

# 2,5-Octadienal, (Z,Z)

Inchi:	InChI=1S/C8H12O/c1-2-3-4-5-6-7-8-9/h3-4,6-8H,2,5H2,1H3/b4-3-,7-6-
InchiKey:	YUPOVSHIQPPSA-CWWKMNTPSA-N
Formula:	C8H12O
SMILES:	CCC=CCC=CC=O
Mol. weight [g/mol]:	124.18

## Physical Properties

Property code	Value	Unit	Source
gf	77.40	kJ/mol	Joback Method
hf	-59.59	kJ/mol	Joback Method
hfus	19.17	kJ/mol	Joback Method
hvap	40.04	kJ/mol	Joback Method
log10ws	-2.16		Crippen Method
logp	2.098		Crippen Method
mcvol	116.550	ml/mol	McGowan Method
pc	3059.17	kPa	Joback Method
ripol	1425.00		NIST Webbook
ripol	1425.00		NIST Webbook
tb	439.42	K	Joback Method
tc	627.33	K	Joback Method
tf	211.76	K	Joback Method
vc	0.461	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	225.21	J/molxK	439.42	Joback Method
cpg	276.76	J/molxK	596.01	Joback Method
cpg	267.58	J/molxK	564.70	Joback Method
cpg	257.87	J/molxK	533.38	Joback Method
cpg	247.60	J/molxK	502.06	Joback Method
cpg	236.72	J/molxK	470.74	Joback Method
cpg	285.43	J/molxK	627.33	Joback Method
dvisc	0.0002188	Paxs	439.42	Joback Method

dvisc	0.0002838	Paxs	401.48	Joback Method
dvisc	0.0003886	Paxs	363.53	Joback Method
dvisc	0.0005725	Paxs	325.59	Joback Method
dvisc	0.0009343	Paxs	287.65	Joback Method
dvisc	0.0017693	Paxs	249.70	Joback Method
dvisc	0.0042123	Paxs	211.76	Joback Method

## Sources

<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=R211528&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=R211528&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>

## 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>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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