

INFN - Istituto Nazionale di Fisica Nucleare
Laboratori Nazionali del Gran Sasso

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**PHYSICS AND THERMODYNAMIC DATA OF n-PENTANE, n-HEXANE
AND PESUDOCUMENE**

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Many detectors being installed at L.N.G.S. are essentially an assembly of limited streamer tubes and/or oil based liquid scintillators. Therefore we think that a short collection of Physical and thermodynamical data on :

n-Pentane,

n-Hexane,

Pseudocumene,

could be of some use for experimental physicists for quick consultation.

Data are shown in tables and they include :

- simple physical properties,
- physical and thermodynamic sizes in relation to temperature in different aggregation states of the substance.

In this note, sizes in relation to temperature are though to be reported in a graphical style, to have a more clear representation. There are also tables with factors of conversion to modify data onto wished sizes. Macintosh disks, containing the same data, are available.

Literature reports many of these data for gases on handbooks and technical papers e.g : Perry's Chemist and Engineer handbook (1), CRC Physic and Chemist handbook (2), Lange's Chemist handbook (3), etc.

TRC Thermodynamic Tables-Hydrocarbons is a collection of 11 volumes, which have been collected in a lot of working years by "Thermodynamic Research Center in the "Texas A & M University System, College Station, TX 77843-3111 U.S.A.

In the past, the TRC was interested in a detailed research of these data, to get precise informations about physical, thermodynamical and spectral properties of hydrocarbons and respective sulphurs and nitrogen derivative, as present in the coal or in the oil. Therefore, a very rich collection is derived from that.

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N-PENTANE, LOW VAPOR PRESSURE AND BOILING POINTS AT 0.0004 TO 10 mmHg

State	T	0.0004	0.0006	0.0008	0.0010	0.0020	0.0040	0.0060
c	P	-131.00						
liq	P		-129.90	-128.50	-127.30	-123.60	-119.70	-117.30
	T	0.0080	0.0100	0.0200	0.0400	0.0600	0.0800	0.1000
liq	P	-115.50	-114.10	-109.50	-104.70	-101.70	-99.50	-97.70
	T	0.2000	0.4000	0.6000	0.8000	1.00	2.00	3.00
liq	P	-92.00	-85.90	-82.10	-79.30	-77.10	-69.70	-65.10
	T	4.0000	5.0000	6.0000	7.0000	8.0000	10.0000	
liq	P	-61.70	-59.03	-56.76	-54.79	-53.05	-50.09	

T = Temperature in °C

P = vapor pressures in mmHg

c = n-Pentane Crystal state

liq = n-Pentane Liquid state

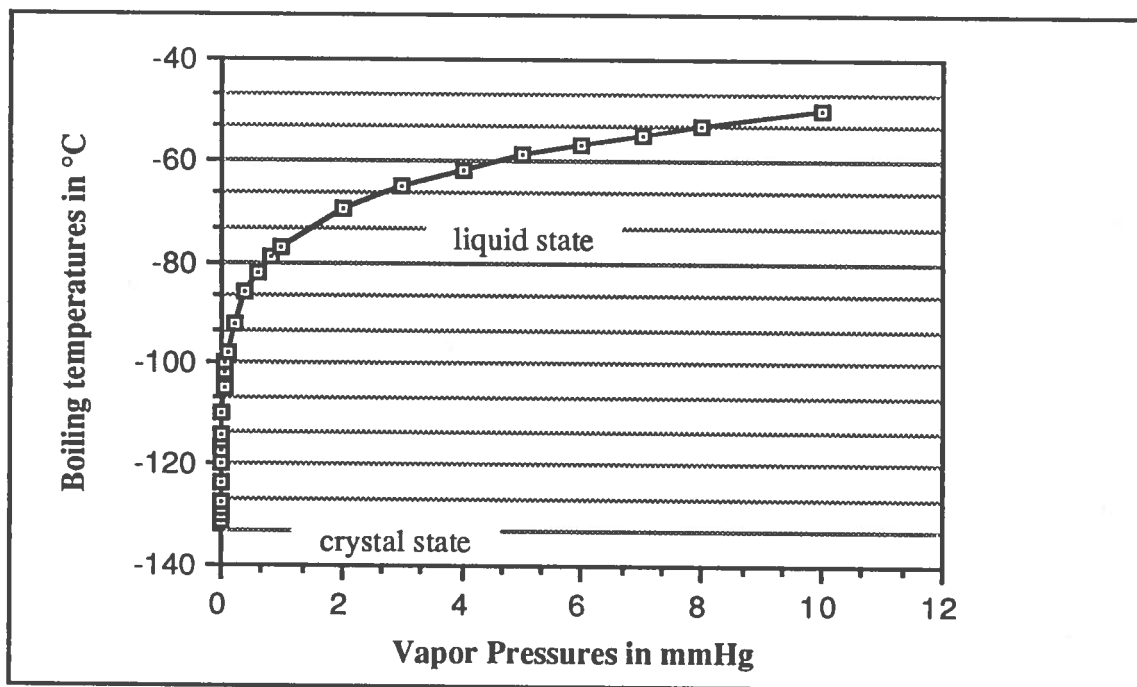
Values of the vapor pressures are calculated from the following constants :

