

# 6-Nonyl-5,6-dihydro-2H-pyran-2-one

<b>Inchi:</b>	InChI=1S/C14H24O2/c1-2-3-4-5-6-7-8-10-13-11-9-12-14(15)16-13/h9,12-13H,2-8,10-11H
<b>InchiKey:</b>	CRCMEDPBLYLQH-UHFFFAOYSA-N
<b>Formula:</b>	C14H24O2
<b>SMILES:</b>	CCCCCCCCC1CC=CC(=O)O1
<b>Mol. weight [g/mol]:</b>	224.34
<b>CAS:</b>	118663-83-5

## Physical Properties

Property code	Value	Unit	Source
gf	-87.30	kJ/mol	Joback Method
hf	-489.89	kJ/mol	Joback Method
hfus	32.56	kJ/mol	Joback Method
hvap	56.24	kJ/mol	Joback Method
log10ws	-4.41		Crippen Method
logp	3.999		Crippen Method
mcvol	200.400	ml/mol	McGowan Method
pc	1898.60	kPa	Joback Method
rinpol	1910.70		NIST Webbook
tb	633.20	K	Joback Method
tc	834.24	K	Joback Method
tf	350.47	K	Joback Method
vc	0.766	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	556.32	J/mol×K	633.20	Joback Method
cpg	575.63	J/mol×K	666.71	Joback Method
cpg	593.92	J/mol×K	700.21	Joback Method
cpg	611.20	J/mol×K	733.72	Joback Method
cpg	627.49	J/mol×K	767.23	Joback Method
cpg	642.79	J/mol×K	800.73	Joback Method
cpg	657.12	J/mol×K	834.24	Joback Method

# Sources

<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=C118663835&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C118663835&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>Joback Method:</b>	<a href="https://en.wikipedia.org/wiki/Joback_method">https://en.wikipedia.org/wiki/Joback_method</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>rinpola:</b>	Non-polar retention indices
<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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