

# Tricyclo[3.2.1.1<sup>3,6</sup>]nonan-7-one

**Other names:** Tricyclo[3.2.1.1.

**InChI:** InChI=1S/C9H12O/c10-9-7-2-5-1-6(4-7)8(9)3-5/h5-8H,1-4H2

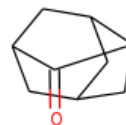
**InChI Key:** QUXWGFTVVNVNFO-UHFFFAOYSA-N

**Formula:** C<sub>9</sub>H<sub>12</sub>O

**SMILES:** O=C1C2CC3CC(CC13)C2

**Molecular Weight:** 136.19

**CAS:** 17931-67-8



## Physical Properties

Property	Value	Unit	Source
$\Delta_f G^\circ$	76.85	kJ/mol	Joback Method
$\Delta_f H^\circ_{\text{gas}}$	-168.73	kJ/mol	Joback Method
$\Delta_{\text{fus}} H^\circ$	14.05	kJ/mol	Joback Method
$\Delta_{\text{vap}} H^\circ$	39.31	kJ/mol	Joback Method
IE	8.81	eV	NIST Webbook
$\log P_{\text{oct/wat}}$	1.62		Crippen Method
$P_c$	3501.28	kPa	Joback Method
$T_{\text{boil}}$	488.69	K	Joback Method
$T_c$	715.13	K	Joback Method
$T_{\text{fus}}$	308.99	K	Joback Method
$V_c$	0.42	m <sup>3</sup> /kg-mol	Joback Method

## Temperature Dependent Properties

Property	Value	Unit	Temperature (K)	Source
$C_{p,\text{gas}}$	264.05	J/mol×K	488.69	Joback Method

## 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/C9H12O/c10-9-7-2-5-1-6\(4-7\)8\(9\)3-5/h5-8H,1-4H2](http://webbook.nist.gov/cgi/inchi/InChI=1S/C9H12O/c10-9-7-2-5-1-6(4-7)8(9)3-5/h5-8H,1-4H2)

**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).

**IE:** Ionization energy (eV).

**logP<sub>oct/wat</sub>**: Octanol/Water partition coefficient .

**P<sub>c</sub>**: Critical Pressure (kPa).

**T<sub>boil</sub>**: Normal Boiling Point Temperature (K).

**T<sub>c</sub>**: Critical Temperature (K).

**T<sub>fus</sub>**: Normal melting (fusion) point (K).

**V<sub>c</sub>**: Critical Volume (m<sup>3</sup>/kg-mol).

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