

1H-Tetrazol-5-amine, 1-methyl-

Other names:	5-Amino-1-methyl-1H-tetrazole 1-Methyl-5-aminotetrazole
Inchi:	InChI=1S/C2H5N5/c1-7-2(3)4-5-6-7/h1H3,(H2,3,4,6)
InchiKey:	GTKOKCQMHAGFSM-UHFFFAOYSA-N
Formula:	C2H5N5
SMILES:	Cn1[nH]nnc1=N
Mol. weight [g/mol]:	99.09
CAS:	5422-44-6

Physical Properties

Property code	Value	Unit	Source
chs	-1683.80 ± 1.10	kJ/mol	NIST Webbook
chs	-1695.20 ± 0.46	kJ/mol	NIST Webbook
hf	302.40 ± 2.80	kJ/mol	NIST Webbook
hf	313.20	kJ/mol	NIST Webbook
hfs	182.20 ± 4.50	kJ/mol	NIST Webbook
hfs	193.00	kJ/mol	NIST Webbook
hsub	120.20 ± 1.70	kJ/mol	NIST Webbook
hsub	120.20	kJ/mol	NIST Webbook
log10ws	-2.50		Crippen Method
logp	-1.859		Crippen Method
mcvol	69.480	ml/mol	McGowan Method
tt	504.00 ± 1.00	K	NIST Webbook

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
hsubt	116.40 ± 1.70	kJ/mol	408.50	NIST Webbook

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C5422446&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

Legend

chs:	Standard solid enthalpy of combustion
hf:	Enthalpy of formation at standard conditions
hfs:	Solid phase enthalpy of formation at standard conditions
hsub:	Enthalpy of sublimation at standard conditions
hsubt:	Enthalpy of sublimation at a given temperature
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
tt:	Triple Point Temperature

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