A = 11.5845; B = 2005.0; C = 265.0 (for the Crystal state)

A = 7.5646; B = 1339.4; C = 254.12 (for the Liquid state)

and the Antoine equation:

$\log_{10}P = A - B / (C+T)$; $T = B / (A - \log_{10}P) - C$; (P in mmHg; T in °C)



**N-PENTANE, VAPOR PRESSURES AND BOILING POINT,
AT 10 TO 1500 mmHg**

State	T	10	20	30	40	50	60	80
liq	P	-50.080	-40.220	-33.930	-29.220	-25.410	-22.180	-16.890
	T	100	150	200	250	300	400	500
liq	P	-12.591	-4.330	+1.920	7.008	11.333	18.486	24.329
	T	600	700	720	740	750	760	770
liq	P	29.311	33.676	34.489	35.285	35.677	36.065	36.448
	T	780	800	900	1000	1200	1500	
liq	P	36.828	37.577	41.110	44.360	50.160	57.590	

T = Temperature in C degrees

P = Vapor pressures, in mmHg

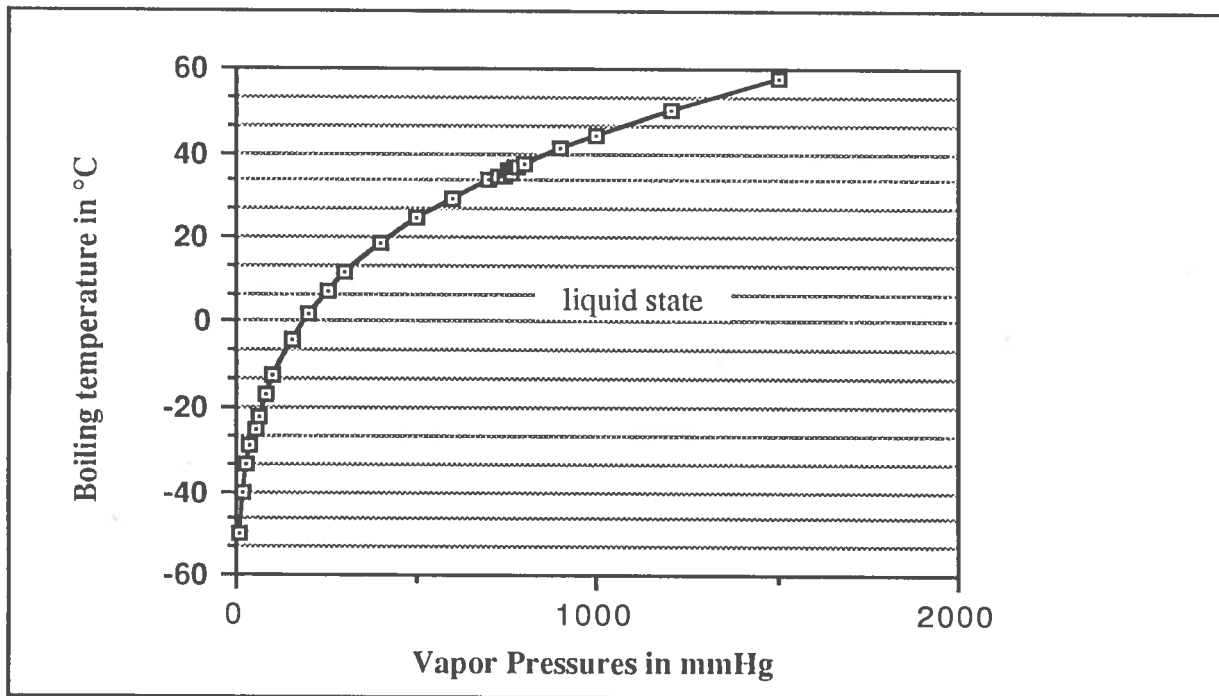
Liq = n-Pentane Liquid State

Values of the vapor pressure are calculated from the following constants :

A = 6.85296; B = 1064.84; C = 232.012

and the Antoine Equationn :

$\log_{10}P = A-B/(C+T)$; $T = B/(A-\log_{10}P) - C$; (P in mmHg, T in °C)



**LIQUID N-PENTANE, HIGH VAPOR PRESSURES (Atm)
AND BOILING POINTS (°C) ABOVE 1 ATM**

T	5.00	10.00	15.00	20.00	25.00	30.00	35.00	40.00
P	1.8285	2.1168	2.4388	2.7969	3.1936	3.6317	4.1140	4.6420
T	45.00	50.00	55.00	60.00	65.00	70.00	80.00	90.00
P	5.2210	5.8510	6.5370	7.2810	8.0860	10.9000	13.1400	15.7200
T	100.00	110.00	130.00	146.55				
P	15.7200	18.6500	25.8000	33.2800				

T = Temperature (T-T_s), in °C

P = Pressure in atm

1 atm = 1.01325 x 10⁵ Pa

Values of the saturated vapor pressures P/atm are calculated from the following constants:

