1-(3-pyridinyl-1-oxide)ethanone

Other names:	Ethanone, 1-(1-oxido-3-pyridinyl)-
	1-(1-oxidopyridin-3-yl)ethanone
Inchi:	InChI=1S/C7H7NO2/c1-6(9)7-3-2-4-8(10)5-7/h2-5H,1H3
InchiKey:	AZFMFGIMDGBJRR-UHFFFAOYSA-N
Formula:	C7H7NO2
SMILES:	CC(=O)c1ccc[n+]([O-])c1
Mol. weight [g/mol]:	137.14
CAS:	14188-94-4

Physical Properties

Property code	Value	Unit	Source
affp	913.10	kJ/mol	NIST Webbook
basg	880.60	kJ/mol	NIST Webbook
log10ws	-3.66		Crippen Method
logp	0.523		Crippen Method
mcvol	103.150	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=C14188944&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

Legend

affp:	Proton affinity
basg:	Gas basicity
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume