n-Docosane

Other names: Normal-docosane; n-Docosane.
InChI: InChI=1S/C22H46/c1-3-5-7-9-11-13-15-17-19-21-22-20-18-16-14-12-10-8-6-4-2/h3-22H2,1-2H3
InChI Key: HOWGUJZVBDQJKV-UHFFFAOYSA-N
Formula: C22H46
SMILES: CCCCCCCCCCCCCCCCCCCCCC
Molecular Weight: 310.60
CAS: 629-97-0

Physical Properties

Property	Value	Unit	Source
$\Delta_f G°$	134.36	kJ/mol	Joback Method
$\Delta_f H°_{gas}$	-497.41	kJ/mol	Joback Method
$\Delta_{fus} H°$	52.74	kJ/mol	Joback Method
$\Delta_{vap} H°$	111.90	kJ/mol	NIST Webbook
$\Delta_{vap} H°$	114.90 ± 0.30	kJ/mol	NIST Webbook
$\Delta_{vap} H°$	115.60 ± 1.90	kJ/mol	NIST Webbook
$\Delta_{vap} H°$	115.60	kJ/mol	NIST Webbook
$logP_{oct/wat}$	8.83		Crippen Method
P_c	1000.00 ± 200.00	kPa	NIST Webbook
P_c	982.00 ± 40.00	kPa	NIST Webbook
T_{boil}	641.80	K	NIST Webbook
T_c	786.00 ± 8.00	K	NIST Webbook
T_c	785.60 ± 3.00	K	NIST Webbook
T_c	763.15 ± 10.00	K	NIST Webbook
T_{fus}	317.05 ± 0.30	K	NIST Webbook
T_{fus}	316.74 ± 0.07	K	NIST Webbook
T_{fus}	316.85 ± 0.15	K	NIST Webbook

Property	Value	Unit	Source
T_{fus}	316.00 ± 0.10	K	NIST Webbook
T_{fus}	316.05 ± 1.00	K	NIST Webbook
T_{fus}	317.30 ± 0.20	K	NIST Webbook
T_{fus}	316.93 ± 0.25	K	NIST Webbook
T_{fus}	318.30 ± 3.00	K	NIST Webbook
T_{fus}	317.07 ± 0.40	K	NIST Webbook
T_{fus}	314.00 ± 4.00	K	NIST Webbook
T_{fus}	317.20 ± 0.30	K	NIST Webbook
T_{fus}	317.06 ± 0.20	K	NIST Webbook
T_{fus}	317.60 ± 0.60	K	NIST Webbook
T_{fus}	317.30 ± 0.60	K	NIST Webbook
T_{fus}	317.00 ± 2.00	K	NIST Webbook
T_{fus}	317.00 ± 0.30	K	NIST Webbook
T_{fus}	317.00 ± 2.00	K	NIST Webbook
T_{fus}	317.70 ± 0.70	K	NIST Webbook
T_{fus}	317.70 ± 2.00	K	NIST Webbook
T_{fus}	313.20 ± 3.00	K	NIST Webbook
T_{fus}	317.70 ± 0.80	K	NIST Webbook
T_{fus}	315.80 ± 4.00	K	NIST Webbook
T_{fus}	317.40 ± 0.70	K	NIST Webbook
T_{fus}	317.60 ± 1.00	K	NIST Webbook
T_{fus}	317.00 ± 2.00	K	NIST Webbook
T_{fus}	317.60 ± 0.80	K	NIST Webbook
T_{fus}	317.60 ± 3.00	K	NIST Webbook
T_{fus}	317.55 ± 1.00	K	NIST Webbook
T_{triple}	315.20 ± 1.00	K	NIST Webbook
V_c	1.27	m^3/kg-mol	Joback Method

Temperature Dependent Properties

Property	Value	Unit	Temperature (K)	Source
$C_{p,gas}$	962.02	J/mol×K	702.76	Joback Method
$C_{p,liquid}$	739.00	J/mol×K	353.0	NIST Webbook
$C_{p,solid}$	563.60	J/mol×K	299.0	NIST Webbook
$C_{p,solid}$	468.00	J/mol×K	300.0	NIST Webbook
η	0.00	Pa×s	702.76	Joback Method
$\Delta_{fus}H$	29.51	kJ/mol	315.2	NIST Webbook
$\Delta_{fus}H$	47.84	kJ/mol	316.1	NIST Webbook
$\Delta_{sub}H$	172.60 ± 2.00	kJ/mol	391.0	NIST Webbook
$\Delta_{vap}H$	124.00 ± 2.00	kJ/mol	391.0	NIST Webbook
$\Delta_{vap}H$	100.90	kJ/mol	407.5	NIST Webbook
$\Delta_{vap}H$	89.90	kJ/mol	424.0	NIST Webbook
$\Delta_{vap}H$	84.30	kJ/mol	513.0	NIST Webbook
$\Delta_{vap}H$	91.30	kJ/mol	536.5	NIST Webbook
$\Delta_{fus}S$	93.62	J/mol×K	315.2	NIST Webbook
$\Delta_{fus}S$	151.36	J/mol×K	316.1	NIST Webbook

Sources

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

NIST Webbook: http://webbook.nist.gov/cgi/inchi/InChI=1S/C22H46/c1-3-5-7-9-11-13-15-17-19-21-22-20-18-16-14-12-10-8-6-4-2/h3-22H2,1-2H3

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

Legend

$C_{p,gas}$: Ideal gas heat capacity (J/mol×K).
$C_{p,liquid}$: Liquid phase heat capacity (J/mol×K).
$C_{p,solid}$: Solid phase heat capacity (J/mol×K).
η: Dynamic viscosity (Pa×s).
Δ_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).
$\Delta_{fus} H$: Enthalpy of fusion at a given temperature (kJ/mol).
$\Delta_{sub} H$: Enthalpy of sublimation at a given temperature (kJ/mol).
$\Delta_{vap} H°$: Enthalpy of vaporization at standard conditions (kJ/mol).
$\Delta_{vap} H$: Enthalpy of vaporization at a given temperature (kJ/mol).
$log P_{oct/wat}$: Octanol/Water partition coefficient .
P_c: Critical Pressure (kPa).
$\Delta_{fus} S$: Entropy of fusion at a given temperature (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).