2H-Tetrazole, 2-methyl-

Other names: 2-Methyltetrazole
Inchi: InChI=1S/C2H4N4/c1-6-4-2-3-5-6/h2H,1H3
InchiKey: VRESBNUEIKZECD-UHFFFAOYSA-N
Formula: C2H4N4
SMILES: Cn1ncnn1
Mol. weight [g/mol]: 84.08
CAS: 16681-78-0

Physical Properties

Property code	Value	Unit	Source
chl	-1640.20 ± 0.50	kJ/mol	NIST Webbook
hf	328.40 ± 0.70	kJ/mol	NIST Webbook
hfl	281.60 ± 0.60	kJ/mol	NIST Webbook
hvap	46.80	kJ/mol	NIST Webbook
hvap	46.80 ± 0.40	kJ/mol	NIST Webbook
ie	10.00	eV	NIST Webbook
log10ws	-2.06		Crippen Method
logp	-0.790		Crippen Method
mcvol	59.500	ml/mol	McGowan Method
tt	286.00 ± 1.00	K	NIST Webbook

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
hfust	12.37	kJ/mol	286.00	NIST Webbook
hfust	12.37	kJ/mol	286.00	NIST Webbook

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C16681780&Units=SI

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

Legend

chl:	Standard liquid enthalpy of combustion
hf:	Enthalpy of formation at standard conditions
hfl:	Liquid phase enthalpy of formation at standard conditions
hfust:	Enthalpy of fusion at a given temperature
hvap:	Enthalpy of vaporization at standard conditions
ie:	Ionization energy
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
tt:	Triple Point Temperature