Hexadecane

Other names: Cetane; n-Cetane; n-Hexadecane.
InChI: InChI=1S/C16H34/c1-3-5-7-9-11-13-15-16-14-12-10-8-6-4-2/h3-16H2,1-2H3
InChI Key: DCAYPVUWAIABOU-UHFFFAOYSA-N
Formula: C16H34
SMILES: CCCCCCCCCCCCCCCC
Molecular Weight: 226.44
CAS: 544-76-3

Physical Properties

Property	Value	Unit	Source
$\Delta_c H°_{liquid}$	-10699.10 ± 1.80	kJ/mol	NIST Webbook
$\Delta_c H°_{liquid}$	-10699.10 ± 4.10	kJ/mol	NIST Webbook
$\Delta_f G°$	83.84	kJ/mol	Joback Method
$\Delta_f H°_{gas}$	-374.90	kJ/mol	NIST Webbook
$\Delta_f H°_{gas}$	-374.70	kJ/mol	NIST Webbook
$\Delta_f H°_{liquid}$	-456.30 ± 2.00	kJ/mol	NIST Webbook
$\Delta_f H°_{liquid}$	-456.10 ± 4.10	kJ/mol	NIST Webbook
$\Delta_{fus} H°$	37.20	kJ/mol	Joback Method
$\Delta_{sub} H°$	135.10	kJ/mol	NIST Webbook
$\Delta_{vap} H°$	81.38	kJ/mol	NIST Webbook
$\Delta_{vap} H°$	81.80 ± 1.30	kJ/mol	NIST Webbook
$\Delta_{vap} H°$	81.40	kJ/mol	NIST Webbook
$\Delta_{vap} H°$	81.40	kJ/mol	NIST Webbook
$\Delta_{vap} H°$	81.20	kJ/mol	NIST Webbook
$\Delta_{vap} H°$	81.40	kJ/mol	NIST Webbook
$\Delta_{vap} H°$	81.40 ± 0.40	kJ/mol	NIST Webbook
$\Delta_{vap} H°$	81.10	kJ/mol	NIST Webbook

Property	Value	Unit	Source
$\Delta_{vap}H°$	80.60 ± 1.50	kJ/mol	NIST Webbook
$logP_{oct/wat}$	6.49		Crippen Method
P_c	1400.00 ± 200.00	kPa	NIST Webbook
P_c	1401.00 ± 50.00	kPa	NIST Webbook
$S°_{gas}$	778.31	J/mol×K	NIST Webbook
$S°_{liquid}$	586.18	J/mol×K	NIST Webbook
$S°_{liquid}$	626.80	J/mol×K	NIST Webbook
T_{boil}	560.20	K	NIST Webbook
T_{boil}	559.00 ± 2.00	K	NIST Webbook
T_{boil}	559.92 ± 0.20	K	NIST Webbook
T_{boil}	553.00 ± 5.00	K	NIST Webbook
T_{boil}	556.00 ± 6.00	K	NIST Webbook
T_{boil}	561.00 ± 4.00	K	NIST Webbook
T_{boil}	548.00 ± 5.00	K	NIST Webbook
T_{boil}	543.00 ± 8.00	K	NIST Webbook
T_{boil}	547.00 ± 5.00	K	NIST Webbook
T_{boil}	551.00 ± 5.00	K	NIST Webbook
T_c	723.00 ± 2.00	K	NIST Webbook
T_c	723.00 ± 1.90	K	NIST Webbook
T_c	722.40 ± 1.10	K	NIST Webbook
T_c	723.00 ± 1.20	K	NIST Webbook
T_c	722.60	K	NIST Webbook
T_c	721.70 ± 2.00	K	NIST Webbook
T_c	723.00 ± 2.00	K	NIST Webbook
T_c	723.00 ± 3.00	K	NIST Webbook
T_c	717.15 ± 3.00	K	NIST Webbook
T_{fus}	291.27 ± 0.02	K	NIST Webbook
T_{fus}	291.32 ± 0.20	K	NIST Webbook

