016/j.fluid.2013.12.017
Molar heat capacities of aqueous solutions of 2-amino-2-ethyl-1,3-propanediol and their ternary mixtures containing piperazine or lithium salts:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C110850&Units=SI
Experiments and theory for the surface tensions of carbonated MDEA - PZ aqueous solutions:	https://www.doi.org/10.1016/j.fluid.2011.11.007
Molar heat capacity of aqueous solutions of 1,3-diaminopropane and 1,4-diaminobutane and their piperazine mixtures:	https://www.doi.org/10.1016/j.tca.2015.08.003
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Density, Viscosity, and Surface Tension of Aqueous Solutions of N-Methyldiethanolamine and Piperazine in the High Gas Loading Region:	https://www.doi.org/10.1021/je101192x
Potassium Glycinate + Piperazine in the Range of (288.15 to 323.15) K:	http://link.springer.com/article/10.1007/BF02311772
Experiments and model for the viscosity of carbonated 2-amino-2-methyl-1-propanol and	https://www.doi.org/10.1016/j.jct.2013.08.025
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Density, Viscosity, and Surface Tension of Aqueous Solution of	https://www.doi.org/10.1021/je400405m
1,4-Bis-(2-hydroxypropyl)-piperazine Sulfate:	https://www.doi.org/10.1021/je700717w
Density and Viscosity of Aqueous Piperazine Solutions	https://www.doi.org/10.1021/je1012263
Aqueous Solubility of Piperazine and 2-Amino-2-methyl-1-propanol plus Their Mixtures Using an Improved	https://www.doi.org/10.1021/acs.jced.6b00576
Freezing Point Depression Method:	https://www.doi.org/10.1021/je1012247
Thermophysical Properties of Aqueous Piperazine and Aqueous	https://www.doi.org/10.1021/je9000069
Absorption capacity and viscosity for CO2 capture processes (298.15 to 338.15) K:	https://www.doi.org/10.1016/j.jct.2016.05.022
CO2 Absorption Rate into Concentrated Aqueous	https://www.doi.org/10.1021/je101234t
Solubility of Carbon Dioxide in Aqueous Solutions of Piperazine and (2-Amino-2-methyl-1-propanol + Piperazine) from (298.15 to 383.15) K:	https://www.doi.org/10.1021/je1012586
	https://www.doi.org/10.1016/j.fluid.2010.01.009

Legend

affp:	Proton affinity
basg:	Gas basicity
chs:	Standard solid enthalpy of combustion
cpg:	Ideal gas heat capacity

cpl:	Liquid phase heat capacity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfs:	Solid phase enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hsub:	Enthalpy of sublimation at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
ie:	Ionization energy
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
psub:	Sublimation pressure
pvap:	Vapor pressure
rhoc:	Critical density
rinpol:	Non-polar retention indices
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
tt:	Triple Point Temperature
vc:	Critical Volume