

# Isonipecotic acid, 2,6-dioxo-

<b>Inchi:</b>	InChI=1S/C6H7NO4/c8-4-1-3(6(10)11)2-5(9)7-4/h3H,1-2H2,(H,10,11)(H,7,8,9)
<b>InchiKey:</b>	QQGLSDQDZJVJSB-UHFFFAOYSA-N
<b>Formula:</b>	C6H7NO4
<b>SMILES:</b>	O=C1CC(C(=O)O)CC(=O)N1
<b>Mol. weight [g/mol]:</b>	157.12
<b>CAS:</b>	6973-55-3

## Physical Properties

Property code	Value	Unit	Source
gf	-399.12	kJ/mol	Joback Method
hf	-615.25	kJ/mol	Joback Method
hfus	17.43	kJ/mol	Joback Method
hvap	68.06	kJ/mol	Joback Method
log10ws	0.17		Crippen Method
logp	-0.876		Crippen Method
mcvol	105.100	ml/mol	McGowan Method
pc	5577.49	kPa	Joback Method
tb	686.47	K	Joback Method
tc	921.72	K	Joback Method
tf	516.98	K	Joback Method
vc	0.381	m3/kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	287.14	J/molxK	686.47	Joback Method
cpg	298.38	J/molxK	725.68	Joback Method
cpg	308.83	J/molxK	764.89	Joback Method
cpg	318.42	J/molxK	804.10	Joback Method
cpg	327.09	J/molxK	843.31	Joback Method
cpg	334.76	J/molxK	882.51	Joback Method
cpg	341.37	J/molxK	921.72	Joback Method

# Sources

<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>
<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=C6973553&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C6973553&amp;Units=SI</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>mccvol:</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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