1H-Pyrazole

Other names:	Pyrazole
	1,2-Diazole
Inchi:	InChI=1S/C3H4N2/c1-2-4-5-3-1/h1-3H,(H,4,5)
InchiKey:	WTKZEGDFNFYCGP-UHFFFAOYSA-N
Formula:	C3H4N2
SMILES:	c1cn[nH]c1
Mol. weight [g/mol]:	68.08
CAS:	288-13-1

Physical Properties

Property code	Value	Unit	Source
affp	894.10	kJ/mol	NIST Webbook
basg	860.50	kJ/mol	NIST Webbook
hf	179.40 ± 0.80	kJ/mol	NIST Webbook
hf	177.40	kJ/mol	NIST Webbook
hf	181.00 ± 8.80	kJ/mol	NIST Webbook
hsub	67.80	kJ/mol	NIST Webbook
hsub	65.00	kJ/mol	NIST Webbook
hsub	62.80 ± 4.20	kJ/mol	NIST Webbook
hsub	74.00 ± 0.40	kJ/mol	NIST Webbook
hsub	74.00	kJ/mol	NIST Webbook
hsub	74.00 ± 0.40	kJ/mol	NIST Webbook
hsub	69.20 ± 0.30	kJ/mol	NIST Webbook
ie	9.15	eV	NIST Webbook
ie	9.15	eV	NIST Webbook
ie	9.27 ± 0.05	eV	NIST Webbook
ie	9.25 ± 0.01	eV	NIST Webbook
ie	9.38 ± 0.03	eV	NIST Webbook
log10ws	-0.46		Crippen Method
logp	-0.072		Crippen Method
mcvol	53.630	ml/mol	McGowan Method
rinpol	864.00		NIST Webbook
rinpol	864.00		NIST Webbook
rinpol	837.00		NIST Webbook
rinpol	837.00		NIST Webbook
rinpol	864.00		NIST Webbook
tb	460.20	K	NIST Webbook

tb	460.15 ± 1.50	K	NIST Webbook
tf	343.20 ± 0.40	K	NIST Webbook
tf	333.10 ± 0.20	K	NIST Webbook

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
hfust	14.20	kJ/mol	343.20	NIST Webbook
hfust	13.80	kJ/mol	333.10	NIST Webbook
hfust	14.20	kJ/mol	343.20	NIST Webbook
hfust	14.20	kJ/mol	343.20	NIST Webbook
hsubt	74.30 ± 0.40	kJ/mol	277.50	NIST Webbook
hsubt	72.70	kJ/mol	263.00	NIST Webbook
sfust	41.43	J/mol×K	333.10	NIST Webbook

Sources

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C288131&Units=SI

Legend

affp: Proton affinity
basg: Gas basicity
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
rinpol: Non-polar retention indices

sfust:	Entropy of fusion at a given temperature
tb:	Normal Boiling Point Temperature
tf:	Normal melting (fusion) point