

# 4-ethyl-6-hepten-3-one

<b>Inchi:</b>	InChI=1S/C9H16O/c1-4-7-8(5-2)9(10)6-3/h4,8H,1,5-7H2,2-3H3
<b>InchiKey:</b>	SUOMOGSVQCEXBO-UHFFFAOYSA-N
<b>Formula:</b>	C9H16O
<b>SMILES:</b>	C=CCC(CC)C(=O)CC
<b>Mol. weight [g/mol]:</b>	140.22
<b>CAS:</b>	131671-56-2

## Physical Properties

Property code	Value	Unit	Source
gf	-18.62	kJ/mol	Joback Method
hf	-221.52	kJ/mol	Joback Method
hfus	15.86	kJ/mol	Joback Method
hvap	41.32	kJ/mol	Joback Method
log10ws	-2.48		Crippen Method
logp	2.568		Crippen Method
mcvol	134.940	ml/mol	McGowan Method
pc	2579.34	kPa	Joback Method
ripol	1468.00		NIST Webbook
ripol	1468.00		NIST Webbook
tb	455.43	K	Joback Method
tc	636.92	K	Joback Method
tf	224.36	K	Joback Method
vc	0.520	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	281.01	J/mol×K	455.43	Joback Method
cpg	294.33	J/mol×K	485.68	Joback Method
cpg	307.06	J/mol×K	515.93	Joback Method
cpg	319.22	J/mol×K	546.18	Joback Method
cpg	330.83	J/mol×K	576.43	Joback Method
cpg	341.89	J/mol×K	606.68	Joback Method
cpg	352.44	J/mol×K	636.92	Joback Method

dvisc	0.0060877	Paxs	224.36	Joback Method
dvisc	0.0024776	Paxs	262.87	Joback Method
dvisc	0.0012688	Paxs	301.38	Joback Method
dvisc	0.0007561	Paxs	339.89	Joback Method
dvisc	0.0005007	Paxs	378.41	Joback Method
dvisc	0.0003578	Paxs	416.92	Joback Method
dvisc	0.0002706	Paxs	455.43	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=C131671562&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C131671562&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>

## 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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