Pyridine, 3-methyl-, 1-oxide

Other names:	«beta»-Picoline N-oxide
	3-Picoline, 1-oxide
	«beta»-Picoline 1-oxide
	3-Methylpyridine N-oxide
	3-Methylpyridine 1-oxide
	3-Picoline N-oxide
Inchi:	InChI=1S/C6H7NO/c1-6-3-2-4-7(8)5-6/h2-5H,1H3
InchiKey:	DMGGLIWGZFZLIY-UHFFFAOYSA-N
Formula:	C6H7NO
SMILES:	Cc1ccc[n+]([O-])c1
Mol. weight [g/mol]:	109.13
CAS:	1003-73-2

Physical Properties

Property code	Value	Unit	Source
affp	935.20	kJ/mol	NIST Webbook
basg	902.80	kJ/mol	NIST Webbook
hfs	8.80 ± 0.70	kJ/mol	NIST Webbook
hsub	82.20 ± 2.40	kJ/mol	NIST Webbook
ie	8.20 ± 0.02	eV	NIST Webbook
log10ws	-3.48		Crippen Method
logp	0.628		Crippen Method
mcvol	87.490	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=C1003732&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
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