2,2-Dimethylindene, 2,3-dihydro-

Other names: 1H-Indene,2,3-dihydro-2,2-dimethyl-.
InChI:
InChI=1S/C11H14/c1-11(2)7-9-5-3-4-6-10(9)8-11/h3-6H,7-8H2,1-2H3
InChI Key: VAMWEVQXIHGFHY-UHFFFAOYSA-N
Formula: C11H14
SMILES: CC1(C)Cc2ccccc2C1
Molecular Weight: 146.23
CAS: 20836-11-7

Physical Properties

Property	Value	Unit	Source
$\Delta_f G°$	199.78	kJ/mol	Joback Method
$\Delta_f H°_{gas}$	42.73	kJ/mol	Joback Method
$\Delta_{fus} H°$	9.73	kJ/mol	Joback Method
$\Delta_{vap} H°$	41.78	kJ/mol	Joback Method
IE	8.47	eV	NIST Webbook
$log P_{oct/wat}$	2.81		Crippen Method
P_c	3145.56	kPa	Joback Method
T_{boil}	489.72	K	Joback Method
T_c	719.26	K	Joback Method
T_{fus}	294.51	K	Joback Method
V_c	0.50	m^3/kg-mol	Joback Method

Temperature Dependent Properties

Property	Value	Unit	Temperature (K)	Source
$C_{p,gas}$	286.80	J/mol×K	489.72	Joback Method

Sources

Joback Method: https://en.wikipedia.org/wiki/Joback_method
NIST Webbook: http://webbook.nist.gov/cgi/inchi/InChI=1S/C11H14/c1-11(2)7-9-5-3-4-6-10(9)8-11/h3-6H,7-8H2,1-2H3
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

$\mathbf{C_{p,gas}}$: Ideal gas heat capacity (J/mol×K).
$\Delta_f\mathbf{G°}$: 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).
IE: Ionization energy (eV).
$\boldsymbol{log}\mathbf{P_{oct/wat}}$: 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).