

# 4-t-Butyl pyridine, 1-oxide

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

<b>Crippen Method:</b>	<a href="https://www.chemeo.com/doc/models/crippen_log10ws">https://www.chemeo.com/doc/models/crippen_log10ws</a>
<b>McGowan Method:</b>	<a href="http://link.springer.com/article/10.1007/BF02311772">http://link.springer.com/article/10.1007/BF02311772</a>
<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=C23569177&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C23569177&amp;Units=SI</a>
<b>Crippen Method:</b>	<a href="http://pubs.acs.org/doi/abs/10.1021/ci9903071">http://pubs.acs.org/doi/abs/10.1021/ci9903071</a>

## Legend

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

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