

# Quinoline, 4-nitro-, 1-oxide

<b>Other names:</b>	Nitrochin 4-Nitroquinoline oxide 4-Nitroquinoline N-oxide 4-Nitroquinoline 1-oxide 4-NQO 4-Nitrochinolin N-oxid NSC 19645
<b>Inchi:</b>	InChI=1S/C9H6N2O3/c12-10-6-5-9(11(13)14)7-3-1-2-4-8(7)10/h1-6H
<b>InchiKey:</b>	YHQDZJICGQWFHK-UHFFFAOYSA-N
<b>Formula:</b>	C9H6N2O3
<b>SMILES:</b>	O=[N+](O-)c1cc[n+](O)c2ccccc12
<b>Mol. weight [g/mol]:</b>	190.16
<b>CAS:</b>	56-57-5

## Physical Properties

Property code	Value	Unit	Source
log10ws	-5.45		Crippen Method
logp	1.381		Crippen Method
mcvol	127.720	ml/mol	McGowan Method
rinpole	330.31		NIST Webbook
rinpole	330.82		NIST Webbook
rinpole	331.55		NIST Webbook

## Sources

<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=C56575&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C56575&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>
<b>Crippen Method:</b>	<a href="https://www.chemeo.com/doc/models/crippen_log10ws">https://www.chemeo.com/doc/models/crippen_log10ws</a>

# Legend

<b>log10ws:</b>	Log10 of Water solubility in mol/l
<b>logp:</b>	Octanol/Water partition coefficient
<b>mcvol:</b>	McGowan's characteristic volume
<b>rinpol:</b>	Non-polar retention indices

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