

Pyridine, 4-methoxy-1-oxide-

Other names:	4-Methoxypyridine-N-oxide Pyridinium,1-hydroxy-4-methoxy-,hydroxide,inner salt
Inchi:	InChI=1S/C6H7NO2/c1-9-6-2-4-7(8)5-3-6/h2-5H,1H3
InchiKey:	BOFAIBPJCWFJFT-UHFFFAOYSA-N
Formula:	C6H7NO2
SMILES:	COc1cc[n+][O-]cc1
Mol. weight [g/mol]:	125.13
CAS:	1122-96-9

Physical Properties

Property code	Value	Unit	Source
ie	7.98 ± 0.05	eV	NIST Webbook
ie	7.89	eV	NIST Webbook
ie	7.74 ± 0.05	eV	NIST Webbook
log10ws	-3.12		Crippen Method
logp	0.329		Crippen Method
mcvol	93.360	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=C1122969&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

Legend

ie:	Ionization energy
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume

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