

1H-Imidazole, 1-ethyl-

Other names:	1-ethyl-1H-imidazole 1-ethylimidazole Imidazole, 1-ethyl- N-Ethylimidazole
Inchi:	InChI=1S/C5H8N2/c1-2-7-4-3-6-5-7/h3-5H,2H2,1H3
InchiKey:	IWDFHWZHHOSSGR-UHFFFAOYSA-N
Formula:	C5H8N2
SMILES:	CCn1ccnc1
Mol. weight [g/mol]:	96.13
CAS:	7098-07-9

Physical Properties

Property code	Value	Unit	Source
hvap	66.00 ± 3.90	kJ/mol	NIST Webbook
log10ws	-1.50		Crippen Method
logp	0.903		Crippen Method
mcvol	81.810	ml/mol	McGowan Method
rinpol	991.00		NIST Webbook
rinpol	991.00		NIST Webbook
rinpol	990.00		NIST Webbook
ripol	1714.00		NIST Webbook
ripol	1714.00		NIST Webbook

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
hvapt	57.53	kJ/mol	298.15	Thermochemistry of 1-alkylimidazoles
rhol	998.60	kg/m ³	293.15	Towards understanding the effect of electrostatic interactions on the density of ionic liquids

rhoI	995.20	kg/m3	298.15	Towards understanding the effect of electrostatic interactions on the density of ionic liquids
rhoI	991.30	kg/m3	303.15	Towards understanding the effect of electrostatic interactions on the density of ionic liquids
rhoI	987.40	kg/m3	308.15	Towards understanding the effect of electrostatic interactions on the density of ionic liquids
rhoI	983.50	kg/m3	313.15	Towards understanding the effect of electrostatic interactions on the density of ionic liquids
rhoI	978.70	kg/m3	318.15	Towards understanding the effect of electrostatic interactions on the density of ionic liquids
rhoI	974.80	kg/m3	323.15	Towards understanding the effect of electrostatic interactions on the density of ionic liquids

Sources

Ternary Liquid-Liquid Equilibria Measurement for Benzene + Cyclohexane + N-Methylimidazole, or N-Ethylimidazole, or N-Methylimidazolium Dibutylphosphate at 298.2 K and Atmospheric Pressure:
Crippen Method:

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

Towards understanding the effect of electrostatic interactions on the density of ionic liquids of 1-alkylimidazoles:

<http://link.springer.com/article/10.1007/BF02311772>

<http://webbook.nist.gov/cgi/cbook.cgi?ID=C7098079&Units=SI>

<http://pubs.acs.org/doi/abs/10.1021/ci9903071>

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

<https://www.doi.org/10.1016/j.fluid.2009.02.011>

<https://www.doi.org/10.1016/j.jct.2014.08.020>

Legend

h_{vap}:	Enthalpy of vaporization at standard conditions
h_{vapt}:	Enthalpy of vaporization at a given temperature
log₁₀w_s:	Log ₁₀ of Water solubility in mol/l
log_p:	Octanol/Water partition coefficient
mc_{vol}:	McGowan's characteristic volume
ρ_{ol}:	Liquid Density
ri_{npol}:	Non-polar retention indices
ri_{pol}:	Polar retention indices

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