

# Cyclopentanone, 2,4,4-trimethyl-

<b>Other names:</b>	2,4,4-Trimethylcyclopentanone 2,4,4-trimethylcyclopentan-1-one
<b>Inchi:</b>	InChI=1S/C8H14O/c1-6-4-8(2,3)5-7(6)9/h6H,4-5H2,1-3H3
<b>InchiKey:</b>	OXTQEWUBDTVSBF-UHFFFAOYSA-N
<b>Formula:</b>	C8H14O
<b>SMILES:</b>	CC1CC(C)(C)CC1=O
<b>Mol. weight [g/mol]:</b>	126.20
<b>CAS:</b>	4694-12-6

## Physical Properties

Property code	Value	Unit	Source
gf	-82.76	kJ/mol	Joback Method
hf	-290.77	kJ/mol	Joback Method
hfus	4.69	kJ/mol	Joback Method
hvap	36.45	kJ/mol	Joback Method
log10ws	-1.86		Crippen Method
logp	2.012		Crippen Method
mvol	114.290	ml/mol	McGowan Method
pc	3231.98	kPa	Joback Method
tb	461.11	K	Joback Method
tc	682.24	K	Joback Method
tf	278.70	K	Joback Method
vc	0.428	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	248.57	J/mol×K	461.11	Joback Method
cpg	265.00	J/mol×K	497.96	Joback Method
cpg	280.47	J/mol×K	534.82	Joback Method
cpg	295.06	J/mol×K	571.67	Joback Method
cpg	308.86	J/mol×K	608.53	Joback Method
cpg	321.95	J/mol×K	645.38	Joback Method
cpg	334.42	J/mol×K	682.24	Joback Method

# Sources

<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=C4694126&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C4694126&amp;Units=SI</a>
<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>

# 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>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>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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