

# (Z)-3-heptenal

Inchi:	InChI=1S/C7H12O/c1-2-3-4-5-6-7-8/h4-5,7H,2-3,6H2,1H3/b5-4-
InchiKey:	ORAQCSKNITWHDW-PLNGDYQASA-N
Formula:	C7H12O
SMILES:	CCCC=CCC=O
Mol. weight [g/mol]:	112.17

## Physical Properties

Property code	Value	Unit	Source
gf	-11.24	kJ/mol	Joback Method
hf	-156.17	kJ/mol	Joback Method
hfus	16.38	kJ/mol	Joback Method
hvap	37.85	kJ/mol	Joback Method
log10ws	-1.89		Crippen Method
logp	1.932		Crippen Method
mcvol	106.760	ml/mol	McGowan Method
pc	3213.68	kPa	Joback Method
ripol	1312.00		NIST Webbook
ripol	1312.00		NIST Webbook
ripol	1295.00		NIST Webbook
ripol	1295.00		NIST Webbook
tb	412.38	K	Joback Method
tc	592.75	K	Joback Method
tf	205.57	K	Joback Method
vc	0.424	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	201.75	J/mol×K	412.38	Joback Method
cpg	212.47	J/mol×K	442.44	Joback Method
cpg	222.70	J/mol×K	472.50	Joback Method
cpg	232.44	J/mol×K	502.57	Joback Method
cpg	241.72	J/mol×K	532.63	Joback Method
cpg	250.55	J/mol×K	562.69	Joback Method

cpg	258.96	J/mol×K	592.75	Joback Method
dvisc	0.0042661	Paxs	205.57	Joback Method
dvisc	0.0019261	Paxs	240.04	Joback Method
dvisc	0.0010618	Paxs	274.51	Joback Method
dvisc	0.0006685	Paxs	308.98	Joback Method
dvisc	0.0004619	Paxs	343.44	Joback Method
dvisc	0.0003414	Paxs	377.91	Joback Method
dvisc	0.0002654	Paxs	412.38	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.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=R298614&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=R298614&amp;Units=SI</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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