4-Pyridinecarbonitrile, 1-oxide

Other names: 4-Cyanopyridine-N-oxide
Isonicotinonitrile, 1-oxide
4-Cyanopyridine oxide
4-Cyanopyridine 1-oxide
Inchi: InChI=1S/C6H4N2O/c7-5-6-1-3-8(9)4-2-6/h1-4H
InchiKey: QNCSFBSIWVBTHE-UHFFFAOYSA-N
Formula: C6H4N2O
SMILES: N#Cc1cc[n+]([O-])cc1
Mol. weight [g/mol]: 120.11
CAS: 14906-59-3

Physical Properties

Property code	Value	Unit	Source
affp	873.40	kJ/mol	NIST Webbook
basg	842.70	kJ/mol	NIST Webbook
hsub	104.40 ± 4.30	kJ/mol	NIST Webbook
ie	8.95 ± 0.02	eV	NIST Webbook
log10ws	-3.35		Crippen Method
logp	0.192		Crippen Method
mcvol	88.870	ml/mol	McGowan Method

Sources

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=C14906593&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

affp: Proton affinity

basg:	Gas basicity
hsub:	Enthalpy of sublimation at standard conditions
ie:	Ionization energy
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume