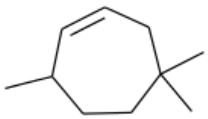
3,6,6-trimethylcycloheptene

InChI: InChI=1S/C10H18/c1-9-5-4-7-10(2,3)8-6-9/h4-5,9H,6-8H2,1-3H3
InChI Key: YCTPMOKNQNWVDT-UHFFFAOYSA-N
Formula: C10H18
SMILES: CC1C=CCC(C)(C)CC1
Molecular Weight: 138.25



Physical Properties

Property	Value	Unit	Source
$\Delta_f G°$	62.43	kJ/mol	Joback Method
$\Delta_f H°_{gas}$	-148.89	kJ/mol	Joback Method
$\Delta_{fus} H°$	7.39	kJ/mol	Joback Method
$\Delta_{vap} H°$	37.29	kJ/mol	Joback Method
$log P_{oct/wat}$	3.39		Crippen Method
P_c	2770.08	kPa	Joback Method
T_{boil}	446.75	K	Joback Method
T_c	662.46	K	Joback Method
T_{fus}	226.74	K	Joback Method
V_c	0.50	m^3/kg-mol	Joback Method

Temperature Dependent Properties

Property	Value	Unit	Temperature (K)	Source
$C_{p,gas}$	285.55	J/mol×K	446.75	Joback Method

Sources

Joback Method: https://en.wikipedia.org/wiki/Joback_method

NIST Webbook: http://webbook.nist.gov/cgi/inchi/InChI=1S/C10H18/c1-9-5-4-7-10(2,3)8-6-9/h4-5,9H,6-8H2,1-3H3

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

Legend

$C_{p,gas}$: Ideal gas heat capacity (J/mol×K).
$\Delta_f G°$: Standard Gibbs free energy of formation (kJ/mol).
$\Delta_f H°_{gas}$: Enthalpy of formation at standard conditions (kJ/mol).
$\Delta_{fus} H°$: Enthalpy of fusion at standard conditions (kJ/mol).
$\Delta_{vap} H°$: Enthalpy of vaporization at standard conditions (kJ/mol).
$log P_{oct/wat}$: 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^3/kg-mol).