

# 1H-Imidazole, 2-methyl-

<b>Other names:</b>	2-Methyl glyoxaline 2-methyl-1H-imidazole 2-methylimidazole 2MZ Imidazole, 2-methyl-
<b>Inchi:</b>	InChI=1S/C4H6N2/c1-4-5-2-3-6-4/h2-3H,1H3,(H,5,6)
<b>InchiKey:</b>	LXBGSDVWAMZHDD-UHFFFAOYSA-N
<b>Formula:</b>	C4H6N2
<b>SMILES:</b>	Cc1ncc[nH]1
<b>Mol. weight [g/mol]:</b>	82.10
<b>CAS:</b>	693-98-1

## Physical Properties

Property code	Value	Unit	Source
affp	963.40	kJ/mol	NIST Webbook
basg	929.60	kJ/mol	NIST Webbook
chs	-2432.90 ± 0.60	kJ/mol	NIST Webbook
hf	89.80 ± 1.10	kJ/mol	NIST Webbook
hfs	1.40 ± 0.80	kJ/mol	NIST Webbook
hsub	88.40	kJ/mol	NIST Webbook
hsub	88.40 ± 0.70	kJ/mol	NIST Webbook
ie	8.50	eV	NIST Webbook
log10ws	-0.93		Crippen Method
logp	0.236		Crippen Method
mcvol	67.720	ml/mol	McGowan Method
rinpol	1050.00		NIST Webbook
rinpol	1050.00		NIST Webbook
rinpol	1050.00		NIST Webbook
ripol	2146.00		NIST Webbook
ripol	2146.00		NIST Webbook
tb	540.20	K	NIST Webbook
tf	419.00	K	Solubility of Imidazoles in Ethers
tf	419.00	K	Solubility of Imidazoles, Benzimidazoles, and Phenylimidazoles in Dichloromethane, 1-Chlorobutane, Toluene, and 2-Nitrotoluene

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cps	2.28	J/molxK	10.17	Heat capacities and thermodynamic functions of the ZIF organic linkers imidazole, 2-methylimidazole, and 2-ethylimidazole
cps	2.59	J/molxK	10.66	Heat capacities and thermodynamic functions of the ZIF organic linkers imidazole, 2-methylimidazole, and 2-ethylimidazole
cps	2.90	J/molxK	11.14	Heat capacities and thermodynamic functions of the ZIF organic linkers imidazole, 2-methylimidazole, and 2-ethylimidazole
cps	3.24	J/molxK	11.63	Heat capacities and thermodynamic functions of the ZIF organic linkers imidazole, 2-methylimidazole, and 2-ethylimidazole
cps	3.61	J/molxK	12.14	Heat capacities and thermodynamic functions of the ZIF organic linkers imidazole, 2-methylimidazole, and 2-ethylimidazole

cps	4.02	J/molxK	12.68	Heat capacities and thermodynamic functions of the ZIF organic linkers imidazole, 2-methylimidazole, and 2-ethylimidazole
cps	4.47	J/molxK	13.25	Heat capacities and thermodynamic functions of the ZIF organic linkers imidazole, 2-methylimidazole, and 2-ethylimidazole
cps	4.96	J/molxK	13.83	Heat capacities and thermodynamic functions of the ZIF organic linkers imidazole, 2-methylimidazole, and 2-ethylimidazole
cps	5.49	J/molxK	14.44	Heat capacities and thermodynamic functions of the ZIF organic linkers imidazole, 2-methylimidazole, and 2-ethylimidazole
cps	6.06	J/molxK	15.08	Heat capacities and thermodynamic functions of the ZIF organic linkers imidazole, 2-methylimidazole, and 2-ethylimidazole
cps	6.52	J/molxK	15.59	Heat capacities and thermodynamic functions of the ZIF organic linkers imidazole, 2-methylimidazole, and 2-ethylimidazole
cps	7.89	J/molxK	17.03	Heat capacities and thermodynamic functions of the ZIF organic linkers imidazole, 2-methylimidazole, and 2-ethylimidazole

