

# 1H-Imidazole, 4-nitro-

<b>Other names:</b>	1H-4-Nitroimidazole 1H-5-Nitroimidazole 4(5)-nitroimidazole 4-nitro-1H-imidazole 4-nitroimidazole 5-nitro-1H-imidazole 5-nitroimidazole Imidazole, 4(or 5)-nitro- Imidazole, 4-nitro-
<b>Inchi:</b>	InChI=1S/C3H3N3O2/c7-6(8)3-1-4-2-5-3/h1-2H,(H,4,5)
<b>InchiKey:</b>	VYDWQPKRHOGLPA-UHFFFAOYSA-N
<b>Formula:</b>	C3H3N3O2
<b>SMILES:</b>	O=[N+][O-]c1c[nH]cn1
<b>Mol. weight [g/mol]:</b>	113.07
<b>CAS:</b>	3034-38-6

## Physical Properties

Property code	Value	Unit	Source
log10ws	-1.11		Crippen Method
logp	-0.164		Crippen Method
mcvol	71.050	ml/mol	McGowan Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
hvapt	122.90	kJ/mol	298.15	Calorimetric and computational studies for three nitroimidazole isomers

# Sources

<b>Crippen Method:</b>	<a href="http://pubs.acs.org/doi/abs/10.1021/ci990307I">http://pubs.acs.org/doi/abs/10.1021/ci990307I</a>
<b>Crippen Method:</b>	<a href="https://www.chemeo.com/doc/models/crippen_log10ws">https://www.chemeo.com/doc/models/crippen_log10ws</a>
<b>Calorimetric and computational studies for three nitroimidazole isomers:</b>	<a href="https://www.doi.org/10.1016/j.jct.2016.10.026">https://www.doi.org/10.1016/j.jct.2016.10.026</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=C3034386&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C3034386&amp;Units=SI</a>

# Legend

<b>hvapt:</b>	Enthalpy of vaporization at a given temperature
<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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