

# Cyclohexanone, 2-(2-propenyl)-

<b>Other names:</b>	2-Allylcyclohexanone 2-allylcyclohexan-1-one Cyclohexanone, 2-allyl-
<b>Inchi:</b>	InChI=1S/C9H14O/c1-2-5-8-6-3-4-7-9(8)10/h2,8H,1,3-7H2
<b>InchiKey:</b>	UPGHEUSRLZSXAE-UHFFFAOYSA-N
<b>Formula:</b>	C9H14O
<b>SMILES:</b>	C=CCC1CCCCC1=O
<b>Mol. weight [g/mol]:</b>	138.21
<b>CAS:</b>	94-66-6

## Physical Properties

Property code	Value	Unit	Source
gf	14.60	kJ/mol	Joback Method
hf	-187.04	kJ/mol	Joback Method
hfus	9.13	kJ/mol	Joback Method
hvap	39.63	kJ/mol	Joback Method
log10ws	-2.38		Crippen Method
logp	2.322		Crippen Method
mcvol	124.080	ml/mol	McGowan Method
pc	3086.42	kPa	Joback Method
tb	489.37	K	Joback Method
tc	711.22	K	Joback Method
tf	265.03	K	Joback Method
vc	0.461	m3/kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	273.58	J/molxK	489.37	Joback Method
cpg	290.93	J/molxK	526.35	Joback Method
cpg	307.44	J/molxK	563.32	Joback Method
cpg	323.11	J/molxK	600.30	Joback Method
cpg	337.93	J/molxK	637.27	Joback Method
cpg	351.92	J/molxK	674.25	Joback Method

## Correlations

Information	Value
Property code	pvap
Equation	$\ln(P_{vp}) = A + B/(T + C)$
Coeff. A	1.50706e+01
Coeff. B	-4.14555e+03
Coeff. C	-7.35340e+01
Temperature range (K), min.	353.96
Temperature range (K), max.	498.32

## Sources

**McGowan Method:**

<http://link.springer.com/article/10.1007/BF02311772>

**NIST Webbook:**

<http://webbook.nist.gov/cgi/cbook.cgi?ID=C94666&Units=SI>

**The Yaws Handbook of Vapor Pressure:**

<https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure>

**Crippen Method:**

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

**Crippen Method:**

[https://www.chemeo.com/doc/models/crippen\\_log10ws](https://www.chemeo.com/doc/models/crippen_log10ws)

**Joback Method:**

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

## Legend

<b>cpg:</b>	Ideal gas heat capacity
<b>gf:</b>	Standard Gibbs free energy of formation
<b>hf:</b>	Enthalpy of formation at standard conditions
<b>hfus:</b>	Enthalpy of fusion at standard conditions
<b>hvap:</b>	Enthalpy of vaporization at standard conditions
<b>log10ws:</b>	Log10 of Water solubility in mol/l
<b>logp:</b>	Octanol/Water partition coefficient
<b>mccvol:</b>	McGowan's characteristic volume
<b>pc:</b>	Critical Pressure
<b>pvap:</b>	Vapor pressure
<b>tb:</b>	Normal Boiling Point Temperature

**tc:** Critical Temperature  
**tf:** Normal melting (fusion) point  
**vc:** Critical Volume

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