A = 6.85296; B = 1064.84; C = 232.012

T^c = 469.7 K; T₀ = +44°C; T_s^a = 50 °C

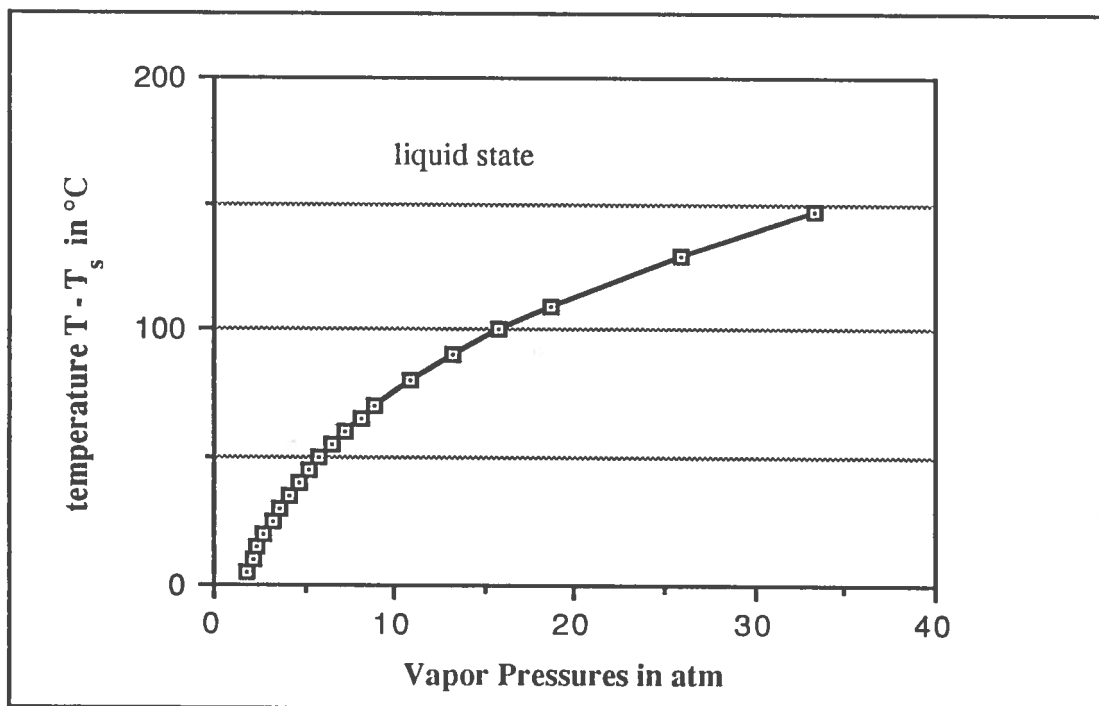
a) t_s = is a fiducial temperature, for temperature below t₀

E = 78.607 °C; F = -1782.3; n = 2.45751

and the equation for temperature t > t₀

$$\log_{10} P - (A - 2.88081) - B / (C + t) + D [(t - t_0) / T^c]^n + E [(t - t_0) / T^c]^8 + F [(t - t_0) / T^c]^{12}$$

where D = log₁₀ c = 0.434294, for t < t₀; set D = E = F = 0



**N-PENTANE, DENSITY FOR THE CONDENSED PHASES
AT ONE ATMOSPHERE OR AT EQUILIBRIUM VAPOR PRESSURE
ABOVE THE BOILING POINT.**