cps	9.44	J/molxK	18.62	Heat capacities and thermodynamic functions of the ZIF organic linkers imidazole, 2-methylimidazole, and 2-ethylimidazole
cps	11.19	J/molxK	20.31	Heat capacities and thermodynamic functions of the ZIF organic linkers imidazole, 2-methylimidazole, and 2-ethylimidazole
cps	13.09	J/molxK	22.25	Heat capacities and thermodynamic functions of the ZIF organic linkers imidazole, 2-methylimidazole, and 2-ethylimidazole
cps	15.20	J/molxK	24.32	Heat capacities and thermodynamic functions of the ZIF organic linkers imidazole, 2-methylimidazole, and 2-ethylimidazole
cps	17.46	J/molxK	26.55	Heat capacities and thermodynamic functions of the ZIF organic linkers imidazole, 2-methylimidazole, and 2-ethylimidazole
cps	19.75	J/molxK	29.03	Heat capacities and thermodynamic functions of the ZIF organic linkers imidazole, 2-methylimidazole, and 2-ethylimidazole
cps	22.15	J/molxK	31.73	Heat capacities and thermodynamic functions of the ZIF organic linkers imidazole, 2-methylimidazole, and 2-ethylimidazole

cps	24.69	J/molxK	34.69	Heat capacities and thermodynamic functions of the ZIF organic linkers imidazole, 2-methylimidazole, and 2-ethylimidazole
cps	27.26	J/molxK	37.92	Heat capacities and thermodynamic functions of the ZIF organic linkers imidazole, 2-methylimidazole, and 2-ethylimidazole
cps	29.75	J/molxK	41.46	Heat capacities and thermodynamic functions of the ZIF organic linkers imidazole, 2-methylimidazole, and 2-ethylimidazole
cps	32.30	J/molxK	45.31	Heat capacities and thermodynamic functions of the ZIF organic linkers imidazole, 2-methylimidazole, and 2-ethylimidazole
cps	34.61	J/molxK	49.53	Heat capacities and thermodynamic functions of the ZIF organic linkers imidazole, 2-methylimidazole, and 2-ethylimidazole
cps	37.01	J/molxK	54.14	Heat capacities and thermodynamic functions of the ZIF organic linkers imidazole, 2-methylimidazole, and 2-ethylimidazole
cps	39.47	J/molxK	59.18	Heat capacities and thermodynamic functions of the ZIF organic linkers imidazole, 2-methylimidazole, and 2-ethylimidazole

cps	41.60	J/molxK	64.67	Heat capacities and thermodynamic functions of the ZIF organic linkers imidazole, 2-methylimidazole, and 2-ethylimidazole
cps	43.65	J/molxK	70.69	Heat capacities and thermodynamic functions of the ZIF organic linkers imidazole, 2-methylimidazole, and 2-ethylimidazole
cps	45.99	J/molxK	77.27	Heat capacities and thermodynamic functions of the ZIF organic linkers imidazole, 2-methylimidazole, and 2-ethylimidazole
cps	48.52	J/molxK	84.43	Heat capacities and thermodynamic functions of the ZIF organic linkers imidazole, 2-methylimidazole, and 2-ethylimidazole
cps	50.82	J/molxK	92.29	Heat capacities and thermodynamic functions of the ZIF organic linkers imidazole, 2-methylimidazole, and 2-ethylimidazole
cps	52.47	J/molxK	100.86	Heat capacities and thermodynamic functions of the ZIF organic linkers imidazole, 2-methylimidazole, and 2-ethylimidazole
cps	54.80	J/molxK	110.94	Heat capacities and thermodynamic functions of the ZIF organic linkers imidazole, 2-methylimidazole, and 2-ethylimidazole

cps	57.30	J/molxK	120.99	Heat capacities and thermodynamic functions of the ZIF organic linkers imidazole, 2-methylimidazole, and 2-ethylimidazole
cps	59.35	J/molxK	131.10	Heat capacities and thermodynamic functions of the ZIF organic linkers imidazole, 2-methylimidazole, and 2-ethylimidazole
cps	61.21	J/molxK	141.18	Heat capacities and thermodynamic functions of the ZIF organic linkers imidazole, 2-methylimidazole, and 2-ethylimidazole
cps	63.48	J/molxK	151.24	Heat capacities and thermodynamic functions of the ZIF organic linkers imidazole, 2-methylimidazole, and 2-ethylimidazole
cps	65.51	J/molxK	161.38	Heat capacities and thermodynamic functions of the ZIF organic linkers imidazole, 2-methylimidazole, and 2-ethylimidazole
cps	67.78	J/molxK	171.49	Heat capacities and thermodynamic functions of the ZIF organic linkers imidazole, 2-methylimidazole, and 2-ethylimidazole
cps	70.38	J/molxK	181.57	Heat capacities and thermodynamic functions of the ZIF organic linkers imidazole, 2-methylimidazole, and 2-ethylimidazole

cps	72.90	J/molxK	191.66	Heat capacities and thermodynamic functions of the ZIF organic linkers imidazole, 2-methylimidazole, and 2-ethylimidazole
cps	105.09	J/molxK	298.15	NIST Webbook
cps	77.88	J/molxK	211.85	Heat capacities and thermodynamic functions of the ZIF organic linkers imidazole, 2-methylimidazole, and 2-ethylimidazole
cps	80.52	J/molxK	221.94	Heat capacities and thermodynamic functions of the ZIF organic linkers imidazole, 2-methylimidazole, and 2-ethylimidazole
cps	83.08	J/molxK	232.03	Heat capacities and thermodynamic functions of the ZIF organic linkers imidazole, 2-methylimidazole, and 2-ethylimidazole
cps	85.92	J/molxK	242.11	Heat capacities and thermodynamic functions of the ZIF organic linkers imidazole, 2-methylimidazole, and 2-ethylimidazole
cps	89.00	J/molxK	252.19	Heat capacities and thermodynamic functions of the ZIF organic linkers imidazole, 2-methylimidazole, and 2-ethylimidazole



cps	91.73	J/mol×K	262.30	Heat capacities and thermodynamic functions of the ZIF organic linkers imidazole, 2-methylimidazole, and 2-ethylimidazole
cps	95.15	J/mol×K	272.43	Heat capacities and thermodynamic functions of the ZIF organic linkers imidazole, 2-methylimidazole, and 2-ethylimidazole
cps	98.26	J/mol×K	282.52	Heat capacities and thermodynamic functions of the ZIF organic linkers imidazole, 2-methylimidazole, and 2-ethylimidazole
cps	101.56	J/mol×K	292.64	Heat capacities and thermodynamic functions of the ZIF organic linkers imidazole, 2-methylimidazole, and 2-ethylimidazole
cps	106.19	J/mol×K	302.80	Heat capacities and thermodynamic functions of the ZIF organic linkers imidazole, 2-methylimidazole, and 2-ethylimidazole
cps	75.42	J/mol×K	201.76	Heat capacities and thermodynamic functions of the ZIF organic linkers imidazole, 2-methylimidazole, and 2-ethylimidazole
hsubt	88.20 ± 0.70	kJ/mol	309.50	NIST Webbook

## Sources

<b>Solubility of Imidazoles in Ethers:</b>	<a href="https://www.doi.org/10.1021/je020113t">https://www.doi.org/10.1021/je020113t</a>
<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=C693981&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C693981&amp;Units=SI</a>
<b>Solubility of Imidazoles, Benzimidazoles, and Phenylimidazoles in Diethyl Ether, 1-Chlorobutane, Toluene, and 2-Nitrotoluene; Viscosity, Density, and Volatility of Binary Mixtures of Imidazole, Methylimidazole, and 2,4,5-Trimethylimidazole with Water. Heat Capacities and thermodynamic functions of the ZIF organic linkers Imidazole, 2-Methylimidazole, and Methylimidazole; Ring Diphenyl Carbonate:</b>	<a href="https://www.doi.org/10.1021/je049907t">https://www.doi.org/10.1021/je049907t</a> <a href="http://pubs.acs.org/doi/abs/10.1021/ci990307l">http://pubs.acs.org/doi/abs/10.1021/ci990307l</a> <a href="https://www.doi.org/10.1021/acs.jced.8b00674">https://www.doi.org/10.1021/acs.jced.8b00674</a> <a href="http://link.springer.com/article/10.1007/BF02311772">http://link.springer.com/article/10.1007/BF02311772</a> <a href="https://www.chemeo.com/doc/models/crippen_log10ws">https://www.chemeo.com/doc/models/crippen_log10ws</a> <a href="https://www.doi.org/10.1016/j.jct.2018.12.024">https://www.doi.org/10.1016/j.jct.2018.12.024</a> <a href="https://www.doi.org/10.1021/je101199g">https://www.doi.org/10.1021/je101199g</a>

## Legend

<b>affp:</b>	Proton affinity
<b>basg:</b>	Gas basicity
<b>chs:</b>	Standard solid enthalpy of combustion
<b>cps:</b>	Solid phase heat capacity
<b>hf:</b>	Enthalpy of formation at standard conditions
<b>hfs:</b>	Solid phase enthalpy of formation at standard conditions
<b>hsub:</b>	Enthalpy of sublimation at standard conditions
<b>hsubt:</b>	Enthalpy of sublimation at a given temperature
<b>ie:</b>	Ionization energy
<b>log10ws:</b>	Log10 of Water solubility in mol/l
<b>logp:</b>	Octanol/Water partition coefficient
<b>mcvol:</b>	McGowan's characteristic volume
<b>rinpol:</b>	Non-polar retention indices
<b>ripol:</b>	Polar retention indices
<b>tb:</b>	Normal Boiling Point Temperature
<b>tf:</b>	Normal melting (fusion) point

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