Property	Value	Unit	Source
T_{fus}	291.19 ± 0.05	K	NIST Webbook
T_{fus}	291.15 ± 0.50	K	NIST Webbook
T_{fus}	291.00 ± 0.30	K	NIST Webbook
T_{fus}	291.33 ± 0.10	K	NIST Webbook
T_{fus}	291.25 ± 0.10	K	NIST Webbook
T_{fus}	290.00 ± 1.66	K	NIST Webbook
T_{fus}	291.00 ± 2.00	K	NIST Webbook
T_{fus}	291.29 ± 0.02	K	NIST Webbook
T_{fus}	291.29 ± 0.02	K	NIST Webbook
T_{fus}	291.30 ± 0.01	K	NIST Webbook
T_{fus}	291.30 ± 0.06	K	NIST Webbook
T_{fus}	291.30 ± 0.04	K	NIST Webbook
T_{fus}	291.31 ± 0.02	K	NIST Webbook
T_{fus}	291.00 ± 2.00	K	NIST Webbook
T_{fus}	290.00 ± 3.00	K	NIST Webbook
T_{fus}	291.21 ± 0.15	K	NIST Webbook
T_{fus}	291.24 ± 0.10	K	NIST Webbook
T_{fus}	291.24 ± 0.20	K	NIST Webbook
T_{fus}	290.80 ± 0.50	K	NIST Webbook
T_{fus}	291.29 ± 0.02	K	NIST Webbook
T_{fus}	291.29 ± 0.01	K	NIST Webbook
T_{fus}	291.24 ± 0.10	K	NIST Webbook
T_{fus}	293.00 ± 0.60	K	NIST Webbook
T_{fus}	291.30 ± 0.02	K	NIST Webbook
T_{fus}	291.20 ± 0.60	K	NIST Webbook
T_{fus}	290.40 ± 1.50	K	NIST Webbook
T_{fus}	291.20 ± 0.40	K	NIST Webbook
T_{fus}	291.00 ± 2.00	K	NIST Webbook

Property	Value	Unit	Source
T_{fus}	291.33 ± 0.20	K	NIST Webbook
T_{fus}	291.30 ± 0.30	K	NIST Webbook
T_{fus}	290.60 ± 0.50	K	NIST Webbook
T_{fus}	291.29 ± 0.10	K	NIST Webbook
T_{fus}	293.00 ± 3.00	K	NIST Webbook
T_{fus}	292.40 ± 0.50	K	NIST Webbook
T_{fus}	290.20 ± 2.00	K	NIST Webbook
T_{fus}	291.00 ± 0.60	K	NIST Webbook
T_{fus}	288.00 ± 3.00	K	NIST Webbook
T_{fus}	291.05 ± 0.40	K	NIST Webbook
T_{fus}	290.10 ± 0.50	K	NIST Webbook
T_{fus}	290.98 ± 0.30	K	NIST Webbook
T_{fus}	288.69 ± 2.00	K	NIST Webbook
T_{fus}	290.70 ± 2.00	K	NIST Webbook
T_{fus}	291.26 ± 0.20	K	NIST Webbook
T_{fus}	290.00 ± 2.00	K	NIST Webbook
T_{fus}	291.26 ± 0.20	K	NIST Webbook
T_{fus}	291.00 ± 2.00	K	NIST Webbook
T_{fus}	293.00 ± 2.00	K	NIST Webbook
T_{fus}	293.00 ± 2.00	K	NIST Webbook
T_{fus}	291.40 ± 2.00	K	NIST Webbook
T_{fus}	292.00 ± 3.00	K	NIST Webbook
T_{fus}	291.00 ± 3.00	K	NIST Webbook
T_{fus}	291.00 ± 2.00	K	NIST Webbook
T_{triple}	291.33 ± 0.05	K	NIST Webbook
T_{triple}	291.32 ± 0.60	K	NIST Webbook
T_{triple}	291.34 ± 0.02	K	NIST Webbook
T_{triple}	291.33 ± 0.40	K	NIST Webbook

Property	Value	Unit	Source
T_{triple}	291.32 ± 0.40	K	NIST Webbook
T_{triple}	291.32 ± 0.20	K	NIST Webbook
T_{triple}	291.34 ± 0.20	K	NIST Webbook
T_{triple}	291.33 ± 0.10	K	NIST Webbook
T_{triple}	291.10 ± 0.20	K	NIST Webbook
V_c	1.03	m^3/kg-mol	NIST Webbook

Temperature Dependent Properties

Property	Value	Unit	Temperature (K)	Source
$C_{p,gas}$	611.73	J/mol×K	565.48	Joback Method
$C_{p,liquid}$	499.00	J/mol×K	297.79	NIST Webbook
$C_{p,liquid}$	498.30	J/mol×K	298.0	NIST Webbook
$C_{p,liquid}$	499.72	J/mol×K	298.15	NIST Webbook
$C_{p,liquid}$	497.16	J/mol×K	298.15	NIST Webbook
$C_{p,liquid}$	499.62	J/mol×K	298.15	NIST Webbook
$C_{p,liquid}$	500.21	J/mol×K	298.15	NIST Webbook
$C_{p,liquid}$	500.21	J/mol×K	298.15	NIST Webbook
$C_{p,liquid}$	499.62	J/mol×K	298.15	NIST Webbook
$C_{p,liquid}$	495.73	J/mol×K	298.15	NIST Webbook
$C_{p,liquid}$	496.45	J/mol×K	298.15	NIST Webbook
$C_{p,liquid}$	499.97	J/mol×K	298.15	NIST Webbook
$C_{p,liquid}$	501.60	J/mol×K	298.15	NIST Webbook
$C_{p,liquid}$	504.58	J/mol×K	298.15	NIST Webbook
$C_{p,liquid}$	501.45	J/mol×K	298.15	NIST Webbook
$C_{p,liquid}$	504.20	J/mol×K	298.15	NIST Webbook
$C_{p,liquid}$	484.90	J/mol×K	311.0	NIST Webbook
$C_{p,liquid}$	512.37	J/mol×K	313.15	NIST Webbook

