Pyridine, 4-methyl-, 1-oxide

Other names:	«gamma»-Picoline N-oxide
	4-Picoline, 1-oxide
	«gamma»-Picoline 1-oxide
	4-Methylpyridine N-oxide
	4-Methylpyridine 1-oxide
	4-Picoline N-oxide
Inchi:	InChI=1S/C6H7NO/c1-6-2-4-7(8)5-3-6/h2-5H,1H3
InchiKey:	IWYYIZOHWPCALJ-UHFFFAOYSA-N
Formula:	C6H7NO
SMILES:	Cc1cc[n+]([O-])cc1
Mol. weight [g/mol]:	109.13
CAS:	1003-67-4

Physical Properties

Property code	Value	Unit	Source
chs	-3360.90 ± 2.10	kJ/mol	NIST Webbook
hfs	-0.50 ± 2.10	kJ/mol	NIST Webbook
hfs	12.90 ± 0.90	kJ/mol	NIST Webbook
hsub	85.30 ± 2.60	kJ/mol	NIST Webbook
hsub	79.10 ± 1.30	kJ/mol	NIST Webbook
ie	8.17	eV	NIST Webbook
ie	8.12 ± 0.02	eV	NIST Webbook
log10ws	-3.48		Crippen Method
logp	0.628		Crippen Method
mcvol	87.490	ml/mol	McGowan Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
hsubt	79.10 ± 1.30	kJ/mol	328.50	NIST Webbook

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C1003674&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

Legend

chs:	Standard solid enthalpy of combustion
hfs:	Solid phase enthalpy of formation at standard conditions
hsub:	Enthalpy of sublimation at standard conditions
hsubt:	Enthalpy of sublimation at a given temperature
ie:	Ionization energy
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume