

# 1H-1,2,4-Triazole

<b>Other names:</b>	1,2,4-1H-Triazole 1,2,4-Triazole 4H-1,2,4-triazole CGA-71019 Pyrrodiazole s-Triazole
<b>Inchi:</b>	InChI=1S/C2H3N3/c1-3-2-5-4-1/h1-2H,(H,3,4,5)
<b>InchiKey:</b>	NSPMIYGKQJPBQR-UHFFFAOYSA-N
<b>Formula:</b>	C2H3N3
<b>SMILES:</b>	<chem>c1nc[nH]n1</chem>
<b>Mol. weight [g/mol]:</b>	69.07
<b>CAS:</b>	288-88-0

## Physical Properties

Property code	Value	Unit	Source
affp	886.00	kJ/mol	NIST Webbook
basg	855.90	kJ/mol	NIST Webbook
chs	-1328.90 ± 1.20	kJ/mol	NIST Webbook
chs	-1325.00	kJ/mol	NIST Webbook
chs	-1324.99 ± 0.90	kJ/mol	NIST Webbook
chs	-1323.66 ± 0.37	kJ/mol	NIST Webbook
chs	-1324.40 ± 0.30	kJ/mol	NIST Webbook
hf	192.70 ± 0.80	kJ/mol	NIST Webbook
hf	189.80	kJ/mol	NIST Webbook
hf	188.50	kJ/mol	NIST Webbook
hf	193.70 ± 1.90	kJ/mol	NIST Webbook
hfs	107.89 ± 0.46	kJ/mol	NIST Webbook
hfs	113.10 ± 1.40	kJ/mol	NIST Webbook
hfs	108.70 ± 0.40	kJ/mol	NIST Webbook
hfs	109.22 ± 0.94	kJ/mol	NIST Webbook
ie	10.00	eV	NIST Webbook
ie	9.80	eV	NIST Webbook
ie	10.10	eV	NIST Webbook
ie	10.60	eV	NIST Webbook
log10ws	-0.22		Crippen Method
logp	-0.677		Crippen Method
mcvol	49.520	ml/mol	McGowan Method

rropol	1116.00		NIST Webbook
rropol	1116.00		NIST Webbook
tb	533.20	K	NIST Webbook
tb	477.15 ± 1.50	K	NIST Webbook
tf	392.00 ± 0.50	K	NIST Webbook
tf	393.50 ± 0.40	K	NIST Webbook
tf	295.15 ± 1.50	K	NIST Webbook

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cps	78.70	J/molxK	298.15	NIST Webbook
hfust	16.10	kJ/mol	393.50	NIST Webbook
hfust	10.76 ± 0.08	kJ/mol	393.30	NIST Webbook
hfust	16.10	kJ/mol	393.50	NIST Webbook
hfust	16.10	kJ/mol	393.50	NIST Webbook

## Sources

McGowan Method:

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

Solubilities and Thermodynamic Properties of CO<sub>2</sub> in Four Azole-Based Deep Eutectic Solvents:

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

Calibration and testing of an isoperibolic micro-combustion calorimeter developed to measure the efficiency of reversible Nitric Oxide absorption by aqueous viscous organic solutions of CO<sub>2</sub> (E. J. Crippen, 2006)

<http://webbook.nist.gov/cgi/cbook.cgi?ID=C288880&Units=SI>

Solubility of CO<sub>2</sub> in Organic Solvents: Ethanol, 1-Propanol, 2-Propanol, 2-Methoxyethanol, and N-Methyl-2-pyrrolidone

<https://www.doi.org/10.1016/j.jct.2012.12.020>

Crippen Method: Ethyl Formate, Methyl Acetate, Ethyl Acetate, and Butyl Acetate at (283 to 363) K:

<https://www.doi.org/10.1021/acs.jced.9b00173>

Calibration and test of an aneroid mini-bomb combustion calorimeter:

<https://www.doi.org/10.1021/je060452c>

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

[https://www.chemeo.com/doc/models/crippen\\_log10ws](https://www.chemeo.com/doc/models/crippen_log10ws)

<https://www.doi.org/10.1016/j.jct.2006.10.013>

## Legend

affp:	Proton affinity
basg:	Gas basicity
chs:	Standard solid enthalpy of combustion
cps:	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>hfust:</b>	Enthalpy of fusion 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>tb:</b>	Normal Boiling Point Temperature
<b>tf:</b>	Normal melting (fusion) point

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