5-methyl-adamantane

InChI: InChI=1S/C11H18/c1-11-5-8-2-9(6-11)4-10(3-8)7-11/h8-10H,2-7H2,1H3/t8-,9+,10-,11+
InChI Key: UZUCFTVAWGRMTQ-DTIDVZRVSA-N
Formula: C11H18
SMILES: CC12CC3CC(CC(C3)C1)C2
Molecular Weight: 150.26

Physical Properties

Property	Value	Unit	Source
$\Delta_f G°$	198.69	kJ/mol	Joback Method
$\Delta_f H°_{gas}$	-63.23	kJ/mol	Joback Method
$\Delta_{fus} H°$	11.32	kJ/mol	Joback Method
$\Delta_{vap} H°$	38.53	kJ/mol	Joback Method
$log P_{oct/wat}$	3.22		Crippen Method
P_c	2931.34	kPa	Joback Method
T_{boil}	471.14	K	Joback Method
T_c	691.15	K	Joback Method
T_{fus}	283.69	K	Joback Method
V_c	0.51	m^3/kg-mol	Joback Method

Temperature Dependent Properties

Property	Value	Unit	Temperature (K)	Source
$C_{p,gas}$	319.89	J/mol×K	471.14	Joback Method

Sources

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

NIST Webbook: http://webbook.nist.gov/cgi/inchi/InChI=1S/C11H18/c1-11-5-8-2-9(6-11)4-10(3-8)7-11/h8-10H,2-7H2,1H3/t8-,9+,10-,11+

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).