

# 1-Allyl-1-cyclohexanol

**Other names:** 1-Allylcyclohexanol; Cyclohexanol, 1-(2-propenyl)-; Cyclohexanol, 1-allyl-

**InChI:** InChI=1S/C9H16O/c1-2-6-9(10)7-4-3-5-8-9/h2,10H,1,3-8H2

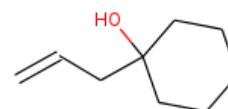
**InChI Key:** ZSLKGUQYEQVKQE-UHFFFAOYSA-N

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

**SMILES:** C=CCC1(O)CCCCC1

**Molecular Weight:** 140.22

**CAS:** 1123-34-8



## Physical Properties

Property	Value	Unit	Source
$\Delta_f G^\circ$	-5.12	kJ/mol	Joback Method
$\Delta_f H^\circ_{\text{gas}}$	-186.33	kJ/mol	Joback Method
$\Delta_{\text{fus}} H^\circ$	7.41	kJ/mol	Joback Method
$\Delta_{\text{vap}} H^\circ$	50.91	kJ/mol	Joback Method
$\log P_{\text{oct/wat}}$	2.258		Crippen Method
$P_c$	3468.36	kPa	Joback Method
$T_{\text{boil}}$	463.20	K	NIST Webbook
$T_c$	713.82	K	Joback Method
$T_{\text{fus}}$	281.53	K	Joback Method
$V_c$	0.470	m <sup>3</sup> /kg-mol	Joback Method

## Temperature Dependent Properties

Property	Value	Unit	Temperature (K)	Source
$C_{p,\text{gas}}$	302.05	J/mol×K	513.97	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/C9H16O/c1-2-6-9\(10\)7-4-3-5-8-9/h2,10H,1,3-8H2](http://webbook.nist.gov/cgi/inchi/InChI=1S/C9H16O/c1-2-6-9(10)7-4-3-5-8-9/h2,10H,1,3-8H2)

**Crippen Method:** <http://pubs.acs.org/doi/abs/10.1021/ci9903071>

## 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).

$\log P_{oct/wat}$ : 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/10-384-4/1-Allyl-1-cyclohexanol>

Generated by Cheméo on Tue, 18 Dec 2018 23:05:35 +0000.

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