

# 4(3H)-Pyrimidonep

<b>Inchi:</b>	InChI=1S/C4H4N2O/c7-4-1-2-5-3-6-4/h2-3H,1H2
<b>InchiKey:</b>	TZYQTWHLVDYPL-UHFFFAOYSA-N
<b>Formula:</b>	C4H4N2O
<b>SMILES:</b>	O=C1CC=NC=N1
<b>Mol. weight [g/mol]:</b>	96.09

## Physical Properties

Property code	Value	Unit	Source
gf	185.85	kJ/mol	Joback Method
hf	68.57	kJ/mol	Joback Method
hfus	9.11	kJ/mol	Joback Method
hvap	42.49	kJ/mol	Joback Method
log10ws	0.59		Aqueous Solubility Prediction Method
logp	0.016		Crippen Method
mcvol	69.290	ml/mol	McGowan Method
pc	6349.11	kPa	Joback Method
tb	488.68	K	Joback Method
tc	753.98	K	Joback Method
tf	359.28	K	Joback Method
vc	0.271	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	153.10	J/mol×K	488.68	Joback Method
cpg	165.98	J/mol×K	532.90	Joback Method
cpg	178.26	J/mol×K	577.11	Joback Method
cpg	189.86	J/mol×K	621.33	Joback Method
cpg	200.70	J/mol×K	665.55	Joback Method
cpg	210.70	J/mol×K	709.77	Joback Method
cpg	219.79	J/mol×K	753.98	Joback Method

# Sources

<b>Joback Method:</b>	<a href="https://en.wikipedia.org/wiki/Joback_method">https://en.wikipedia.org/wiki/Joback_method</a>
<b>Aqueous Solubility Prediction Method:</b>	<a href="http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDataset002.xlsx">http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDataset002.xlsx</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>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>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>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
<b>tf:</b>	Normal melting (fusion) point
<b>vc:</b>	Critical Volume

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