C31-Hopane, 17bH, 21bH

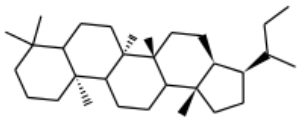
InChI: InChI=1S/C31H54/c1-9-21(2)22-13-18-28(5)23(22)14-19-30(7)25(28)11-12-26-29(6)17-10-16-27(3,4)24(29)15-20-31(26,30)8/h21-26H,9-20H2,1-8H3/t21?,22-,23+,24?,25?,26?,28+,29+,30-,31-/m0/s1

InChI Key: QFBGIDMRCNNMIW-OFQVYJJRSA-N

Formula: C31H54

SMILES: CCC(C)C1CCC2(C)C1CCC1(C)C2CCC2C3(C)CCCC(C)(C)C3CCC21C

Molecular Weight: 426.76



Physical Properties

Property	Value	Unit	Source
$\Delta_f G°$	372.85	kJ/mol	Joback Method
$\Delta_f H°_{gas}$	-386.91	kJ/mol	Joback Method
$\Delta_{fus} H°$	24.46	kJ/mol	Joback Method
$\Delta_{vap} H°$	77.51	kJ/mol	Joback Method
$log P_{oct/wat}$	9.52		Crippen Method
P_c	903.97	kPa	Joback Method
T_{boil}	945.41	K	Joback Method
T_c	1186.91	K	Joback Method
T_{fus}	591.01	K	Joback Method
V_c	1.49	m^3/kg-mol	Joback Method

Temperature Dependent Properties

Property	Value	Unit	Temperature (K)	Source
$C_{p,gas}$	1530.77	J/mol×K	945.41	Joback Method

Sources

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

NIST Webbook: http://webbook.nist.gov/cgi/inchi/InChI=1S/C31H54/c1-9-21(2)22-13-18-28(5)23(22)14-19-30(7)25(28)11-12-26-29(6)17-10-16-27(3,4)24(29)15-20-31(26,30)8/h21-26H,9-20H2,1-8H3/t21?,22-,23+,24?,25?,26?,28+,29+,30-,31-/m0/s1

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).