

2-AMINOPYRIDINE 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]:	110.12

Physical Properties

Property code	Value	Unit	Source
hf	153.00	kJ/mol	Cheméo Relay (1.0)
ie	8.04 ± 0.05	eV	NIST Webbook
logp	-0.098		Crippen Method
mcvol	83.380	ml/mol	McGowan Method
tf	411.49	K	Cheméo Relay (1.0)

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C14150959&Units=SI
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.cheméo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	

Legend

hf:	Enthalpy of formation at standard conditions
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ie:	Ionization energy
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
tf:	Normal melting (fusion) point

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