

# 3,5-undecadien-2-one

<b>Inchi:</b>	InChI=1S/C11H18O/c1-3-4-5-6-7-8-9-10-11(2)12/h7-10H,3-6H2,1-2H3/b8-7+,10-9+
<b>InchiKey:</b>	RCFOEQFXUGQOMT-XBLVEGMJSA-N
<b>Formula:</b>	C11H18O
<b>SMILES:</b>	CCCCC=CC=CC(C)=O
<b>Mol. weight [g/mol]:</b>	166.26
<b>CAS:</b>	68973-20-6

## Physical Properties

Property code	Value	Unit	Source
gf	73.26	kJ/mol	Joback Method
hf	-148.51	kJ/mol	Joback Method
hfus	26.25	kJ/mol	Joback Method
hvap	46.74	kJ/mol	Joback Method
log10ws	-3.41		Crippen Method
logp	3.268		Crippen Method
mcvol	158.820	ml/mol	McGowan Method
pc	2252.53	kPa	Joback Method
rinpol	1342.00		NIST Webbook
rinpol	1386.00		NIST Webbook
rinpol	1379.00		NIST Webbook
rinpol	1344.00		NIST Webbook
rinpol	1344.00		NIST Webbook
tb	513.27	K	Joback Method
tc	700.01	K	Joback Method
tf	253.50	K	Joback Method
vc	0.618	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	353.56	J/mol×K	513.27	Joback Method
cpg	368.13	J/mol×K	544.39	Joback Method
cpg	381.94	J/mol×K	575.52	Joback Method
cpg	395.05	J/mol×K	606.64	Joback Method

cpg	407.47	J/molxK	637.77	Joback Method
cpg	419.25	J/molxK	668.89	Joback Method
cpg	430.43	J/molxK	700.01	Joback Method
dvisc	0.0039020	Paxs	253.50	Joback Method
dvisc	0.0016040	Paxs	296.80	Joback Method
dvisc	0.0008268	Paxs	340.09	Joback Method
dvisc	0.0004950	Paxs	383.38	Joback Method
dvisc	0.0003289	Paxs	426.68	Joback Method
dvisc	0.0002356	Paxs	469.97	Joback Method
dvisc	0.0001786	Paxs	513.27	Joback Method

## Sources

<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=C68973206&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C68973206&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

<b>cpg:</b>	Ideal gas heat capacity
<b>dvisc:</b>	Dynamic viscosity
<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>rinpol:</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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