4-Nitropyridine

Inchi: InChI=1S/C5H4N2O2/c8-7(9)5-1-3-6-4-2-5/h1-4H
InchiKey: FEXIEMAAKBNTFK-UHFFFAOYSA-N
Formula: C5H4N2O2
SMILES: O=[N+]([O-])c1ccncc1
Mol. weight [g/mol]: 124.10
CAS: 1122-61-8

Physical Properties

Property code	Value	Unit	Source
affp	874.30	kJ/mol	NIST Webbook
basg	842.50	kJ/mol	NIST Webbook
ie	10.20 ± 0.10	eV	NIST Webbook
ie	10.40	eV	NIST Webbook
log10ws	-1.89		Crippen Method
logp	0.990		Crippen Method
mcvol	84.950	ml/mol	McGowan Method

Sources

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
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C1122618&Units=SI&Mask=3FFF

Legend

affp: Proton affinity
basg: Gas basicity
ie: Ionization energy
log10ws: Log10 of Water solubility in mol/l
logp: Octanol/Water partition coefficient

mcvol: McGowan's characteristic volume