# 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-trimethyi-cyclohexanone; Dihydroisophorone.

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

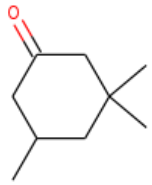
**InChI Key**: POSWICCRDBKBMH-UHFFFAOYSA-N

**Formula**: C9H16O

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

**Molecular Weight**: 140.22

**CAS**: 873-94-9



## Physical Properties

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

## Temperature Dependent Properties

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

## Sources

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

## Legend

$\mathbf{C_{p,gas}}$: Ideal gas heat capacity (J/mol×K).
$\Delta_f\mathbf{G°}$: Standard Gibbs free energy of formation (kJ/mol).
$\Delta_f\mathbf{H°_{gas}}$: Enthalpy of formation at standard conditions (kJ/mol).
$\Delta_{fus}\mathbf{H°}$: Enthalpy of fusion at standard conditions (kJ/mol).
$\Delta_{vap}\mathbf{H°}$: Enthalpy of vaporization at standard conditions (kJ/mol).
$\Delta_{vap}\mathbf{H}$: Enthalpy of vaporization at a given temperature (kJ/mol).
$\boldsymbol{log}\mathbf{P_{oct/wat}}$: Octanol/Water partition coefficient .
$\mathbf{P_c}$: Critical Pressure (kPa).
$\mathbf{T_{boil}}$: Normal Boiling Point Temperature (K).
$\mathbf{T_c}$: Critical Temperature (K).
$\mathbf{T_{fus}}$: Normal melting (fusion) point (K).
$\mathbf{V_c}$: Critical Volume ($m^3$/kg-mol).