

1H-1,2,3-Triazolo[4,5-b]pyridine

Other names:	1,2,3-Triazolo(5,4-b)pyridine
Inchi:	InChI=1S/C5H4N4/c1-2-4-5(6-3-1)8-9-7-4/h1-3H,(H,6,7,8,9)
InchiKey:	VQNDBXJTIJKJPV-UHFFFAOYSA-N
Formula:	C5H4N4
SMILES:	<chem>c1cnc2[nH]nnc2c1</chem>
Mol. weight [g/mol]:	120.11
CAS:	273-34-7

Physical Properties

Property code	Value	Unit	Source
ie	9.20 ± 0.05	eV	NIST Webbook
log10ws	-1.79		Crippen Method
logp	-0.129		Crippen Method
mcvol	82.310	ml/mol	McGowan Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C273347&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

Legend

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

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