3,5-Diamino-1,2,4-triazole

Other names:	1,2,4-Triazolidine, 3,5-diimino-
	1H-1,2,4-triazole-3,5-diamine
	3,5-diamino-1H-1,2,4-triazole
	3,5-diamino-s-triazole
	MC 51762
	NCI-C04819
	NSC 1895
	guanazole
	s-triazole, 3,5-diamino-
Inchi:	InChI=1S/C2H5N5/c3-1-5-2(4)7-6-1/h(H5,3,4,5,6,7)
InchiKey:	PKWIYNIDEDLDCJ-UHFFFAOYSA-N
Formula:	C2H5N5
SMILES:	N=c1[nH][nH]c(=N)[nH]1
Mol. weight [g/mol]:	99.09
CAS:	1455-77-2

Physical Properties

Property code	Value	Unit	Source
chs	-1548.00	kJ/mol	NIST Webbook
log10ws	-1.11		Crippen Method
logp	-2.816		Crippen Method
mcvol	69.480	ml/mol	McGowan Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C1455772&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
A 2D nickel-based energetic MOFs incorporating 3,5-diamino-1,2,4-triazole and malonic acid: Synthesis, crystal structure and thermochemical study:	https://www.doi.org/10.1016/j.jct.2015.09.009
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

Legend

chs:	Standard solid enthalpy of combustion
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume