

# 1H-Imidazole, 2-ethyl-

Other names:	2-ethyl-1H-imidazole 2-ethylimidazole imidazole, 2-ethyl-
Inchi:	InChI=1S/C5H8N2/c1-2-5-6-3-4-7-5/h3-4H,2H2,1H3,(H,6,7)
InchiKey:	PQAMFDRRWURCFQ-UHFFFAOYSA-N
Formula:	C5H8N2
SMILES:	CCc1ncc[nH]1
Mol. weight [g/mol]:	96.13
CAS:	1072-62-4

## Physical Properties

Property code	Value	Unit	Source
chs	-3089.60 ± 1.00	kJ/mol	NIST Webbook
hf	68.30 ± 1.30	kJ/mol	NIST Webbook
hfs	-21.30 ± 1.20	kJ/mol	NIST Webbook
hsub	89.60	kJ/mol	NIST Webbook
hsub	89.60 ± 0.40	kJ/mol	NIST Webbook
hsub	89.60 ± 0.40	kJ/mol	NIST Webbook
log10ws	-1.26		Crippen Method
logp	0.490		Crippen Method
mcvol	81.810	ml/mol	McGowan Method
tb	541.20	K	NIST Webbook
tt	282.00	K	Heat capacities and thermodynamic functions of the ZIF organic linkers imidazole, 2-methylimidazole, and 2-ethylimidazole

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cps	147.08	J/mol×K	298.15	NIST Webbook
hsbt	89.20 ± 0.40	kJ/mol	312.00	NIST Webbook

# Sources

<b>Crippen Method:</b>	<a href="https://www.chemeo.com/doc/models/crippen_log10ws">https://www.chemeo.com/doc/models/crippen_log10ws</a>
<b>Heat capacities and thermodynamic functions of the ZIF organic linkers McGowan Method</b>	<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>
<b>McGowan Method</b>	<a href="http://link.springer.com/article/10.1007/BF02311772">http://link.springer.com/article/10.1007/BF02311772</a>
<b>2-ethylimidazole, and NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=C1072624&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C1072624&amp;Units=SI</a>
<b>Crippen Method:</b>	<a href="http://pubs.acs.org/doi/abs/10.1021/ci990307l">http://pubs.acs.org/doi/abs/10.1021/ci990307l</a>

# Legend

<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>log10ws:</b>	Log10 of Water solubility in mol/l
<b>logp:</b>	Octanol/Water partition coefficient
<b>mcvol:</b>	McGowan's characteristic volume
<b>tb:</b>	Normal Boiling Point Temperature
<b>tt:</b>	Triple Point Temperature

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