

# 1,3-Dinitro-2-imidazolidinone

<b>Other names:</b>	1,3-Dinitro-2-imidazolidone 2-Imidazolidinone, 1,3-dinitro- N,N'-Dinitro-N,N'-ethyleneurea 1,3-Diazacyclopentan-2-one 1,3-dinitro-
<b>Inchi:</b>	InChI=1S/C3H4N4O5/c8-3-4(6(9)10)1-2-5(3)7(11)12/h1-2H2
<b>InchiKey:</b>	XIWMHAHUHIHAER-UHFFFAOYSA-N
<b>Formula:</b>	C3H4N4O5
<b>SMILES:</b>	O=C1N([N+](=O)[O-])CCN1[N+](=O)[O-]
<b>Mol. weight [g/mol]:</b>	176.09
<b>CAS:</b>	2536-18-7

## Physical Properties

Property code	Value	Unit	Source
log10ws	-1.02		Crippen Method
logp	-0.893		Crippen Method
mcvol	98.640	ml/mol	McGowan Method

## Sources

<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=C2536187&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C2536187&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>
<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

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