

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

<b>Inchi:</b>	InChI=1S/C9H12O/c1-2-3-4-5-6-7-8-9-10/h3-9H,2H2,1H3/b4-3-,6-5+,8-7+
<b>InchiKey:</b>	XHDSWFFUGPJMMN-ZRGCPWHVSA-N
<b>Formula:</b>	C9H12O
<b>SMILES:</b>	CCC=CC=CC=CC=O
<b>Mol. weight [g/mol]:</b>	136.19

## Physical Properties

Property code	Value	Unit	Source
gf	166.04	kJ/mol	Joback Method
hf	36.99	kJ/mol	Joback Method
hfus	21.96	kJ/mol	Joback Method
hvap	42.22	kJ/mol	Joback Method
log10ws	-2.43		Crippen Method
logp	2.264		Crippen Method
mcvol	126.340	ml/mol	McGowan Method
pc	2915.53	kPa	Joback Method
rinpol	1269.00		NIST Webbook
rinpol	1276.00		NIST Webbook
ripol	1877.00		NIST Webbook
tb	466.46	K	Joback Method
tc	661.54	K	Joback Method
tf	217.95	K	Joback Method
vc	0.496	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	249.68	J/mol×K	466.46	Joback Method
cpg	261.80	J/mol×K	498.97	Joback Method
cpg	273.16	J/mol×K	531.49	Joback Method
cpg	283.82	J/mol×K	564.00	Joback Method
cpg	293.82	J/mol×K	596.51	Joback Method
cpg	303.21	J/mol×K	629.02	Joback Method
cpg	312.04	J/mol×K	661.54	Joback Method

dvisc	0.0040805	Paxs	217.95	Joback Method
dvisc	0.0015983	Paxs	259.37	Joback Method
dvisc	0.0008104	Paxs	300.79	Joback Method
dvisc	0.0004843	Paxs	342.20	Joback Method
dvisc	0.0003235	Paxs	383.62	Joback Method
dvisc	0.0002337	Paxs	425.04	Joback Method
dvisc	0.0001789	Paxs	466.46	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=R417919&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=R417919&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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