

# 3-Nitraza-1,5-pentanediiisocyanate

Inchi:	InChI=1S/C6H8N4O4/c11-5-7-1-3-9(10(13)14)4-2-8-6-12/h1-4H2
InchiKey:	PMZAXZNFRDOMGE-UHFFFAOYSA-N
Formula:	C6H8N4O4
SMILES:	O=C=NCCN(CCN=C=O)[N+](=O)[O-]
Mol. weight [g/mol]:	200.15
CAS:	7046-61-9

## Physical Properties

Property code	Value	Unit	Source
chs	-3242.35	kJ/mol	NIST Webbook
hf	-121.22	kJ/mol	Joback Method
hfs	-142.10 ± 2.90	kJ/mol	NIST Webbook
hvap	66.65	kJ/mol	Joback Method
log10ws	-8.97		Crippen Method
logp	-0.848		Crippen Method
mcvol	137.300	ml/mol	McGowan Method
pc	3736.23	kPa	Joback Method
tb	634.30	K	Joback Method
tc	847.51	K	Joback Method

## Sources

<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=C7046619&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C7046619&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>Joback Method:</b>	<a href="https://en.wikipedia.org/wiki/Joback_method">https://en.wikipedia.org/wiki/Joback_method</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

**chs:** Standard solid enthalpy of combustion

<b>hf:</b>	Enthalpy of formation at standard conditions
<b>hfs:</b>	Solid phase enthalpy of formation at standard conditions
<b>hvap:</b>	Enthalpy of vaporization at standard conditions
<b>log10ws:</b>	Log10 of Water solubility in mol/l
<b>logp:</b>	Octanol/Water partition coefficient
<b>mcvol:</b>	McGowan's characteristic volume
<b>pc:</b>	Critical Pressure
<b>tb:</b>	Normal Boiling Point Temperature
<b>tc:</b>	Critical Temperature

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