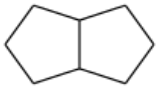
Pentalene, octahydro-

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
$\Delta_f G°$	113.78	kJ/mol	Joback Method
$\Delta_f H°_{gas}$	-75.17	kJ/mol	Joback Method
$\Delta_{fus} H°$	8.55	kJ/mol	Joback Method
$\Delta_{vap} H°$	33.57	kJ/mol	Joback Method
$log P_{oct/wat}$	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
$C_{p,gas}$	198.70	J/mol×K	404.46	Joback Method
η	0.0004750	Pa×s	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
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

$\mathbf{C_{p,gas}}$: Ideal gas heat capacity (J/mol×K).
η: Dynamic viscosity (Pa×s).
$\Delta_f\mathbf{G°}$: Standard Gibbs free energy of formation (kJ/mol).
$\Delta_f\mathbf{H°_{gas}}$: Enthalpy of formation at standard conditions (kJ/mol).
$\Delta_{fus}\mathbf{H°}$: Enthalpy of fusion at standard conditions (kJ/mol).
$\Delta_{vap}\mathbf{H°}$: Enthalpy of vaporization at standard conditions (kJ/mol).
$\boldsymbol{log}\mathbf{P_{oct/wat}}$: Octanol/Water partition coefficient .
$\mathbf{P_c}$: Critical Pressure (kPa).
$\mathbf{T_{boil}}$: Normal Boiling Point Temperature (K).
$\mathbf{T_c}$: Critical Temperature (K).
$\mathbf{T_{fus}}$: Normal melting (fusion) point (K).
$\mathbf{V_c}$: Critical Volume (m^3/kg-mol).