Property	Value	Unit	Temperature (K)	Source
η	0.00	Pa×s	565.48	Joback Method
$\Delta_{fus}H$	51.46	kJ/mol	291.1	NIST Webbook
$\Delta_{fus}H$	53.35	kJ/mol	291.3	NIST Webbook
$\Delta_{sub}H$	80.00 ± 3.00	kJ/mol	288.0	NIST Webbook
$\Delta_{sub}H$	83.00 ± 8.00	kJ/mol	289.0	NIST Webbook
$\Delta_{sub}H$	134.90	kJ/mol	291.0	NIST Webbook
$\Delta_{vap}H$	80.20	kJ/mol	300.5	NIST Webbook
$\Delta_{vap}H$	93.40	kJ/mol	311.5	NIST Webbook
$\Delta_{vap}H$	66.90	kJ/mol	343.0	NIST Webbook
$\Delta_{vap}H$	66.20	kJ/mol	353.0	NIST Webbook
$\Delta_{vap}H$	65.60	kJ/mol	363.0	NIST Webbook
$\Delta_{vap}H$	74.90	kJ/mol	373.0	NIST Webbook
$\Delta_{vap}H$	64.90	kJ/mol	373.0	NIST Webbook
$\Delta_{vap}H$	64.20	kJ/mol	383.0	NIST Webbook
$\Delta_{vap}H$	65.70	kJ/mol	455.5	NIST Webbook
$\Delta_{vap}H$	68.50	kJ/mol	488.0	NIST Webbook
$\Delta_{vap}H$	61.70	kJ/mol	515.0	NIST Webbook
$\Delta_{vap}H$	59.80	kJ/mol	547.0	NIST Webbook
$\Delta_{fus}S$	176.79	J/mol×K	291.1	NIST Webbook
$\Delta_{fus}S$	183.13	J/mol×K	291.3	NIST Webbook

Sources

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

NIST Webbook: http://webbook.nist.gov/cgi/inchi/InChI=1S/C16H34/c1-3-5-7-9-11-13-15-16-14-12-10-8-6-4-2/h3-16H2,1-2H3

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

Legend

Δ_c**H°**$_{liquid}$: Standard liquid enthalpy of combustion (kJ/mol).
C$_{p,gas}$: Ideal gas heat capacity (J/mol×K).
C$_{p,liquid}$: Liquid phase heat capacity (J/mol×K).
η: Dynamic viscosity (Pa×s).
Δ_f**G°**: Standard Gibbs free energy of formation (kJ/mol).
Δ_f**H°**$_{gas}$: Enthalpy of formation at standard conditions (kJ/mol).
Δ_f**H°**$_{liquid}$: Liquid phase enthalpy of formation at standard conditions (kJ/mol).
Δ_{fus}**H°**: Enthalpy of fusion at standard conditions (kJ/mol).
Δ_{fus}**H**: Enthalpy of fusion at a given temperature (kJ/mol).
Δ_{sub}**H°**: Enthalpy of sublimation at standard conditions (kJ/mol).
Δ_{sub}**H**: Enthalpy of sublimation at a given temperature (kJ/mol).
Δ_{vap}**H°**: Enthalpy of vaporization at standard conditions (kJ/mol).
Δ_{vap}**H**: Enthalpy of vaporization at a given temperature (kJ/mol).
***log*P**$_{oct/wat}$: Octanol/Water partition coefficient .
P$_c$: Critical Pressure (kPa).
Δ_{fus}**S**: Entropy of fusion at a given temperature (J/mol×K).
S°$_{gas}$: Molar entropy at standard conditions (J/mol×K).
S°$_{liquid}$: Liquid phase molar entropy at standard conditions (J/mol×K).
T$_{boil}$: Normal Boiling Point Temperature (K).
T$_c$: Critical Temperature (K).
T$_{fus}$: Normal melting (fusion) point (K).
T$_{triple}$: Triple Point Temperature (K).
V$_c$: Critical Volume (m^3/kg-mol).