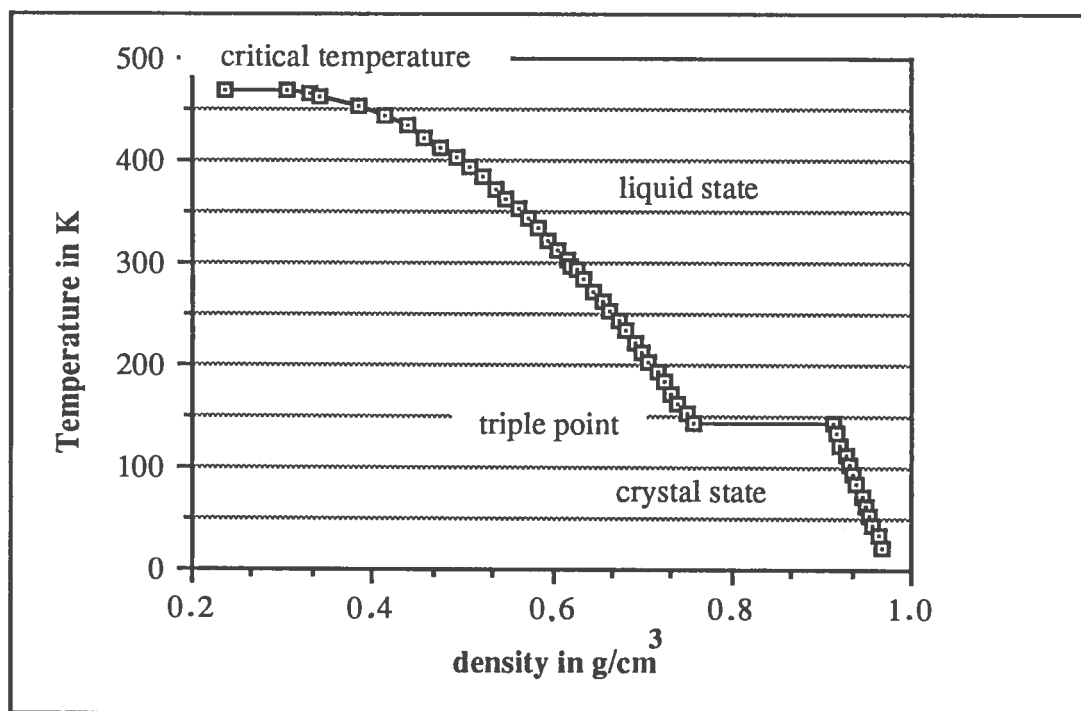
State	K	23.15	33.15	43.15	53.15	63.15	73.15	83.15
c	D	0.9660	0.9620	0.9580	0.9530	0.9490	0.9440	0.9400
	K	93.15	103.15	113.15	123.15	133.15	143.15	143.46
c	D	0.9360	0.9310	0.9270	0.9220	0.9180	0.9140	0.9140a
liq	D							0.7570a
	K	153.15	163.15	173.15	183.15	193.15	203.15	213.15
liq	D	0.7490	0.7410	0.7330	0.7250	0.7163	0.7079	0.6993
	K	223.15	233.15	243.15	253.15	263.15	273.15	283.15
liq	D	0.6907	0.6819	0.6730	0.6640	0.6548	0.6454	0.6359
	K	293.15	298.15	303.15	313.15	323.15	333.15	343.15
liq	D	0.6261	0.6212	0.6161	0.6059	0.5952	0.5843	0.5729
	K	353.15	363.15	373.15	383.15	393.15	403.15	413.15
liq	D	0.5611	0.5488	0.5359	0.5224	0.5081	0.4928	0.4762
	K	423.15	433.15	443.15	453.15	463.15	464.65	467.65
liq	D	0.4581	0.4378	0.4141	0.3850	0.3420	0.3320	0.305
	K	469.65						
liq	D	0.2370b						

K = Temperature in K

D = Density in g/cm³

c= crystal state, liq= liquid state

a) At the triple point; b) At the critical temperature



TRC

Page d-1010 table 23-2-(1.101)-d, Page 1

TRC

Page d-1011 table 23-2-(1.101)-d, page 2

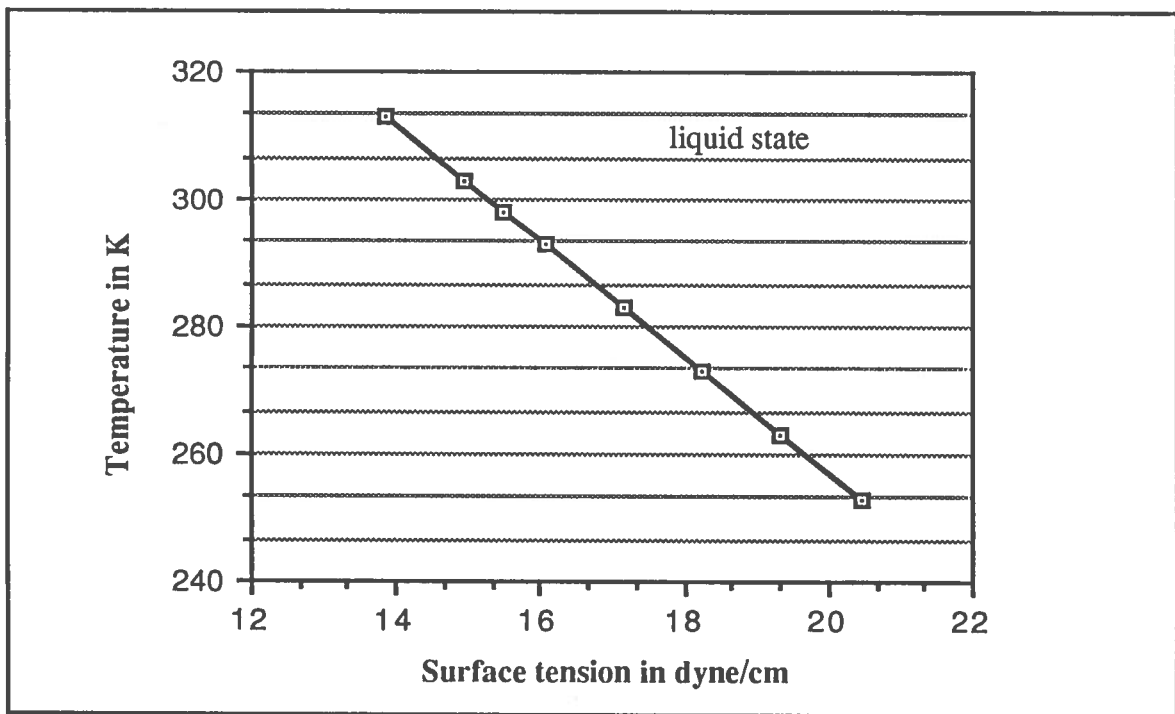
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Page d-1012 table 23-2-(1.101)-d, Page 3

