

# (Z)-2-Hexene, 3-ethyl

Inchi:	InChI=1S/C9H18/c1-4-7-8-9(5-2)6-3/h5H,4,6-8H2,1-3H3/b9-5-
InchiKey:	JUUIRFQGSUFDPY-UITAMQMPSA-N
Formula:	C9H18
SMILES:	CC=C(CC)CCCC
Mol. weight [g/mol]:	126.24

## Physical Properties

Property code	Value	Unit	Source
gf	96.57	kJ/mol	Joback Method
hf	-121.66	kJ/mol	Joback Method
hfus	17.96	kJ/mol	Joback Method
hvap	35.67	kJ/mol	Joback Method
log10ws	-3.44		Crippen Method
logp	3.533		Crippen Method
mcvol	133.370	ml/mol	McGowan Method
pc	2438.65	kPa	Joback Method
rinpol	794.00		NIST Webbook
rinpol	794.00		NIST Webbook
rinpol	794.00		NIST Webbook
rinpol	794.00		NIST Webbook
tb	409.36	K	Joback Method
tc	583.79	K	Joback Method
tf	172.15	K	Joback Method
vc	0.520	m3/kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	258.03	J/molxK	409.36	Joback Method
cpg	272.25	J/molxK	438.43	Joback Method
cpg	285.86	J/molxK	467.50	Joback Method
cpg	298.88	J/molxK	496.58	Joback Method
cpg	311.33	J/molxK	525.65	Joback Method
cpg	323.24	J/molxK	554.72	Joback Method

## Sources

<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=R568611&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=R568611&amp;Units=SI</a>
<b>Crippen Method:</b>	<a href="http://pubs.acs.org/doi/abs/10.1021/ci990307I">http://pubs.acs.org/doi/abs/10.1021/ci990307I</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>

## 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>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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