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/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
tb: Normal Boiling Point Temperature