

# 1H-1,2,4-Triazole, 3-nitro-

<b>Other names:</b>	s-Triazole, 3-nitro- 3-Nitro-1,2,4-triazole 3-Nitro-1H-1,2,4-triazole 3-Nitro-4H-[1,2,4]triazole
<b>Inchi:</b>	InChI=1S/C2H2N4O2/c7-6(8)2-3-1-4-5-2/h1H,(H,3,4,5)
<b>InchiKey:</b>	KUEFXPHXHHANKS-UHFFFAOYSA-N
<b>Formula:</b>	C2H2N4O2
<b>SMILES:</b>	O=[N+](O)c1nc[nH]n1
<b>Mol. weight [g/mol]:</b>	114.06
<b>CAS:</b>	24807-55-4

## Physical Properties

Property code	Value	Unit	Source
log10ws	-0.87		Crippen Method
logp	-0.769		Crippen Method
mcvol	66.940	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=C24807554&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C24807554&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>

## 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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