

C33-25-Norhopane, 17aH, 21bH, 22R

InChI: InChI=1S/C32H56/c1-8-9-11-22(2)23-15-19-30(5)26(23)17-21-32(7)28(30)14-13-27-24-12-10-18-29(3,4)25(24)16-20-31(27,32)6/h22-28H,8-21H2,1-7H3/t22-,23-,24?,25?,26-,27?,28?,30+,31-,32-/m0/s1

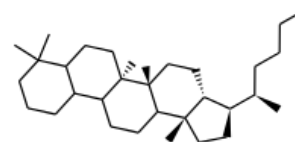
InChI Key: XCRHOWRYNNGKCR-XDDOIUQPSA-N

Formula: C₃₂H₅₆

SMILES:

CCCC(C)C1CCC2(C)C1CCC1(C)C2CCC2C3CCCC(C)(C)C3CCC21C

Molecular Weight: 440.79



Physical Properties

Property	Value	Unit	Source
$\Delta_f G^\circ$	386.76	kJ/mol	Joback Method
$\Delta_f H^\circ_{\text{gas}}$	-422.79	kJ/mol	Joback Method
$\Delta_{\text{fus}} H^\circ$	33.35	kJ/mol	Joback Method
$\Delta_{\text{vap}} H^\circ$	80.89	kJ/mol	Joback Method
$\log P_{\text{oct/wat}}$	9.91		Crippen Method
P_c	831.94	kPa	Joback Method
T_{boil}	968.05	K	Joback Method
T_c	1203.22	K	Joback Method
T_{fus}	578.38	K	Joback Method
V_c	1.55	m ³ /kg-mol	Joback Method

Temperature Dependent Properties

Property	Value	Unit	Temperature (K)	Source
$C_{p,\text{gas}}$	1605.16	J/mol×K	968.05	Joback Method

Sources

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

NIST Webbook: [http://webbook.nist.gov/cgi/inchi/InChI=1S/C32H56/c1-8-9-11-22\(2\)23-15-19-30\(5\)26\(23\)17-21-32\(7\)28\(30\)14-13-27-24-12-10-18-29\(3,4\)25\(24\)16-20-31\(27,32\)6/h22-28H,8-21H2,1-7H3/t22-,23-,24?,25?,26-,27?,28?,30+,31-,32-/m0/s1](http://webbook.nist.gov/cgi/inchi/InChI=1S/C32H56/c1-8-9-11-22(2)23-15-19-30(5)26(23)17-21-32(7)28(30)14-13-27-24-12-10-18-29(3,4)25(24)16-20-31(27,32)6/h22-28H,8-21H2,1-7H3/t22-,23-,24?,25?,26-,27?,28?,30+,31-,32-/m0/s1)

Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>

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).

$\log P_{oct/wat}$: 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 (m³/kg-mol).

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