

# 5,7-Dinitro-8-quinolinol

<b>Other names:</b>	8-Quinolinol, 5,7-dinitro-
<b>Inchi:</b>	InChI=1S/C9H5N3O5/c13-9-7(12(16)17)4-6(11(14)15)5-2-1-3-10-8(5)9/h1-4,13H
<b>InchiKey:</b>	YPEUTQKEMPFKO-UHFFFAOYSA-N
<b>Formula:</b>	C9H5N3O5
<b>SMILES:</b>	O=[N+]([O-])c1cc([N+](=O)[O-])c2cccnc2c1O
<b>Mol. weight [g/mol]:</b>	235.15
<b>CAS:</b>	1084-32-8

## Physical Properties

Property code	Value	Unit	Source
log10ws	-3.89		Crippen Method
logp	1.757		Crippen Method
mcvol	145.140	ml/mol	McGowan Method

## 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=C1084328&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C1084328&amp;Units=SI</a>
<b>Crippen Method:</b>	<a href="http://pubs.acs.org/doi/abs/10.1021/ci990307l">http://pubs.acs.org/doi/abs/10.1021/ci990307l</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

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