

1H-Imidazole

Other names:	1,3-diaza-2,4-cyclopentadiene 1,3-diazole Formamidine, N,N'-vinylene- IMD Imidazol Iminazole Imutex Miazole NSC 60522 Pyrro(b)monazole USAF EK-4733 glyoxalin glyoxaline imidazole methanimidamide, N,N'-1,2-ethenediyl-
Inchi:	InChI=1S/C3H4N2/c1-2-5-3-4-1/h1-3H,(H,4,5)
InchiKey:	RAXXELZNTBOGNW-UHFFFAOYSA-N
Formula:	C3H4N2
SMILES:	c1c[nH]cn1
Mol. weight [g/mol]:	68.08
CAS:	288-32-4

Physical Properties

Property code	Value	Unit	Source
affp	942.80	kJ/mol	NIST Webbook
basg	909.20	kJ/mol	NIST Webbook
hf	128.00 ± 7.50	kJ/mol	NIST Webbook
hf	129.50	kJ/mol	NIST Webbook
hf	139.30 ± 1.90	kJ/mol	NIST Webbook
hf	132.90 ± 0.60	kJ/mol	NIST Webbook
hsub	85.40	kJ/mol	NIST Webbook
hsub	83.10 ± 0.20	kJ/mol	NIST Webbook
hsub	83.10	kJ/mol	NIST Webbook
hsub	83.10 ± 0.20	kJ/mol	NIST Webbook
hsub	74.50 ± 0.40	kJ/mol	NIST Webbook
hsub	66.90 ± 4.20	kJ/mol	NIST Webbook
hsub	69.50	kJ/mol	NIST Webbook

hsub	85.30	kJ/mol	NIST Webbook
ie	8.81 ± 0.01	eV	NIST Webbook
ie	9.12	eV	NIST Webbook
ie	8.78	eV	NIST Webbook
ie	8.96	eV	NIST Webbook
ie	8.81 ± 0.01	eV	NIST Webbook
log10ws	-0.46		Crippen Method
logp	-0.072		Crippen Method
mcvol	53.630	ml/mol	McGowan Method
rinpol	1055.00		NIST Webbook
rinpol	1095.00		NIST Webbook
rinpol	1095.00		NIST Webbook
rinpol	1055.00		NIST Webbook
rinpol	1095.00		NIST Webbook
rinpol	1069.00		NIST Webbook
rinpol	1069.00		NIST Webbook
rinpol	1042.00		NIST Webbook
ripol	2200.00		NIST Webbook
ripol	2172.00		NIST Webbook
ripol	2200.00		NIST Webbook
tb	530.20	K	NIST Webbook
tf	363.70 ± 0.40	K	NIST Webbook
tf	362.25	K	Solubility of Imidazoles in Ethers
tf	361.90 ± 0.20	K	NIST Webbook
tt	362.69 ± 0.02	K	NIST Webbook

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cps	84.90	J/mol×K	302.82	Heat capacities and thermodynamic functions of the ZIF organic linkers imidazole, 2-methylimidazole, and 2-ethylimidazole

cps	81.87	J/mol×K	292.36	Heat capacities and thermodynamic functions of the ZIF organic linkers imidazole, 2-methylimidazole, and 2-ethylimidazole
cps	80.30	J/mol×K	282.40	Heat capacities and thermodynamic functions of the ZIF organic linkers imidazole, 2-methylimidazole, and 2-ethylimidazole
cps	78.25	J/mol×K	272.36	Heat capacities and thermodynamic functions of the ZIF organic linkers imidazole, 2-methylimidazole, and 2-ethylimidazole
cps	75.44	J/mol×K	262.27	Heat capacities and thermodynamic functions of the ZIF organic linkers imidazole, 2-methylimidazole, and 2-ethylimidazole
cps	73.06	J/mol×K	252.18	Heat capacities and thermodynamic functions of the ZIF organic linkers imidazole, 2-methylimidazole, and 2-ethylimidazole
cps	70.27	J/mol×K	242.09	Heat capacities and thermodynamic functions of the ZIF organic linkers imidazole, 2-methylimidazole, and 2-ethylimidazole
cps	1.52	J/mol×K	12.69	Heat capacities and thermodynamic functions of the ZIF organic linkers imidazole, 2-methylimidazole, and 2-ethylimidazole

