

# 2-Hepten-4-one, 6-methyl-

Other names:	6-methyl-2-hepten-4-one
Inchi:	InChI=1S/C8H14O/c1-4-5-8(9)6-7(2)3/h4-5,7H,6H2,1-3H3/b5-4+
InchiKey:	VJQKJGLHKJYTQM-SNAWJCMRSA-N
Formula:	C8H14O
SMILES:	CC=CC(=O)CC(C)C
Mol. weight [g/mol]:	126.20
CAS:	49852-35-9

## Physical Properties

Property code	Value	Unit	Source
gf	-34.66	kJ/mol	Joback Method
hf	-209.09	kJ/mol	Joback Method
hfus	14.75	kJ/mol	Joback Method
hvap	39.72	kJ/mol	Joback Method
log10ws	-2.06		Crippen Method
logp	2.178		Crippen Method
mcvol	120.850	ml/mol	McGowan Method
pc	2881.21	kPa	Joback Method
tb	440.03	K	Joback Method
tc	628.20	K	Joback Method
tf	209.77	K	Joback Method
vc	0.464	m3/kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	239.81	J/molxK	440.03	Joback Method
cpg	252.37	J/molxK	471.39	Joback Method
cpg	264.33	J/molxK	502.75	Joback Method
cpg	275.70	J/molxK	534.12	Joback Method
cpg	286.51	J/molxK	565.48	Joback Method
cpg	296.79	J/molxK	596.84	Joback Method
cpg	306.55	J/molxK	628.20	Joback Method
dvisc	0.0063735	Paxs	209.77	Joback Method

dvisc	0.0024014	Paxs	248.15	Joback Method
dvisc	0.0011752	Paxs	286.52	Joback Method
dvisc	0.0006809	Paxs	324.90	Joback Method
dvisc	0.0004427	Paxs	363.28	Joback Method
dvisc	0.0003125	Paxs	401.65	Joback Method
dvisc	0.0002344	Paxs	440.03	Joback Method

## Correlations

Information	Value
Property code	pvap
Equation	$\ln(P_{vp}) = A + B/(T + C)$
Coeff. A	1.32542e+01
Coeff. B	-3.43841e+03
Coeff. C	-6.43460e+01
Temperature range (K), min.	329.52
Temperature range (K), max.	497.25

## Sources

Joback Method:	<a href="https://en.wikipedia.org/wiki/Joback_method">https://en.wikipedia.org/wiki/Joback_method</a>
McGowan Method:	<a href="http://link.springer.com/article/10.1007/BF02311772">http://link.springer.com/article/10.1007/BF02311772</a>
NIST Webbook:	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=C49852359&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C49852359&amp;Units=SI</a>
The Yaws Handbook of Vapor Pressure:	<a href="https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure">https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure</a>
Crippen Method:	<a href="http://pubs.acs.org/doi/abs/10.1021/ci990307l">http://pubs.acs.org/doi/abs/10.1021/ci990307l</a>
Crippen Method:	<a href="https://www.chemeo.com/doc/models/crippen_log10ws">https://www.chemeo.com/doc/models/crippen_log10ws</a>

## Legend

cp <sub>g</sub> :	Ideal gas heat capacity
dvisc:	Dynamic viscosity
g <sub>f</sub> :	Standard Gibbs free energy of formation
h <sub>f</sub> :	Enthalpy of formation at standard conditions
h <sub>fus</sub> :	Enthalpy of fusion at standard conditions
h <sub>vap</sub> :	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>pvap:</b>	Vapor pressure
<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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