

# 2,2,4-Trimethyl-3-pentanone

<b>Other names:</b>	3-Pentanone, 2,2,4-trimethyl- Isopropyl tert-butyl ketone Pentamethylacetone tert-Butyl isopropyl ketone tert-C <sub>4</sub> H <sub>9</sub> CO(iso-C <sub>3</sub> H <sub>7</sub> )
<b>Inchi:</b>	InChI=1S/C8H16O/c1-6(2)7(9)8(3,4)5/h6H,1-5H3
<b>InchiKey:</b>	OVCHQRXVZXVQNQ-UHFFFAOYSA-N
<b>Formula:</b>	C <sub>8</sub> H <sub>16</sub> O
<b>SMILES:</b>	CC(C)C(=O)C(C)(C)C
<b>Mol. weight [g/mol]:</b>	128.21
<b>CAS:</b>	5857-36-3

## Physical Properties

Property code	Value	Unit	Source
affp	856.90	kJ/mol	NIST Webbook
basg	825.00	kJ/mol	NIST Webbook
chl	-5053.20 ± 1.20	kJ/mol	NIST Webbook
gf	-112.04	kJ/mol	Joback Method
hf	-338.30 ± 1.20	kJ/mol	NIST Webbook
hfl	-381.60 ± 1.20	kJ/mol	NIST Webbook
hfus	7.14	kJ/mol	Joback Method
hvap	43.30 ± 0.20	kJ/mol	NIST Webbook
hvap	43.30 ± 0.10	kJ/mol	NIST Webbook
hvap	43.30 ± 0.10	kJ/mol	NIST Webbook
ie	8.80 ± 0.01	eV	NIST Webbook
log10ws	-1.97		Crippen Method
logp	2.258		Crippen Method
mcvol	125.150	ml/mol	McGowan Method
pc	2781.78	kPa	Joback Method
tb	408.00 ± 5.00	K	NIST Webbook
tb	409.00 ± 2.00	K	NIST Webbook
tb	407.00 ± 2.00	K	NIST Webbook
tb	407.00 ± 2.00	K	NIST Webbook
tb	399.34 ± 0.10	K	NIST Webbook
tb	409.40 ± 2.00	K	NIST Webbook
tb	406.00 ± 4.00	K	NIST Webbook
tb	408.00 ± 3.00	K	NIST Webbook

tb	407.00 ± 3.00	K	NIST Webbook
tc	623.69	K	Joback Method
tf	244.13 ± 0.10	K	NIST Webbook
vc	0.472	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	332.61	J/mol×K	623.69	Joback Method
cpg	257.77	J/mol×K	432.64	Joback Method
cpg	271.99	J/mol×K	464.48	Joback Method
cpg	285.48	J/mol×K	496.32	Joback Method
cpg	298.26	J/mol×K	528.17	Joback Method
cpg	310.35	J/mol×K	560.01	Joback Method
cpg	321.79	J/mol×K	591.85	Joback Method
dvisc	0.0002951	Paxs	432.64	Joback Method
dvisc	0.0112300	Paxs	217.27	Joback Method
dvisc	0.0039833	Paxs	253.16	Joback Method
dvisc	0.0018277	Paxs	289.06	Joback Method
dvisc	0.0009961	Paxs	324.95	Joback Method
dvisc	0.0006126	Paxs	360.85	Joback Method
dvisc	0.0004114	Paxs	396.75	Joback Method
hvapt	55.70	kJ/mol	347.50	NIST Webbook

## Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	332.70	K	6.70	NIST Webbook

## Correlations

Information	Value
Property code	pvap
Equation	$\ln(P_{vp}) = A + B/(T + C)$
Coeff. A	1.51172e+01

Coeff. B	-3.69933e+03
Coeff. C	-5.46430e+01
Temperature range (K), min.	304.10
Temperature range (K), max.	431.91

## Sources

<b>Crippen Method:</b>	<a href="http://pubs.acs.org/doi/abs/10.1021/ci990307l">http://pubs.acs.org/doi/abs/10.1021/ci990307l</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>
<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=C5857363&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C5857363&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>

## Legend

<b>affp:</b>	Proton affinity
<b>basg:</b>	Gas basicity
<b>chl:</b>	Standard liquid enthalpy of combustion
<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>hfl:</b>	Liquid phase 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>hvapt:</b>	Enthalpy of vaporization at a given temperature
<b>ie:</b>	Ionization energy
<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>tbrp:</b>	Boiling point at reduced pressure
<b>tc:</b>	Critical Temperature
<b>tf:</b>	Normal melting (fusion) point
<b>vc:</b>	Critical Volume

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