1H-Tetrazole

Other names: 1,2,3,4-tetrazole
Tetraazacyclopentadiene
tetrazole
Inchi: InChI=1S/CH2N4/c1-2-4-5-3-1/h1H,(H,2,3,4,5)
InchiKey: KJUGUADJHNHALS-UHFFFAOYSA-N
Formula: CH2N4
SMILES: c1nnn[nH]1
Mol. weight [g/mol]: 70.05
CAS: 288-94-8

Physical Properties

Property code	Value	Unit	Source
chs	-915.50 ± 0.40	kJ/mol	NIST Webbook
chs	-916.30	kJ/mol	NIST Webbook
chs	-916.42 ± 0.88	kJ/mol	NIST Webbook
hf	320.00 ± 3.00	kJ/mol	NIST Webbook
hf	321.10	kJ/mol	NIST Webbook
hfs	236.00 ± 0.40	kJ/mol	NIST Webbook
hfs	237.10	kJ/mol	NIST Webbook
hsub	85.00 ± 3.00	kJ/mol	NIST Webbook
hsub	97.50	kJ/mol	NIST Webbook
hsub	84.00	kJ/mol	NIST Webbook
ie	11.30	eV	NIST Webbook
ie	11.00	eV	NIST Webbook
ie	10.95	eV	NIST Webbook
ie	11.30	eV	NIST Webbook
log10ws	0.01		Crippen Method
logp	-1.282		Crippen Method
mcvol	45.410	ml/mol	McGowan Method
ss	96.36	J/mol×K	NIST Webbook
tf	430.70 ± 0.40	K	NIST Webbook
tt	429.00 ± 1.00	K	NIST Webbook
tt	430.00 ± 1.00	K	NIST Webbook

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cps	76.52	J/mol×K	298.15	NIST Webbook
hfust	18.40	kJ/mol	430.70	NIST Webbook
hfust	17.70	kJ/mol	432.10	NIST Webbook
hsubt	88.16	kJ/mol	353.00	NIST Webbook
hsubt	87.80 ± 1.40	kJ/mol	369.00	NIST Webbook
hsubt	88.00 ± 1.60	kJ/mol	368.50	NIST Webbook
hsubt	97.32	kJ/mol	333.00	NIST Webbook
hsubt	97.50 ± 4.20	kJ/mol	348.00	NIST Webbook

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C288948&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Efficient and Reversible Nitric Oxide Absorption by Low-Viscosity, Azole-Derived Deep Eutectic Solvents:	https://www.doi.org/10.1021/acs.jced.9b00173
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

Legend

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
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
ss:	Solid phase molar entropy at standard conditions
tf:	Normal melting (fusion) point
tt:	Triple Point Temperature

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