**SURFACE TENSION, FOR THE N-PENTANE NORMAL LIQUID RANGE,
AT ATMOSPHERIC PRESSURE.**

K	253.15	263.15	273.15	283.15	293.15	298.15	303.15	313.15
S.T.	20.45	19.35	18.25	17.15	16.05	15.49	14.94	13.84

K = Temperature in K
S.T. = Surface Tension, in dyne/cm



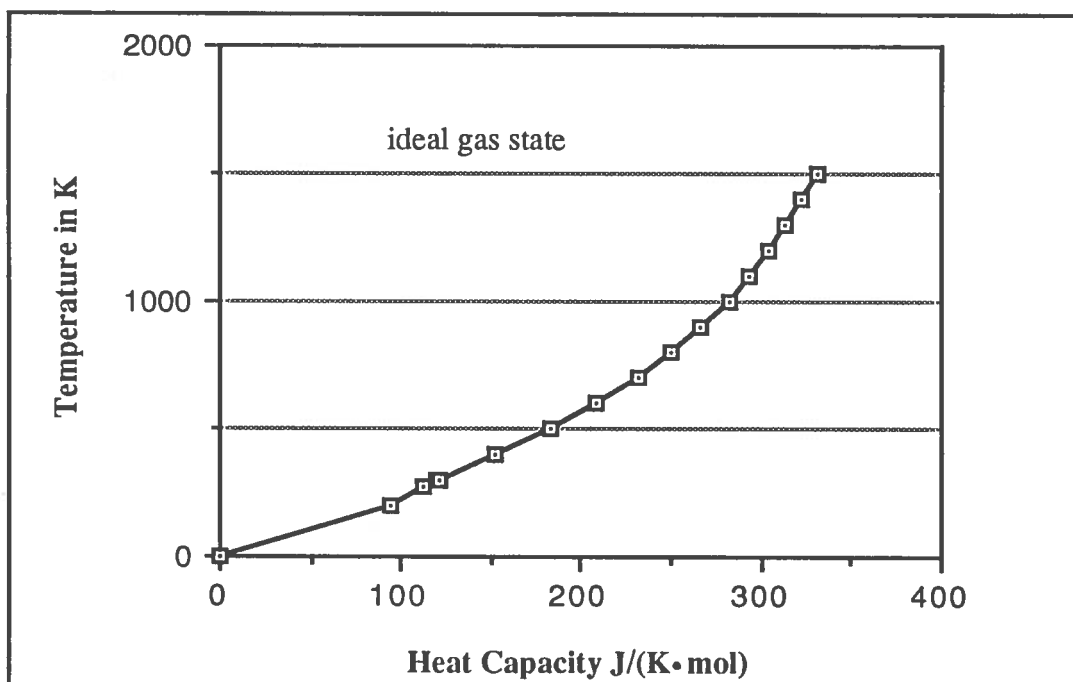
HEAT CAPACITY, " $C_p^\circ(T)$ ", FOR THE N-PENTANE IDEAL GAS STATE.

K	0	200	298.15	300	400	500	600	700
C	0	93.55	120.04	120.62	152.55	182.59	208.78	231.38
K	800	900	1000	1100	1200	1300	1400	1500
C	250.62	266.94	281.58	293.72	304.60	313.80	322.17	330.54

$C_p^\circ(T)$ is independent of pressure

K = Temperature in K

C = Heat Capacity in J/(K · mol)



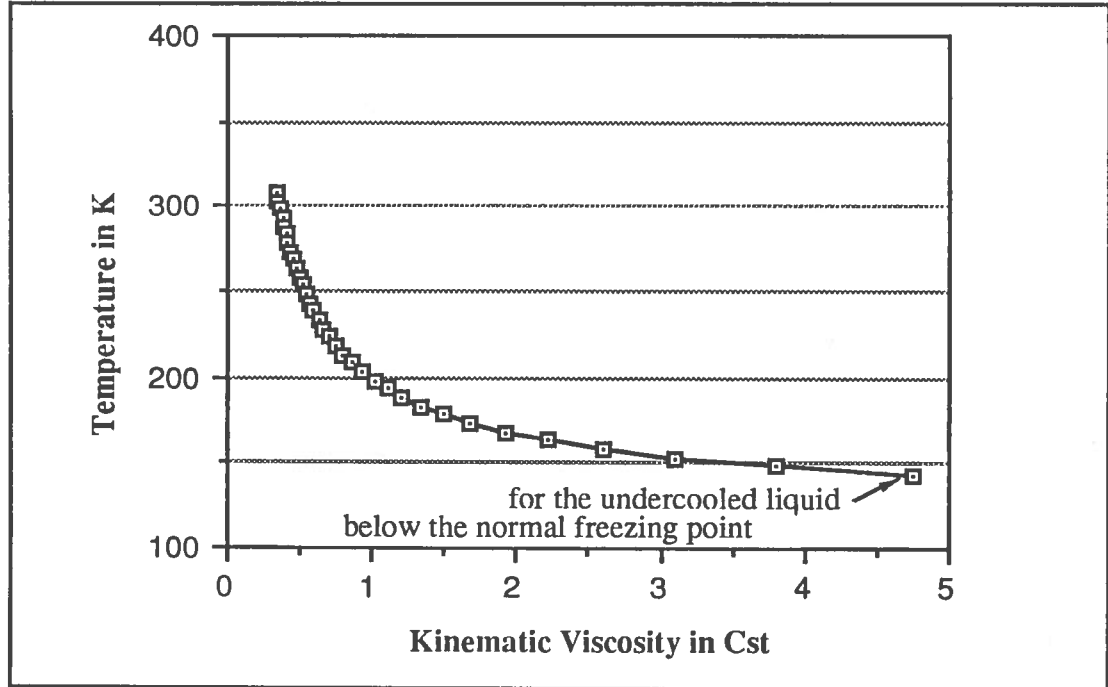
N-PENTANE, KINEMATIC VISCOSITY, FOR THE NORMAL LIQUID RANGE AT ATMOSPHERIC PRESSURE.

