Pyridine, 1-oxide

Other names:	Pyridine oxide
	Pyridine N-oxide
Inchi:	InChI=1S/C5H5NO/c7-6-4-2-1-3-5-6/h1-5H
InchiKey:	ILVXOBCQQYKLDS-UHFFFAOYSA-N
Formula:	C5H5NO
SMILES:	[O-][n+]1ccccc1
Mol. weight [g/mol]:	95.10
CAS:	694-59-7

Physical Properties

Property code	Value	Unit	Source
affp	923.60	kJ/mol	NIST Webbook
basg	892.90	kJ/mol	NIST Webbook
hf	87.90 ± 2.50	kJ/mol	NIST Webbook
hf	87.90 ± 2.50	kJ/mol	NIST Webbook
hfs	8.60 ± 2.30	kJ/mol	NIST Webbook
hfs	8.60 ± 2.30	kJ/mol	NIST Webbook
hfs	7.70	kJ/mol	NIST Webbook
hsub	79.30 ± 1.00	kJ/mol	NIST Webbook
hsub	79.30 ± 1.00	kJ/mol	NIST Webbook
hsub	81.90 ± 1.50	kJ/mol	NIST Webbook
hsub	79.30 ± 1.00	kJ/mol	NIST Webbook
ie	8.46	eV	NIST Webbook
ie	8.38 ± 0.02	eV	NIST Webbook
ie	8.38 ± 0.02	eV	NIST Webbook
log10ws	-3.00		Crippen Method
logp	0.320		Crippen Method
mcvol	73.400	ml/mol	McGowan Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C694597&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

affp:	Proton affinity
basg:	Gas basicity
hf:	Enthalpy of formation at standard conditions
hfs:	Solid phase enthalpy of formation at standard conditions
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