

(1H)-1,2,4-triazole-3-amino, 5-imino-1-(pyridin-2-yl)-

Inchi:	InChI=1S/C7H8N6/c8-6-11-7(9)13(12-6)5-3-1-2-4-10-5/h1-4H,(H4,8,9,11,12)
InchiKey:	IVUXBPCZNBDZGC-UHFFFAOYSA-N
Formula:	C7H8N6
SMILES:	N=c1[nH]c(N)nn1-c1cccn1
Mol. weight [g/mol]:	176.18

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.50		Crippen Method
logp	-0.825		Crippen Method
mcvol	126.150	ml/mol	McGowan Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=B6010401&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

Legend

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

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