

# 3H-1,2,4-Triazol-3-one, 1,2-dihydro-5-nitro-

<b>Other names:</b>	s-Triazol-3-ol, 5-nitro- 5-Nitro-2,4-dihydro-(1,2,4)triazol-3-one 1,2-dihydro-5-nitro-3H-1,2,4-triazol-3-one
<b>Inchi:</b>	InChI=1S/C2H2N4O3/c7-2-3-1(4-5-2)6(8)9/h(H2,3,4,5,7)
<b>InchiKey:</b>	QJTIRVUEVSKJTK-UHFFFAOYSA-N
<b>Formula:</b>	C2H2N4O3
<b>SMILES:</b>	O=[N+][O-]c1nc(O)n[nH]1
<b>Mol. weight [g/mol]:</b>	130.06
<b>CAS:</b>	932-64-9

## Physical Properties

Property code	Value	Unit	Source
log10ws	-0.42		Crippen Method
logp	-1.063		Crippen Method
mcvol	72.810	ml/mol	McGowan Method

## Sources

<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=C932649&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C932649&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>
<b>McGowan Method:</b>	<a href="http://link.springer.com/article/10.1007/BF02311772">http://link.springer.com/article/10.1007/BF02311772</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

Latest version available from:

<https://www.chemeo.com/cid/96-970-9/3H-1-2-4-Triazol-3-one-1-2-dihydro-5-nitro.pdf>

Generated by Cheméo on 2024-05-05 06:47:02.464174114 +0000 UTC m=+17180871.384751429.

Cheméo (<https://www.chemeo.com>) is the biggest free database of chemical and physical data for the process industry.