K	143.15	148.15	153.15	158.15	163.15	168.15	173.15	178.15
V	4.750a	3.810	3.110	2.610	2.220	1.920	1.680	1.490
K	183.15	188.15	193.15	198.15	203.15	208.15	213.15	218.15
V	1.337	1.207	1.100	1.007	0.927	0.859	0.801	0.749
K	223.15	228.15	233.15	238.15	243.15	248.15	253.15	258.15
V	0.703	0.661	0.626	0.593	0.563	0.535	0.512	0.489
K	263.15	268.15	273.15	278.15	283.15	288.15	293.15	298.15
V	0.468	0.450	0.431	0.416	0.400	0.387	0.374	0.361
K	303.15	308.15						
V	0.350	0.338						

K = Temperature in K

V = Kinematic Viscosity in Centistokes

a) For the undercooled liquid below the normal freezing point



N-PENTANE, VISCOSITY (ABSOLUTE), FOR THE NORMAL LIQUID RANGE, AT ATMOSPHERIC PRESSURE.

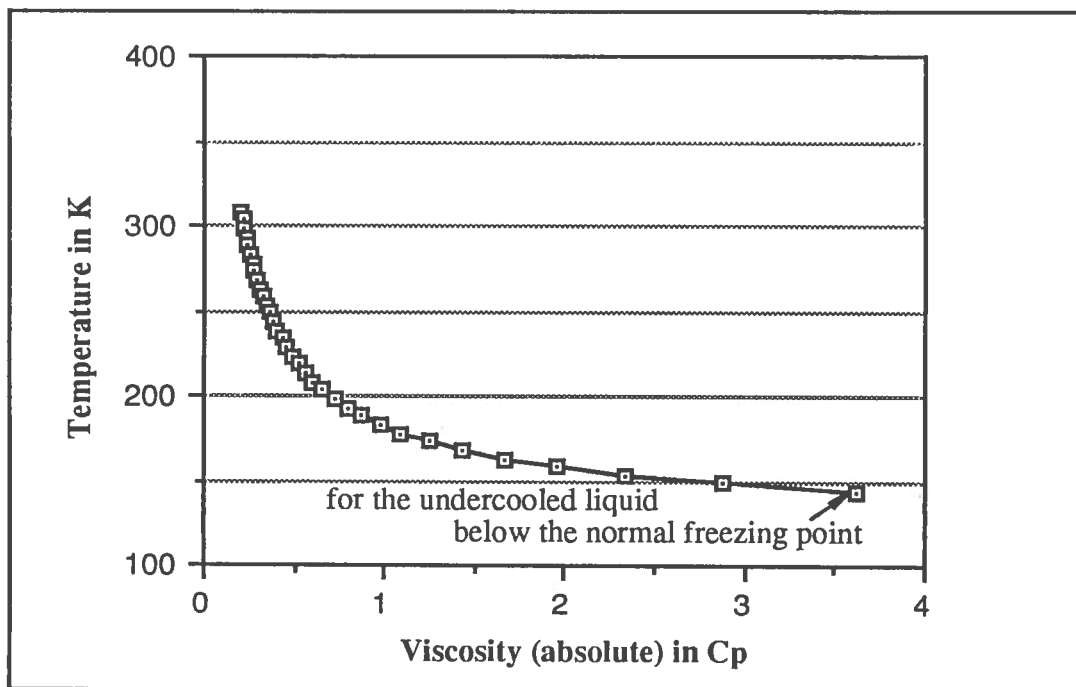
K	143.15	148.15	153.15	158.15	163.15	168.15	173.15	178.15
V	3.620b	2.880	2.340	1.950	1.660	1.430	1.240	1.090
K	183.15	188.15	193.15	198.15	203.15	208.15	213.15	218.15
V	0.970	0.871	0.789	0.718	0.657	0.605	0.560	0.520
K	223.15	228.15	233.15	238.15	243.15	248.15	253.15	258.15
V	0.486	0.454	0.427	0.402	0.379	0.358	0.340	0.322
K	263.15	268.15	273.15	278.15	283.15	288.15	293.15	298.15
V	0.306	0.292	0.278	0.266	0.254	0.244	0.234	0.224
K	303.15	308.15						
V	0.215	0.206						

K = Temperature in K

V = Absolute viscosity in Centipoises

a) The values of absolute viscosity in this table are referred to a value of 1.002 centipoises for water at 20°C. This value was adopted on July 1, 1953 by the National Bureau of Standards as the primary standard for determinations of viscosity. The American Society for Testing Materials, the National Physical Laboratory in England, and the Physikalisch-Technische Bundesanstalt in Germany have concurred in this action.

b) For the undercooled liquid below the normal freezing point.



These values are drawn from the TRC Thermodynamic Tables-Hydrocarbons

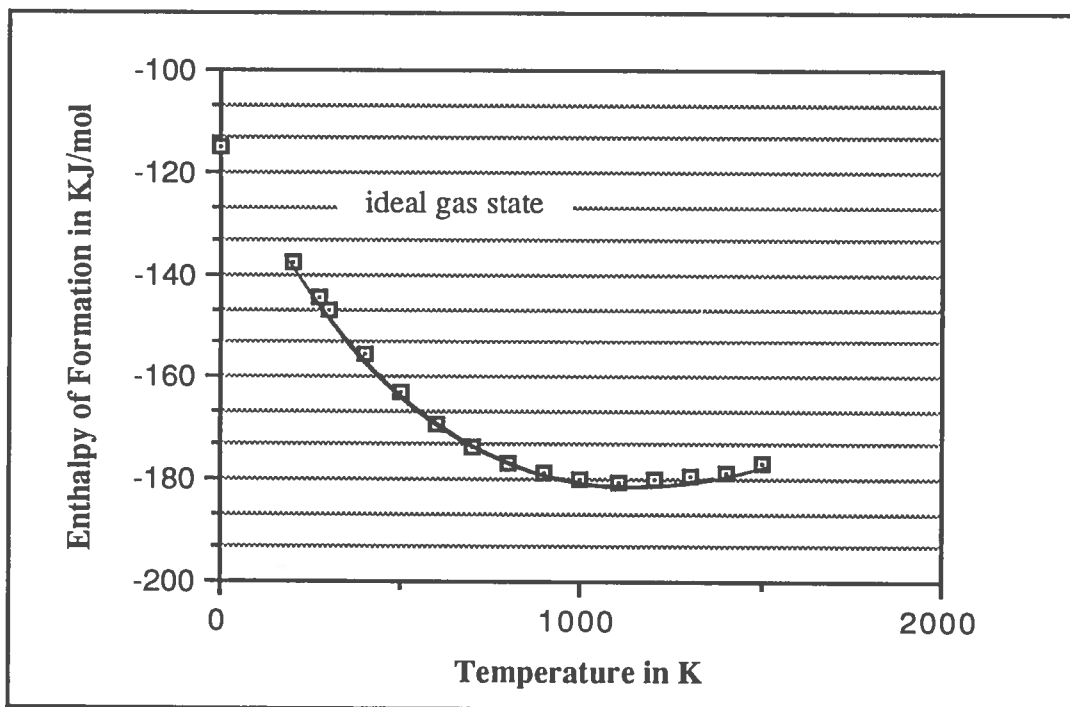
ENTHALPY OF FORMATION, " $\Delta_f H^\circ(T)$ ", FOR THE N-PENTANE IDEAL GAS STATE.

K	0	200	273.15	298.15	300	400	500	600
H	-114.89	-137.20	-144.36	-146.76	-146.95	-155.82	-163.25	-169.09
K	700	800	900	1000	1100	1200	1300	1400
H	-173.54	-176.84	-178.92	-179.94	-180.69	-180.30	-179.55	-178.44
K	1500							
H	-176.92							

$\Delta_f H^\circ(T)$ is independent of pressure

K = Temperature in K

H = Enthalpy of Formation in KJ/mol



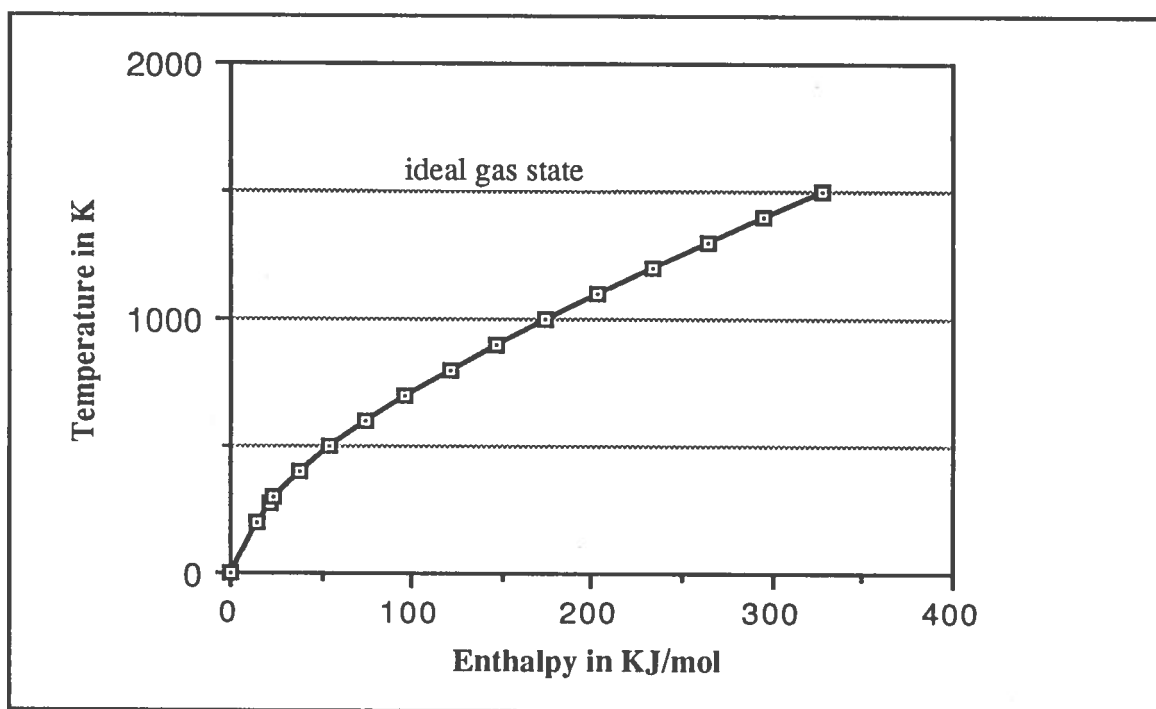
ENTHALPY, " $H^\circ(T)-H^\circ(0)$ ", FOR N-PENTANE IDEAL GAS STATE

