1-Aminotetrazole

Other names:	1H-tetrazole, 5-amino- 1H-tetrazole-5-amine 5-amino-1,2,3,4-tetrazole 5-amino-1H-tetrazole 5-aminotetrazole aminotetrazole tetrazole, 5-amino-
Inchi:	InChI=1S/CH3N5/c2-6-1-3-4-5-6/h1H,2H2
InchiKey:	KNRUQUSSDKZTSQ-UHFFFAOYSA-N
Formula:	CH3N5
SMILES:	Nn1cnnn1
Mol. weight [g/mol]:	85.07
CAS:	5378-49-4

Physical Properties

Property code	Value	Unit	Source
hf	323.80 ± 2.60	kJ/mol	NIST Webbook
hfs	207.80 ± 2.30	kJ/mol	NIST Webbook
hsub	116.00	kJ/mol	NIST Webbook
hsub	116.00 ± 1.20	kJ/mol	NIST Webbook
log10ws	0.14		Crippen Method
logp	-1.613		Crippen Method
mcvol	55.390	ml/mol	McGowan Method

Sources

Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Solubility Determination, Correlation, and Solute-Solvent Molecular Interactions of 5-Aminotetrazole in Various Pure Solvents:	https://www.doi.org/10.1021/acs.jced.9b00385
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C5378494&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

hf:	Enthalpy of formation at standard conditions
hfs:	Solid phase enthalpy of formation at standard conditions
hsub:	Enthalpy of sublimation at standard conditions
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume