

# (E,E,Z)-2,4,6-undecatrienal

<b>Inchi:</b>	InChI=1S/C11H16O/c1-2-3-4-5-6-7-8-9-10-11-12/h5-11H,2-4H2,1H3/b6-5-,8-7+,10-9+
<b>InchiKey:</b>	IYJQORLVRUQEIH-WJTNUVGISA-N
<b>Formula:</b>	C11H16O
<b>SMILES:</b>	CCCCC=CC=CC=CC=O
<b>Mol. weight [g/mol]:</b>	164.24

## Physical Properties

Property code	Value	Unit	Source
gf	182.88	kJ/mol	Joback Method
hf	-4.29	kJ/mol	Joback Method
hfus	27.14	kJ/mol	Joback Method
hvap	46.67	kJ/mol	Joback Method
log10ws	-3.27		Crippen Method
logp	3.044		Crippen Method
mcvol	154.520	ml/mol	McGowan Method
pc	2393.53	kPa	Joback Method
ripol	1472.00		NIST Webbook
ripol	2078.00		NIST Webbook
ripol	2078.00		NIST Webbook
tb	512.22	K	Joback Method
tc	702.68	K	Joback Method
tf	240.49	K	Joback Method
vc	0.609	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	336.68	J/molxK	512.22	Joback Method
cpg	350.51	J/molxK	543.96	Joback Method
cpg	363.54	J/molxK	575.71	Joback Method
cpg	375.83	J/molxK	607.45	Joback Method
cpg	387.42	J/molxK	639.19	Joback Method
cpg	398.37	J/molxK	670.94	Joback Method
cpg	408.72	J/molxK	702.68	Joback Method

dvisc	0.0041723	Paxs	240.49	Joback Method
dvisc	0.0015863	Paxs	285.78	Joback Method
dvisc	0.0007858	Paxs	331.07	Joback Method
dvisc	0.0004609	Paxs	376.36	Joback Method
dvisc	0.0003032	Paxs	421.64	Joback Method
dvisc	0.0002163	Paxs	466.93	Joback Method
dvisc	0.0001639	Paxs	512.22	Joback Method

## Sources

<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=R237015&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=R237015&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>

## 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>ripol:</b>	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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