cps	67.60	J/mol×K	232.01	Heat capacities and thermodynamic functions of the ZIF organic linkers imidazole, 2-methylimidazole, and 2-ethylimidazole
cps	0.77	J/mol×K	10.18	Heat capacities and thermodynamic functions of the ZIF organic linkers imidazole, 2-methylimidazole, and 2-ethylimidazole
cps	0.90	J/mol×K	10.66	Heat capacities and thermodynamic functions of the ZIF organic linkers imidazole, 2-methylimidazole, and 2-ethylimidazole
cps	1.03	J/mol×K	11.15	Heat capacities and thermodynamic functions of the ZIF organic linkers imidazole, 2-methylimidazole, and 2-ethylimidazole
cps	1.17	J/mol×K	11.64	Heat capacities and thermodynamic functions of the ZIF organic linkers imidazole, 2-methylimidazole, and 2-ethylimidazole
cps	1.34	J/mol×K	12.15	Heat capacities and thermodynamic functions of the ZIF organic linkers imidazole, 2-methylimidazole, and 2-ethylimidazole
cps	65.02	J/mol×K	221.93	Heat capacities and thermodynamic functions of the ZIF organic linkers imidazole, 2-methylimidazole, and 2-ethylimidazole

cps	1.73	J/mol×K	13.25	Heat capacities and thermodynamic functions of the ZIF organic linkers imidazole, 2-methylimidazole, and 2-ethylimidazole
cps	1.96	J/mol×K	13.83	Heat capacities and thermodynamic functions of the ZIF organic linkers imidazole, 2-methylimidazole, and 2-ethylimidazole
cps	2.23	J/mol×K	14.45	Heat capacities and thermodynamic functions of the ZIF organic linkers imidazole, 2-methylimidazole, and 2-ethylimidazole
cps	2.52	J/mol×K	15.09	Heat capacities and thermodynamic functions of the ZIF organic linkers imidazole, 2-methylimidazole, and 2-ethylimidazole
cps	2.76	J/mol×K	15.59	Heat capacities and thermodynamic functions of the ZIF organic linkers imidazole, 2-methylimidazole, and 2-ethylimidazole
cps	3.50	J/mol×K	17.03	Heat capacities and thermodynamic functions of the ZIF organic linkers imidazole, 2-methylimidazole, and 2-ethylimidazole
cps	4.40	J/mol×K	18.62	Heat capacities and thermodynamic functions of the ZIF organic linkers imidazole, 2-methylimidazole, and 2-ethylimidazole

cps	5.44	J/mol×K	20.32	Heat capacities and thermodynamic functions of the ZIF organic linkers imidazole, 2-methylimidazole, and 2-ethylimidazole
cps	6.72	J/mol×K	22.25	Heat capacities and thermodynamic functions of the ZIF organic linkers imidazole, 2-methylimidazole, and 2-ethylimidazole
cps	8.16	J/mol×K	24.32	Heat capacities and thermodynamic functions of the ZIF organic linkers imidazole, 2-methylimidazole, and 2-ethylimidazole
cps	9.80	J/mol×K	26.56	Heat capacities and thermodynamic functions of the ZIF organic linkers imidazole, 2-methylimidazole, and 2-ethylimidazole
cps	11.60	J/mol×K	29.04	Heat capacities and thermodynamic functions of the ZIF organic linkers imidazole, 2-methylimidazole, and 2-ethylimidazole
cps	13.60	J/mol×K	31.74	Heat capacities and thermodynamic functions of the ZIF organic linkers imidazole, 2-methylimidazole, and 2-ethylimidazole
cps	15.78	J/mol×K	34.70	Heat capacities and thermodynamic functions of the ZIF organic linkers imidazole, 2-methylimidazole, and 2-ethylimidazole

cps	18.12	J/mol×K	37.93	Heat capacities and thermodynamic functions of the ZIF organic linkers imidazole, 2-methylimidazole, and 2-ethylimidazole
cps	60.47	J/mol×K	201.76	Heat capacities and thermodynamic functions of the ZIF organic linkers imidazole, 2-methylimidazole, and 2-ethylimidazole
cps	22.98	J/mol×K	45.33	Heat capacities and thermodynamic functions of the ZIF organic linkers imidazole, 2-methylimidazole, and 2-ethylimidazole
cps	25.37	J/mol×K	49.55	Heat capacities and thermodynamic functions of the ZIF organic linkers imidazole, 2-methylimidazole, and 2-ethylimidazole
cps	27.86	J/mol×K	54.15	Heat capacities and thermodynamic functions of the ZIF organic linkers imidazole, 2-methylimidazole, and 2-ethylimidazole
cps	30.35	J/mol×K	59.19	Heat capacities and thermodynamic functions of the ZIF organic linkers imidazole, 2-methylimidazole, and 2-ethylimidazole
cps	32.58	J/mol×K	64.68	Heat capacities and thermodynamic functions of the ZIF organic linkers imidazole, 2-methylimidazole, and 2-ethylimidazole

