

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

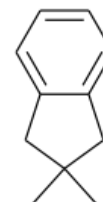
InChI Key: VAMWEVQXIHGFHY-UHFFFAOYSA-N

Formula: C11H14

SMILES: CC1(C)Cc2ccccc2C1

Molecular Weight: 146.23

CAS: 20836-11-7



Physical Properties

Property	Value	Unit	Source
$\Delta_f G^\circ$	199.78	kJ/mol	Joback Method
$\Delta_f H^\circ_{\text{gas}}$	42.73	kJ/mol	Joback Method
$\Delta_{\text{fus}} H^\circ$	9.73	kJ/mol	Joback Method
$\Delta_{\text{vap}} H^\circ$	41.78	kJ/mol	Joback Method
IE	8.47	eV	NIST Webbook
$\log P_{\text{oct/wat}}$	2.811		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	0.498	m ³ /kg-mol	Joback Method

Temperature Dependent Properties

Property	Value	Unit	Temperature (K)	Source
$C_{p,\text{gas}}$	286.80	J/molxK	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](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

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

$\Delta_f G^\circ$: 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).

IE: Ionization energy (eV).

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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