

# Pentalene, octahydro-

**Other names:** Bicyclo[3.3.0]octane; Octahydropentalene.

**InChI:** InChI=1S/C8H14/c1-3-7-5-2-6-8(7)4-1/h7-8H,1-6H2

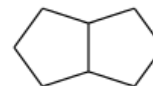
**InChI Key:** AEBWATHAIVJLTA-UHFFFAOYSA-N

**Formula:** C<sub>8</sub>H<sub>14</sub>

**SMILES:** C1CC2CCCC2C1

**Molecular Weight:** 110.20

**CAS:** 694-72-4



## Physical Properties

Property	Value	Unit	Source
$\Delta_f G^\circ$	113.78	kJ/mol	Joback Method
$\Delta_f H^\circ_{\text{gas}}$	-75.17	kJ/mol	Joback Method
$\Delta_{\text{fus}} H^\circ$	8.55	kJ/mol	Joback Method
$\Delta_{\text{vap}} H^\circ$	33.57	kJ/mol	Joback Method
$\log P_{\text{oct/wat}}$	2.59		Crippen Method
$P_c$	3560.02	kPa	Joback Method
$T_{\text{boil}}$	404.46	K	Joback Method
$T_c$	614.38	K	Joback Method
$T_{\text{fus}}$	208.76	K	Joback Method
$V_c$	0.38	m <sup>3</sup> /kg-mol	Joback Method

## Temperature Dependent Properties

Property	Value	Unit	Temperature (K)	Source
$C_{p,\text{gas}}$	198.70	J/mol×K	404.46	Joback Method
$\eta$	0.00	Paxs	404.46	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/C8H14/c1-3-7-5-2-6-8\(7\)4-1/h7-8H,1-6H2](http://webbook.nist.gov/cgi/inchi/InChI=1S/C8H14/c1-3-7-5-2-6-8(7)4-1/h7-8H,1-6H2)

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

## Legend

$C_{p, gas}$ : Ideal gas heat capacity (J/mol×K).

$\eta$ : Dynamic viscosity (Pa×s).

$\Delta_f G^\circ$ : 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).

$logP_{oct/wat}$ : 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).

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