4-t-Butyl pyridine, 1-oxide

Other names:	Pyridine,4-(1,1-dimethylethyl)-,1-oxide
	4-t-Butylpyridine-N-oxide
Inchi:	InChI=1S/C9H13NO/c1-9(2,3)8-4-6-10(11)7-5-8/h4-7H,1-3H3
InchiKey:	CMFQXPIZAKBRCG-UHFFFAOYSA-N
Formula:	C9H13NO
SMILES:	CC(C)(C)c1cc[n+]([O-])cc1
Mol. weight [g/mol]:	151.21
CAS:	23569-17-7

Physical Properties

Property code	Value	Unit	Source
ie	7.80	eV	NIST Webbook
ie	8.00	eV	NIST Webbook
log10ws	-4.31		Crippen Method
logp	1.617		Crippen Method
mcvol	129.760	ml/mol	McGowan Method

Sources

Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C23569177&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

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