

1H-Tetrazol-5-amine

Other names:	1H-Tetrazole, 5-amino- 5-Amino-1,2,3,4-tetrazole 5-Amino-1H-tetrazole 5-Aminotetrazole Tetrazole, 5-amino- 1H-Tetrazol-5-ylamine 5-Tetrazolamine 5-Amino-2H-tetrazole 2H-Tetrazol-5-amine Aminotetrazole NSC 3004 tetrazol-5-ylamine
Inchi:	InChI=1S/CH3N5/c2-1-3-5-6-4-1/h(H3,2,3,4,5,6)
InchiKey:	ULRPISSMEBPJLN-UHFFFAOYSA-N
Formula:	CH3N5
SMILES:	<chem>Nc1nnn[nH]1</chem>
Mol. weight [g/mol]:	85.07
CAS:	4418-61-5

Physical Properties

Property code	Value	Unit	Source
chs	-1069.13	kJ/mol	NIST Webbook
chs	-1030.10 ± 2.30	kJ/mol	NIST Webbook
hfs	207.80	kJ/mol	NIST Webbook
log10ws	0.38		Crippen Method
logp	-1.700		Crippen Method
mcvol	55.390	ml/mol	McGowan Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
hsubt	112.60 ± 1.20	kJ/mol	413.00	NIST Webbook

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307I
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=C4418615&Units=SI

Legend

chs:	Standard solid enthalpy of combustion
hfs:	Solid phase enthalpy of formation 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

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