

# 2,2,5,5-Tetramethyltetrahydro-3-ketofuran

<b>Other names:</b>	Dihydro-2,2,5,5-tetramethyl-3(2H)-furanone 3(2H)-Furanone,dihydro-2,2,5,5-tetramethyl-
<b>Inchi:</b>	InChI=1S/C8H14O2/c1-7(2)5-6(9)8(3,4)10-7/h5H2,1-4H3
<b>InchiKey:</b>	HWFLEGUPVIFSJN-UHFFFAOYSA-N
<b>Formula:</b>	C8H14O2
<b>SMILES:</b>	CC1(C)CC(=O)C(C)(C)O1
<b>Mol. weight [g/mol]:</b>	142.20
<b>CAS:</b>	5455-94-7

## Physical Properties

Property code	Value	Unit	Source
gf	-174.37	kJ/mol	Joback Method
hf	-407.53	kJ/mol	Joback Method
hfus	6.37	kJ/mol	Joback Method
hvap	39.81	kJ/mol	Joback Method
ie	9.29 ± 0.03	eV	NIST Webbook
log10ws	-1.66		Crippen Method
logp	1.533		Crippen Method
mcvol	120.160	ml/mol	McGowan Method
pc	3368.44	kPa	Joback Method
tb	488.30	K	Joback Method
tc	717.80	K	Joback Method
tf	329.17	K	Joback Method
vc	0.448	m3/kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	279.20	J/molxK	488.30	Joback Method
cpg	294.96	J/molxK	526.55	Joback Method
cpg	309.57	J/molxK	564.80	Joback Method
cpg	323.23	J/molxK	603.05	Joback Method
cpg	336.12	J/molxK	641.30	Joback Method
cpg	348.45	J/molxK	679.55	Joback Method

cpg

360.40

J/mol×K

717.80

Joback Method

## Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	315.70	K	1.50	NIST Webbook

## 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=C5455947&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C5455947&amp;Units=SI</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>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>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>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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