

# 6-Nitroindole

<b>Other names:</b>	1H-Indole, 6-nitro- 6-nitro-1H-indole
<b>Inchi:</b>	InChI=1S/C8H6N2O2/c11-10(12)7-2-1-6-3-4-9-8(6)5-7/h1-5,9H
<b>InchiKey:</b>	PSWCIARYGITEOY-UHFFFAOYSA-N
<b>Formula:</b>	C8H6N2O2
<b>SMILES:</b>	O=[N+](O-)c1ccc2cc[nH]c2c1
<b>Mol. weight [g/mol]:</b>	162.15
<b>CAS:</b>	4769-96-4

## Physical Properties

Property code	Value	Unit	Source
log10ws	-3.15		Crippen Method
logp	1.594		Crippen Method
mvol	112.060	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=C4769964&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C4769964&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>log10ws:</b>	Log10 of Water solubility in mol/l
<b>logp:</b>	Octanol/Water partition coefficient
<b>mvol:</b>	McGowan's characteristic volume

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