

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

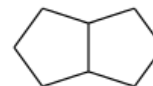
InChI Key: AEBWATHAIVJLTA-UHFFFAOYSA-N

Formula: C₈H₁₄

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
$\log P_{\text{oct/wat}}$	2.587		Crippen Method
P_c	3560.02	kPa	Joback Method
T_{boil}	404.46	K	Joback Method
T_c	614.38	K	Joback Method
T_{fus}	208.76	K	Joback Method
V_c	0.382	m ³ /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
η	0.0004750	Paxs	404.46	Joback Method

Sources

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/ci9903071>

Legend

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

η : Dynamic viscosity (Paxs).

$\Delta_f G^\circ$: 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 (m³/kg-mol).

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