

2-Pyridinamine, 1-oxide

Other names:	2-Aminopyridine N-oxide 2-Amino-1-pyridine 1-oxide 2-Aminopyridine 1-oxide 2-Aminopyridine oxide Pyridine, 2-amino-, 1-oxide
Inchi:	InChI=1S/C5H6N2O/c6-5-3-1-2-4-7(5)8/h1-4H,6H2
InchiKey:	NNDASDMUUQRZKG-UHFFFAOYSA-N
Formula:	C5H6N2O
SMILES:	<chem>Nc1cccc[n+][O-]</chem>
Mol. weight [g/mol]:	110.11
CAS:	14150-95-9

Physical Properties

Property code	Value	Unit	Source
ie	8.04 ± 0.05	eV	NIST Webbook
log10ws	-2.63		Crippen Method
logp	-0.098		Crippen Method
mvol	83.380	ml/mol	McGowan Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C14150959&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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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