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

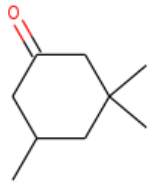
InChI Key: POSWICCRDBKBMH-UHFFFAOYSA-N

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
$log P_{oct/wat}$	2.402		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	0.476	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).