

# 3-Hexanone, 4,4-dimethyl-

<b>Other names:</b>	4,4-Dimethyl-3-hexanone
<b>Inchi:</b>	InChI=1S/C8H16O/c1-5-7(9)8(3,4)6-2/h5-6H2,1-4H3
<b>InchiKey:</b>	YEDJXYBDQSVPFJ-UHFFFAOYSA-N
<b>Formula:</b>	C8H16O
<b>SMILES:</b>	CCC(=O)C(C)(C)CC
<b>Mol. weight [g/mol]:</b>	128.21
<b>CAS:</b>	19550-14-2

## Physical Properties

Property code	Value	Unit	Source
gf	-109.60	kJ/mol	Joback Method
hf	-329.78	kJ/mol	Joback Method
hfus	10.66	kJ/mol	Joback Method
hvap	38.85	kJ/mol	Joback Method
log10ws	-2.21		Crippen Method
logp	2.402		Crippen Method
mcvol	125.150	ml/mol	McGowan Method
pc	2758.46	kPa	Joback Method
tb	424.00 ± 3.00	K	NIST Webbook
tb	424.20	K	NIST Webbook
tb	424.20 ± 3.00	K	NIST Webbook
tb	426.65 ± 1.50	K	NIST Webbook
tc	619.80	K	Joback Method
tf	232.27	K	Joback Method
vc	0.478	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	257.73	J/mol×K	433.08	Joback Method
cpg	271.54	J/mol×K	464.20	Joback Method
cpg	284.66	J/mol×K	495.32	Joback Method
cpg	297.11	J/mol×K	526.44	Joback Method
cpg	308.91	J/mol×K	557.56	Joback Method

cpg	320.09	J/mol×K	588.68	Joback Method
cpg	330.68	J/mol×K	619.80	Joback Method
dvisc	0.0068051	Paxs	232.27	Joback Method
dvisc	0.0029357	Paxs	265.74	Joback Method
dvisc	0.0015286	Paxs	299.21	Joback Method
dvisc	0.0009076	Paxs	332.67	Joback Method
dvisc	0.0005927	Paxs	366.14	Joback Method
dvisc	0.0004158	Paxs	399.61	Joback Method
dvisc	0.0003081	Paxs	433.08	Joback Method

## Correlations

Information	Value
Property code	pvap
Equation	$\ln(P_{vp}) = A + B/(T + C)$
Coeff. A	1.47248e+01
Coeff. B	-3.69868e+03
Coeff. C	-5.82300e+01
Temperature range (K), min.	314.42
Temperature range (K), max.	451.15

## Sources

<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=C19550142&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C19550142&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>
<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>

## 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>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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