

Pyridine, 2-nitro-

Other names:	2-Nitropyridine
Inchi:	InChI=1S/C5H4N2O2/c8-7(9)5-3-1-2-4-6-5/h1-4H
InchiKey:	HLTDBMHJSBSAOM-UHFFFAOYSA-N
Formula:	C5H4N2O2
SMILES:	O=[N+]([O-])c1ccccn1
Mol. weight [g/mol]:	124.10
CAS:	15009-91-3

Physical Properties

Property code	Value	Unit	Source
ie	10.10 ± 0.10	eV	NIST Webbook
log10ws	-1.89		Crippen Method
logp	0.990		Crippen Method
mcvol	84.950	ml/mol	McGowan Method
tb	529.20	K	NIST Webbook

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C15009913&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

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

Latest version available from:

<https://www.cheméo.com/cid/32-510-9/Pyridine-2-nitro.pdf>

Generated by Cheméo on 2024-05-02 20:40:27.3094997 +0000 UTC m=+16971676.230077018.

Cheméo (<https://www.cheméo.com>) is the biggest free database of chemical and physical data for the process industry.