

# 2-ethyl-2-hexenal (Z)

<b>Other names:</b>	(Z)-2-Ethylhex-2-enal
<b>Inchi:</b>	InChI=1S/C8H14O/c1-3-5-6-8(4-2)7-9/h6-7H,3-5H2,1-2H3/b8-6-
<b>InchiKey:</b>	PYLMCYQHBRSDND-VURMDHGXSA-N
<b>Formula:</b>	C8H14O
<b>SMILES:</b>	CCCC=C(C=O)CC
<b>Mol. weight [g/mol]:</b>	126.20

## Physical Properties

Property code	Value	Unit	Source
gf	-11.37	kJ/mol	Joback Method
hf	-186.60	kJ/mol	Joback Method
hfus	17.66	kJ/mol	Joback Method
hvap	40.16	kJ/mol	Joback Method
log10ws	-2.30		Crippen Method
logp	2.322		Crippen Method
mcvol	120.850	ml/mol	McGowan Method
pc	2906.11	kPa	Joback Method
rinpol	1021.00		NIST Webbook
rinpol	982.00		NIST Webbook
rinpol	982.00		NIST Webbook
ripol	1318.00		NIST Webbook
ripol	1318.00		NIST Webbook
tb	435.14	K	Joback Method
tc	617.65	K	Joback Method
tf	202.88	K	Joback Method
vc	0.481	m3/kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	241.01	J/molxK	435.14	Joback Method
cpg	253.06	J/molxK	465.56	Joback Method
cpg	264.55	J/molxK	495.98	Joback Method
cpg	275.48	J/molxK	526.39	Joback Method

cpg	285.90	J/mol×K	556.81	Joback Method
cpg	295.81	J/mol×K	587.23	Joback Method
cpg	305.24	J/mol×K	617.65	Joback Method

## Sources

<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.cheméo.com/doc/models/crippen_log10ws">https://www.cheméo.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=R333425&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=R333425&amp;Units=SI</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>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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