1H-Imidazole, 1-methyl-

Other names:	1-Methyl-1H-imidazole
	1-Methylimidazole
	Imidazole, 1-methyl-
	N-Methylimidazole
Inchi:	InChI=1S/C4H6N2/c1-6-3-2-5-4-6/h2-4H,1H3
InchiKey:	MCTWTZJPVLRJOU-UHFFFAOYSA-N
Formula:	C4H6N2
SMILES:	Cn1ccnc1
Mol. weight [g/mol]:	82.10
CAS:	616-47-7

Physical Properties

Property code	Value	Unit	Source
affp	959.60	kJ/mol	NIST Webbook
basg	927.70	kJ/mol	NIST Webbook
ie	8.66	eV	NIST Webbook
log10ws	-2.53		Crippen Method
logp	0.420		Crippen Method
mcvol	67.720	ml/mol	McGowan Method
rinpol	929.00		NIST Webbook
rinpol	929.00		NIST Webbook
rinpol	929.00		NIST Webbook
ripol	1681.00		NIST Webbook
ripol	1638.00		NIST Webbook
ripol	1700.00		NIST Webbook
tb	471.20	K	NIST Webbook
tb	471.60	K	Vapor-liquid equilibrium in the production of the ionic liquid, 1-hexyl-3-methylimidazolium bromide ([HMIm][Br]), in acetone

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source

pvap	101.33	kPa	471.60	Vapor-liquid equilibrium in the production of the ionic liquid, 1-hexyl-3-methylimidazolium bromide ([HMIm][Br]), in acetone
rhol	1011.90	kg/m3	323.15	Towards understanding the effect of electrostatic interactions on the density of ionic liquids
rhol	1033.20	kg/m3	298.15	Towards understanding the effect of electrostatic interactions on the density of ionic liquids
rhol	1029.20	kg/m3	303.15	Towards understanding the effect of electrostatic interactions on the density of ionic liquids
rhol	1025.00	kg/m3	308.15	Towards understanding the effect of electrostatic interactions on the density of ionic liquids
rhol	1020.70	kg/m3	313.15	Towards understanding the effect of electrostatic interactions on the density of ionic liquids
rhol	1015.50	kg/m3	318.15	Towards understanding the effect of electrostatic interactions on the density of ionic liquids
rhol	1037.00	kg/m3	293.15	Towards understanding the effect of electrostatic interactions on the density of ionic liquids

rhol	1039.36	kg/m3	288.15	Mass density, sound velocity, mixing enthalpy, 1H NMR, Ab initio calculations and intermolecular interactions in binary mixtures of N-methylimidazole + water, +methanol, +ethanol, +1-propanol, +2-propanol
rhol	1030.52	kg/m3	298.15	Mass density, sound velocity, mixing enthalpy, 1H NMR, Ab initio calculations and intermolecular interactions in binary mixtures of N-methylimidazole + water, +methanol, +ethanol, +1-propanol, +2-propanol
rhol	1021.66	kg/m3	308.15	Mass density, sound velocity, mixing enthalpy, 1H NMR, Ab initio calculations and intermolecular interactions in binary mixtures of N-methylimidazole + water, +methanol, +ethanol, +1-propanol, +2-propanol
rhol	1012.76	kg/m3	318.15	Mass density, sound velocity, mixing enthalpy, 1H NMR, Ab initio calculations and intermolecular interactions in binary mixtures of N-methylimidazole + water, +methanol, +ethanol, +1-propanol, +2-propanol

rhol	1003.83	kg/m3	328.15	Mass density, sound velocity, mixing enthalpy, 1H NMR, Ab initio calculations and intermolecular interactions in binary mixtures of N-methylimidazole + water, +methanol, +ethanol, +1-propanol, +2-propanol
rhol	1031.14	kg/m3	298.15	Determination of Infinite Dilution Partial Molar Excess Enthalpies and Volumes for Some Ionic Liquid Precursors in Water and Methanol Using Tandem Flow Mixing Calorimetry and Vibrating-Tube Densimetry