cps	34.67	J/mol×K	70.69	Heat capacities and thermodynamic functions of the ZIF organic linkers imidazole, 2-methylimidazole, and 2-ethylimidazole
cps	36.89	J/mol×K	77.27	Heat capacities and thermodynamic functions of the ZIF organic linkers imidazole, 2-methylimidazole, and 2-ethylimidazole
cps	39.12	J/mol×K	84.43	Heat capacities and thermodynamic functions of the ZIF organic linkers imidazole, 2-methylimidazole, and 2-ethylimidazole
cps	41.04	J/mol×K	92.28	Heat capacities and thermodynamic functions of the ZIF organic linkers imidazole, 2-methylimidazole, and 2-ethylimidazole
cps	42.43	J/mol×K	100.87	Heat capacities and thermodynamic functions of the ZIF organic linkers imidazole, 2-methylimidazole, and 2-ethylimidazole
cps	44.28	J/mol×K	110.96	Heat capacities and thermodynamic functions of the ZIF organic linkers imidazole, 2-methylimidazole, and 2-ethylimidazole
cps	46.09	J/mol×K	121.01	Heat capacities and thermodynamic functions of the ZIF organic linkers imidazole, 2-methylimidazole, and 2-ethylimidazole

cps	47.65	J/mol×K	131.13	Heat capacities and thermodynamic functions of the ZIF organic linkers imidazole, 2-methylimidazole, and 2-ethylimidazole
cps	49.12	J/mol×K	141.20	Heat capacities and thermodynamic functions of the ZIF organic linkers imidazole, 2-methylimidazole, and 2-ethylimidazole
cps	50.76	J/mol×K	151.26	Heat capacities and thermodynamic functions of the ZIF organic linkers imidazole, 2-methylimidazole, and 2-ethylimidazole
cps	52.37	J/mol×K	161.40	Heat capacities and thermodynamic functions of the ZIF organic linkers imidazole, 2-methylimidazole, and 2-ethylimidazole
cps	54.19	J/mol×K	171.53	Heat capacities and thermodynamic functions of the ZIF organic linkers imidazole, 2-methylimidazole, and 2-ethylimidazole
cps	56.27	J/mol×K	181.59	Heat capacities and thermodynamic functions of the ZIF organic linkers imidazole, 2-methylimidazole, and 2-ethylimidazole
cps	58.38	J/mol×K	191.67	Heat capacities and thermodynamic functions of the ZIF organic linkers imidazole, 2-methylimidazole, and 2-ethylimidazole

cps	20.50	J/mol×K	41.46	Heat capacities and thermodynamic functions of the ZIF organic linkers imidazole, 2-methylimidazole, and 2-ethylimidazole
cps	62.61	J/mol×K	211.85	Heat capacities and thermodynamic functions of the ZIF organic linkers imidazole, 2-methylimidazole, and 2-ethylimidazole
hfust	12.80	kJ/mol	361.90	NIST Webbook
hfust	12.82	kJ/mol	362.69	NIST Webbook
hfust	12.50	kJ/mol	363.70	NIST Webbook
hfust	12.80	kJ/mol	361.90	NIST Webbook
hfust	12.80	kJ/mol	361.90	NIST Webbook
hsubt	83.10 ± 0.20	kJ/mol	300.50	NIST Webbook
hsubt	80.80	kJ/mol	299.00	NIST Webbook
sfust	35.35	J/mol×K	362.69	NIST Webbook
sfust	35.37	J/mol×K	361.90	NIST Webbook

Sources

Solubility of Imidazoles in Ethers:

Thermochemistry of triimidazolium nonaborate:
Solubility of Imidazoles, Benzimidazoles, and Phenylimidazoles in Common Media, 1-Chlorobutane, Toluene, and 2-Nitrotoluene:
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<http://webbook.nist.gov/cgi/cbook.cgi?ID=C288324&Units=SI>

Efficient and Reversible Nitric Oxide Absorption by Low-Viscosity, Heat-Exchangeable Thermodynamic Functions of the ZIF organic linkers imidazole, 2-ethylimidazole, and 2-methylimidazole, and tetraethylammonium bromide based ionic liquid solvents: Experimental Properties of CO₂ in Flow Simulations: Deep Eutectic Solvents:

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<https://www.doi.org/10.1021/acs.jced.8b00098>

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Viscosity, Density, and Volatility of Binary Mixtures of Imidazole, 2-methylimidazole, and 2-ethylimidazole: Thermophysical Properties and Solubility of Different Sugar Derived Deep Eutectic Solvents: 1,2,4,5-Tetraethylimidazole with Water:

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<https://www.doi.org/10.1021/acs.jced.7b00184>

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Legend

affp:	Proton affinity
basg:	Gas basicity
cps:	Solid phase heat capacity
hf:	Enthalpy of formation at standard conditions
hfust:	Enthalpy of fusion at a given temperature
hsub:	Enthalpy of sublimation at standard conditions
hsubt:	Enthalpy of sublimation 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
rnpol:	Non-polar retention indices
ripol:	Polar retention indices
sfust:	Entropy of fusion at a given temperature
tb:	Normal Boiling Point Temperature
tf:	Normal melting (fusion) point
tt:	Triple Point Temperature

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