1H-1,2,4-Triazole

Other names:	1,2,4-1H-Triazole
	1,2,4-Triazole
	4H-1,2,4-triazole
	CGA-71019
	Pyrrodiazole
	s-Triazole
Inchi:	InChI=1S/C2H3N3/c1-3-2-5-4-1/h1-2H,(H,3,4,5)
InchiKey:	NSPMIYGKQJPBQR-UHFFFAOYSA-N
Formula:	C2H3N3
SMILES:	c1nc[nH]n1
Mol. weight [g/mol]:	69.07
CAS:	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	-1324.40 ± 0.30	kJ/mol	NIST Webbook
chs	-1323.66 ± 0.37	kJ/mol	NIST Webbook
chs	-1324.99 ± 0.90	kJ/mol	NIST Webbook
chs	-1325.00	kJ/mol	NIST Webbook
chs	-1328.90 ± 1.20	kJ/mol	NIST Webbook
hf	192.70 ± 0.80	kJ/mol	NIST Webbook
hf	188.50	kJ/mol	NIST Webbook
hf	193.70 ± 1.90	kJ/mol	NIST Webbook
hf	189.80	kJ/mol	NIST Webbook
hfs	113.10 ± 1.40	kJ/mol	NIST Webbook
hfs	109.22 ± 0.94	kJ/mol	NIST Webbook
hfs	107.89 ± 0.46	kJ/mol	NIST Webbook
hfs	108.70 ± 0.40	kJ/mol	NIST Webbook
ie	10.00	eV	NIST Webbook
ie	10.60	eV	NIST Webbook
ie	9.80	eV	NIST Webbook
ie	10.10	eV	NIST Webbook
log10ws	-0.22		Crippen Method
logp	-0.677		Crippen Method
mcvol	49.520	ml/mol	McGowan Method

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

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cps	78.70	J/mol×K	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

Efficient and Reversible Nitric Oxide Absorption by Low-Viscosity, Azole Derived Deep Eutectic Solvents:	https://www.doi.org/10.1021/acs.jced.9b00173
Solubility of 1H-1,2,4-Triazole in Ethanol, 1-Propanol, 2-Propanol, 1,2-Propanediol, Ethyl Formate, Methyl Acetate, Ethyl Acetate, and Butyl Acetate at (283 to 363) K:	https://www.doi.org/10.1021/je060452c
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Calibration and test of an aneroid mini-bomb combustion calorimeter:	https://www.doi.org/10.1016/j.jct.2006.10.013
Calibration and testing of an isoperibolic micro-combustion calorimeter developed to measure the enthalpy of combustion of organic compounds containing C, H, O and N:	https://www.doi.org/10.1016/j.jct.2012.12.020
Solubilities and Thermodynamic Properties of CO2 in Four Azole-Based Deep Eutectic Solvents:	https://www.doi.org/10.1021/acs.jced.8b00098
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C288880&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

affp:	Proton affinity
basg:	Gas basicity
chs:	Standard solid enthalpy of combustion
cps:	Solid phase heat capacity

hf:	Enthalpy of formation at standard conditions
hfs:	Solid phase enthalpy of formation at standard conditions
hfust:	Enthalpy of fusion 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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tf:	Normal melting (fusion) point