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C616477&Units=SI
Does Alkyl Chain Length Really Matter? Structure-Property Relationships in Thermochemistry of Ionic Liquids.:	https://www.doi.org/10.1016/j.tca.2013.04.003
Limiting activity coefficients of 1-chlorobutane in water and in aqueous solutions of substances involved in synthesis of ionic liquids:	https://www.doi.org/10.1016/j.fluid.2010.09.026
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Mass density, sound velocity, mixing enthalpy, 1H NMR, Ab initio calculations and intermolecular interactions in binary mixtures of N-methylimidazole + water, +methanol, +ethanol, +1-propanol, +2-propanol:	https://www.doi.org/10.1016/j.jct.2018.12.019
Towards understanding the effect of electrostatic interactions on the density of ionic liquids:	https://www.doi.org/10.1016/j.fluid.2009.02.011
A combined experimental and theoretical approach to the study of hydrogen bond interaction in the binary mixture of N-methylimidazole with water:	https://www.doi.org/10.1016/j.jct.2012.06.015
Phase equilibria in systems with ionic liquids: An example for the downstream process of the Biphasic Acid Scavenging utilizing Ionic Liquids (BASIL) process. Part I: Experimental data:	https://www.doi.org/10.1016/j.jct.2011.05.027
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Influence of Typical Impurities on the Surface Tension Measurements of Binary Mixtures of Water and the Ionic Liquids 1-Butyl-3-Methylimidazolium Tetrafluoroborate and Chloride:	https://www.doi.org/10.1021/je100949x
Thermal Conductivities of Imidazolium-Based Ionic Liquid + CO2 Mixtures:	https://www.doi.org/10.1007/s10765-008-0506-x
Phase Behavior, Densities, and Isothermal Compressibility of Carbon Dioxide + 1-Bromobutane, Carbon Dioxide + 1-Chlorobutane, and Carbon Dioxide + 1-Methylimidazole:	https://www.doi.org/10.1021/je900387e
Experimental liquid-liquid equilibria of 1-methylimidazole with hydrocarbons and ionic liquids:	https://www.doi.org/10.1016/j.fluid.2005.09.021
Experimental and modelling investigation of H2S solubility in N-methylimidazole and gamma-butyrolactone:	https://www.doi.org/10.1016/j.jct.2019.03.031
Comparative Study of the Solubilities of SO2 in Five Low Volatile Organic Solvents (Sulfolane, Ethylene Glycol, Propylene Carbonate, N-Methylimidazole, and N-Methylpyrrolidone):	https://www.doi.org/10.1021/je4007713
Liquid-Liquid Equilibrium in Systems with an Ionic Liquid: Experimental Data for the Example of the Biphasic Acid Scavenging Process:	https://www.doi.org/10.1021/je1004966
Determination of Infinite Dilution Partial Molar Excess Enthalpies and Volumes for Some Ionic Liquid Precursors in Water and Methanol Using Tandem Flow Mixing Calorimetry and Vibrating-Tube Densimetry:	https://www.doi.org/10.1021/je200093f

Ternary Liquid-Liquid Equilibria Measurement for Benzene + Cyclohexane + N-Methylimidazole, or N-Ethylimidazole, or N-Methylimidazolium.

https://www.doi.org/10.1021/je800376f

Crippen Method

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

Vapor-liquid equilibrium in the production of the ionic liquid 1-hexyl-3-methylimidazolium bromide ([HMIm][Br]), in acetone: Dibutylphosphate at 298.2 K and Atmospheric Pressure.

https://www.doi.org/10.1016/j.fluid.2013.11.030

Legend

affp:	Proton affinity
basg:	Gas basicity
ie:	Ionization energy
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pvap:	Vapor pressure
rhol:	Liquid Density
rinpol:	Non-polar retention indices
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature