

# Nitroxide, bis(1,1-dimethylethyl)

<b>Other names:</b>	di-t-Butylnitroxyl (tert-C <sub>4</sub> H <sub>9</sub> ) <sub>2</sub> NO di-tert-Butylnitroxide di-tert-Butyl nitroxyl Nitroxide, di-tert-butyl Dtn di(tert-butyl)aminyl oxide
<b>Inchi:</b>	InChI=1S/C <sub>8</sub> H <sub>18</sub> NO/c1-7(2,3)9(10)8(4,5)6/h1-6H3
<b>InchiKey:</b>	CKJMHSMEPSUICM-UHFFFAOYSA-N
<b>Formula:</b>	C <sub>8</sub> H <sub>18</sub> NO
<b>SMILES:</b>	CC(C)(C)N([O])C(C)(C)C
<b>Mol. weight [g/mol]:</b>	144.23
<b>CAS:</b>	2406-25-9

## Physical Properties

Property code	Value	Unit	Source
ie	6.77	eV	NIST Webbook
log10ws	-6.85		Crippen Method
logp	2.231		Crippen Method
mvol	137.280	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=C2406259&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C2406259&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

**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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