

# 3-Heptanone, 5-methyl-

<b>Other names:</b>	3-Methyl-5-heptanone 5-Methyl-3-heptanone 5-Methylheptan-3-one 5-Methylheptanone-(3) Ethyl 2-methylbutyl ketone Ethyl sec-amyl ketone
<b>Inchi:</b>	InChI=1S/C8H16O/c1-4-7(3)6-8(9)5-2/h7H,4-6H2,1-3H3
<b>InchiKey:</b>	PSBKJPTZCVYXSD-UHFFFAOYSA-N
<b>Formula:</b>	C8H16O
<b>SMILES:</b>	CCC(=O)CC(C)CC
<b>Mol. weight [g/mol]:</b>	128.21
<b>CAS:</b>	541-85-5

## Physical Properties

Property code	Value	Unit	Source
gf	-114.88	kJ/mol	Joback Method
hf	-326.31	kJ/mol	Joback Method
hfus	14.55	kJ/mol	Joback Method
hvap	39.76	kJ/mol	Joback Method
log10ws	-2.21		Crippen Method
logp	2.402		Crippen Method
mcvol	125.150	ml/mol	McGowan Method
pc	2726.86	kPa	Joback Method
rinpol	931.00		NIST Webbook
rinpol	922.00		NIST Webbook
rinpol	149.25		NIST Webbook
rinpol	922.00		NIST Webbook
rinpol	922.00		NIST Webbook
rinpol	954.00		NIST Webbook
rinpol	960.00		NIST Webbook
rinpol	952.00		NIST Webbook
rinpol	962.00		NIST Webbook
rinpol	149.25		NIST Webbook
rinpol	922.00		NIST Webbook
rinpol	944.00		NIST Webbook
rinpol	944.00		NIST Webbook
rinpol	944.00		NIST Webbook

rinpol	944.00		NIST Webbook
rinpol	926.00		NIST Webbook
rinpol	922.00		NIST Webbook
rinpol	923.00		NIST Webbook
rinpol	924.00		NIST Webbook
rinpol	943.00		NIST Webbook
rinpol	939.00		NIST Webbook
rinpol	962.00		NIST Webbook
rinpol	926.00		NIST Webbook
ripol	1265.00		NIST Webbook
ripol	1219.50		NIST Webbook
ripol	1213.00		NIST Webbook
ripol	1266.00		NIST Webbook
ripol	1265.00		NIST Webbook
ripol	1265.00		NIST Webbook
ripol	1266.00		NIST Webbook
ripol	1219.50		NIST Webbook
ripol	1267.00		NIST Webbook
ripol	1266.00		NIST Webbook
ripol	1266.00		NIST Webbook
tb	432.70	K	NIST Webbook
tb	431.00 ± 2.00	K	NIST Webbook
tb	435.00 ± 3.00	K	NIST Webbook
tb	431.00 ± 3.00	K	NIST Webbook
tc	615.20	K	Joback Method
tf	214.85	K	Joback Method
vc	0.483	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	255.56	J/mol×K	435.87	Joback Method
cpg	268.41	J/mol×K	465.76	Joback Method
cpg	280.75	J/mol×K	495.65	Joback Method
cpg	292.58	J/mol×K	525.54	Joback Method
cpg	303.91	J/mol×K	555.42	Joback Method
cpg	314.75	J/mol×K	585.31	Joback Method
cpg	325.12	J/mol×K	615.20	Joback Method
dvisc	0.0067893	Paxs	214.85	Joback Method
dvisc	0.0027108	Paxs	251.69	Joback Method
dvisc	0.0013683	Paxs	288.52	Joback Method

dvisc	0.0008063	Paxs	325.36	Joback Method
dvisc	0.0005291	Paxs	362.20	Joback Method
dvisc	0.0003753	Paxs	399.03	Joback Method
dvisc	0.0002821	Paxs	435.87	Joback Method

## Correlations

Information	Value
Property code	pvap
Equation	$\ln(P_{vp}) = A + B/(T + C)$
Coeff. A	1.48779e+01
Coeff. B	-3.81556e+03
Coeff. C	-6.07980e+01
Temperature range (K), min.	322.31
Temperature range (K), max.	459.65

## 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=C541855&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C541855&amp;Units=SI</a>
<b>The Yaws Handbook of Vapor Pressure:</b>	<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>
<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>

## 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>h vap:</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>pvap:</b>	Vapor 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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