1H-Tetrazole, 1,5-dimethyl-

Other names: 1,5-Dimethyltetrazole
1,5-dimethyl-1H-tetrazole
Inchi: InChI=1S/C3H6N4/c1-3-4-5-6-7(3)2/h1-2H3
InchiKey: HWHNFJYQDMSYAF-UHFFFAOYSA-N
Formula: C3H6N4
SMILES: Cc1nnnn1C
Mol. weight [g/mol]: 98.11
CAS: 5144-11-6

Physical Properties

Property code	Value	Unit	Source
chl	-2224.20 ± 2.60	kJ/mol	NIST Webbook
chs	-2226.70 ± 3.60	kJ/mol	NIST Webbook
hf	273.20 ± 2.90	kJ/mol	NIST Webbook
hfl	186.10 ± 2.70	kJ/mol	NIST Webbook
hfs	188.60	kJ/mol	NIST Webbook
hvap	87.10 ± 1.00	kJ/mol	NIST Webbook
hvap	87.10	kJ/mol	NIST Webbook
log10ws	-2.53		Crippen Method
logp	-0.481		Crippen Method
mcvol	73.590	ml/mol	McGowan Method
tt	349.00 ± 1.00	K	NIST Webbook
tt	350.00 ± 1.00	K	NIST Webbook

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
hfust	14.70	kJ/mol	349.00	NIST Webbook
hfust	14.70	kJ/mol	349.00	NIST Webbook
hsubt	86.20 ± 1.00	kJ/mol	323.00	NIST Webbook

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C5144116&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
chs:	Standard solid enthalpy of combustion
hf:	Enthalpy of formation at standard conditions
hfl:	Liquid phase enthalpy of formation at standard conditions
hfs:	Solid phase enthalpy of formation at standard conditions
hfust:	Enthalpy of fusion at a given temperature
hsubt:	Enthalpy of sublimation at a given temperature
hvap:	Enthalpy of vaporization at standard conditions
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
tt:	Triple Point Temperature