

# Cyclohexanone, 3,3,5-trimethyl-

**Other names:** (dl) 3,5,5-trimethylcyclohexanone;  
3,3,5-Trimethylcyclohexan-1-one; 3,3,5-Trimethylcyclohexanone;  
3,3,5-trimethyl-cyclohexanone; Dihydroisophorone.

**InChI:** InChI=1S/C9H16O/c1-7-4-8(10)6-9(2,3)5-7/h7H,4-6H2,1-3H3

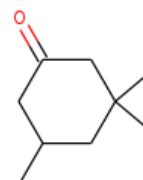
**InChI Key:** POSWICCRDBKBMH-UHFFFAOYSA-N

**Formula:** C<sub>9</sub>H<sub>16</sub>O

**SMILES:** CC1CC(=O)CC(C)(C)C1

**Molecular Weight:** 140.22

**CAS:** 873-94-9



## Physical Properties

Property	Value	Unit	Source
$\Delta_f G^\circ$	-86.44	kJ/mol	Joback Method
$\Delta_f H^\circ_{\text{gas}}$	-317.57	kJ/mol	Joback Method
$\Delta_{\text{fus}} H^\circ$	5.18	kJ/mol	Joback Method
$\Delta_{\text{vap}} H^\circ$	38.84	kJ/mol	Joback Method
$\log P_{\text{oct/wat}}$	2.40		Crippen Method
$P_c$	2986.06	kPa	Joback Method
$T_{\text{boil}}$	488.26	K	Joback Method
$T_c$	714.57	K	Joback Method
$T_{\text{fus}}$	286.45	K	Joback Method
$V_c$	0.48	m <sup>3</sup> /kg-mol	Joback Method

## Temperature Dependent Properties

Property	Value	Unit	Temperature (K)	Source
$C_{p,\text{gas}}$	292.44	J/mol×K	488.26	Joback Method
$\Delta_{\text{vap}} H$	39.30	kJ/mol	443.0	NIST Webbook

## Sources

**Joback Method:** [https://en.wikipedia.org/wiki/Joback\\_method](https://en.wikipedia.org/wiki/Joback_method)

**NIST Webbook:**

[http://webbook.nist.gov/cgi/inchi/InChI=1S/C9H16O/c1-7-4-8\(10\)6-9\(2,3\)5-7/h7H,4-6H2,1-3H3](http://webbook.nist.gov/cgi/inchi/InChI=1S/C9H16O/c1-7-4-8(10)6-9(2,3)5-7/h7H,4-6H2,1-3H3)

**Crippen Method:** <http://pubs.acs.org/doi/abs/10.1021/ci990307l>

## Legend

$C_{p,gas}$ : Ideal gas heat capacity (J/mol×K).

$\Delta_f G^\circ$ : Standard Gibbs free energy of formation (kJ/mol).

$\Delta_f H^\circ_{gas}$ : Enthalpy of formation at standard conditions (kJ/mol).

$\Delta_{fus} H^\circ$ : Enthalpy of fusion at standard conditions (kJ/mol).

$\Delta_{vap} H^\circ$ : Enthalpy of vaporization at standard conditions (kJ/mol).

$\Delta_{vap} H$ : Enthalpy of vaporization at a given temperature (kJ/mol).

$logP_{oct/wat}$ : Octanol/Water partition coefficient .

$P_c$ : Critical Pressure (kPa).

$T_{boil}$ : Normal Boiling Point Temperature (K).

$T_c$ : Critical Temperature (K).

$T_{fus}$ : Normal melting (fusion) point (K).

$V_c$ : Critical Volume (m<sup>3</sup>/kg-mol).

Latest version available from:

<https://www.cheméo.com/cid/10-651-7/Cyclohexanone%2C%203%2C3%2C5-trimethyl->

Generated by Cheméo on Mon, 19 Feb 2018 15:50:59 +0000.

**Cheméo** (<https://www.cheméo.com>) is the biggest free database of chemical and physical data for the process industry.