

# 2-Imidazolidinone

<b>Other names:</b>	1,3-Ethyleneurea 2-Oxoimidazolidine 2-imidazolidone Imidazolid-2-one Imidazoliden-2-one N,N'-ethyleneurea NSC 21314 SD 6073 Urea, 1,3-ethylene- Urea, N,N'-(1,2-Ethanediyl)- ethyleneurea urea, ethylene-
<b>Inchi:</b>	InChI=1S/C3H6N2O/c6-3-4-1-2-5-3/h1-2H2,(H2,4,5,6)
<b>InchiKey:</b>	YAMHXTCMCPHKLN-UHFFFAOYSA-N
<b>Formula:</b>	C3H6N2O
<b>SMILES:</b>	O=C1NCCN1
<b>Mol. weight [g/mol]:</b>	86.09
<b>CAS:</b>	120-93-4

## Physical Properties

Property code	Value	Unit	Source
gf	71.47	kJ/mol	Joback Method
hf	-86.51	kJ/mol	Joback Method
hfus	13.20	kJ/mol	Structural studies of cyclic ureas: 1. Enthalpies of formation of imidazolidin-2-one and N,N0-trimethyleneurea
hsub	83.70	kJ/mol	NIST Webbook
hsub	96.60 ± 0.80	kJ/mol	NIST Webbook
hvap	40.60	kJ/mol	Joback Method
ie	8.90	eV	NIST Webbook
ie	9.55	eV	NIST Webbook
log10ws	-0.10		Crippen Method
logp	-0.701		Crippen Method
mcvol	63.800	ml/mol	McGowan Method
pc	6852.77	kPa	Joback Method
tb	452.91	K	Joback Method

tc	696.51	K	Joback Method
tf	416.99	K	Joback Method
tt	397.30 ± 1.50	K	NIST Webbook
vc	0.227	m3/kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	118.87	J/mol×K	452.91	Joback Method
cpg	128.39	J/mol×K	493.51	Joback Method
cpg	137.62	J/mol×K	534.11	Joback Method
cpg	146.54	J/mol×K	574.71	Joback Method
cpg	155.11	J/mol×K	615.31	Joback Method
cpg	163.30	J/mol×K	655.91	Joback Method
cpg	171.06	J/mol×K	696.51	Joback Method
hfust	11.50	kJ/mol	401.20	NIST Webbook
hfust	5.11	kJ/mol	397.30	NIST Webbook

## Sources

**Crippen Method:** [https://www.chemeo.com/doc/models/crippen\\_log10ws](https://www.chemeo.com/doc/models/crippen_log10ws)

**Structural studies of cyclic ureas: 1.** <https://www.doi.org/10.1016/j.jct.2007.08.004>

**Enthalpies of formation of** [https://en.wikipedia.org/wiki/Joback\\_method](https://en.wikipedia.org/wiki/Joback_method)

**Joback Method** <http://link.springer.com/article/10.1007/BF02311772>

**N,N,N,N-tetramethylurea:** <http://link.springer.com/article/10.1007/BF02311772>

**McGowan Method:** <http://link.springer.com/article/10.1007/BF02311772>

**NIST Webbook:** <http://webbook.nist.gov/cgi/cbook.cgi?ID=C120934&Units=SI>

**Crippen Method:** <http://pubs.acs.org/doi/abs/10.1021/ci990307l>

## Legend

<b>cpg:</b>	Ideal gas heat capacity
<b>gf:</b>	Standard Gibbs free energy of formation
<b>hf:</b>	Enthalpy of formation at standard conditions
<b>hfus:</b>	Enthalpy of fusion at standard conditions
<b>hfust:</b>	Enthalpy of fusion at a given temperature
<b>hsub:</b>	Enthalpy of sublimation at standard conditions

<b>hvap:</b>	Enthalpy of vaporization at standard conditions
<b>ie:</b>	Ionization energy
<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
<b>tf:</b>	Normal melting (fusion) point
<b>tt:</b>	Triple Point Temperature
<b>vc:</b>	Critical Volume

Latest version available from:

<https://www.chemeo.com/cid/17-911-1/2-Imidazolidinone.pdf>

Generated by Cheméo on 2024-04-09 09:01:26.75519566 +0000 UTC m=+14942535.675772972.

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