K	0	200	273.15	298.15	300	400	500	600
H	0	13.770	21.267	24.184	24.393	38.074	54.810	74.430
K	700	800	900	1000	1100	1200	1300	1400
H	96.480	120.500	146.440	174.050	202.510	232.630	263.590	295.390
K	1500							
H	328.030							

K = Temperature in K

H = Enthalpy in KJ/mol

$H^\circ(T)-H^\circ(0)$ is independent of pressure



These values are drawn from the TRC Thermodynamic Tables-Hydrocarbons

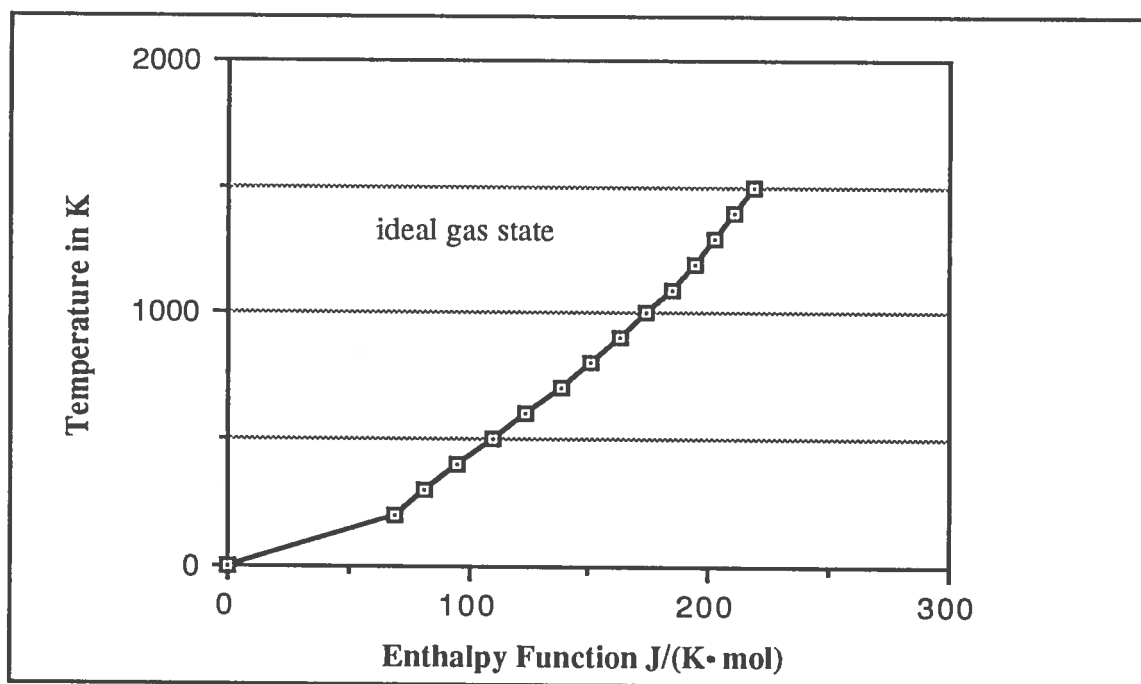
ENTHALPY FUNCTION, " $\{H^\circ(T)-H^\circ(0)\}/T$ ", FOR THE N-PENTANE IDEAL GAS STATE.

K	0	200	273.15	298.15	300	400	500	600
H	0	68.848	77.859	81.112	81.309	95.186	109.621	124.060
K	700	800	900	1000	1100	1200	1300	1400
H	137.830	150.620	162.710	174.050	184.100	193.860	202.760	210.990
K	1500							
H	218.680							

K = Temperature in K

H = Enthalpy Function in J/(K · mol)

$\{H^\circ(T)-H^\circ(0)\}/T$ is independent of pressure



These values are drawn from the TRC Thermodynamic Tables-Hydrocarbons

ENTROPY, " $S^\circ(T)-S^\circ(0)$ ", FOR N-PENTANE IDEAL GAS STATE, AT 1 BAR.

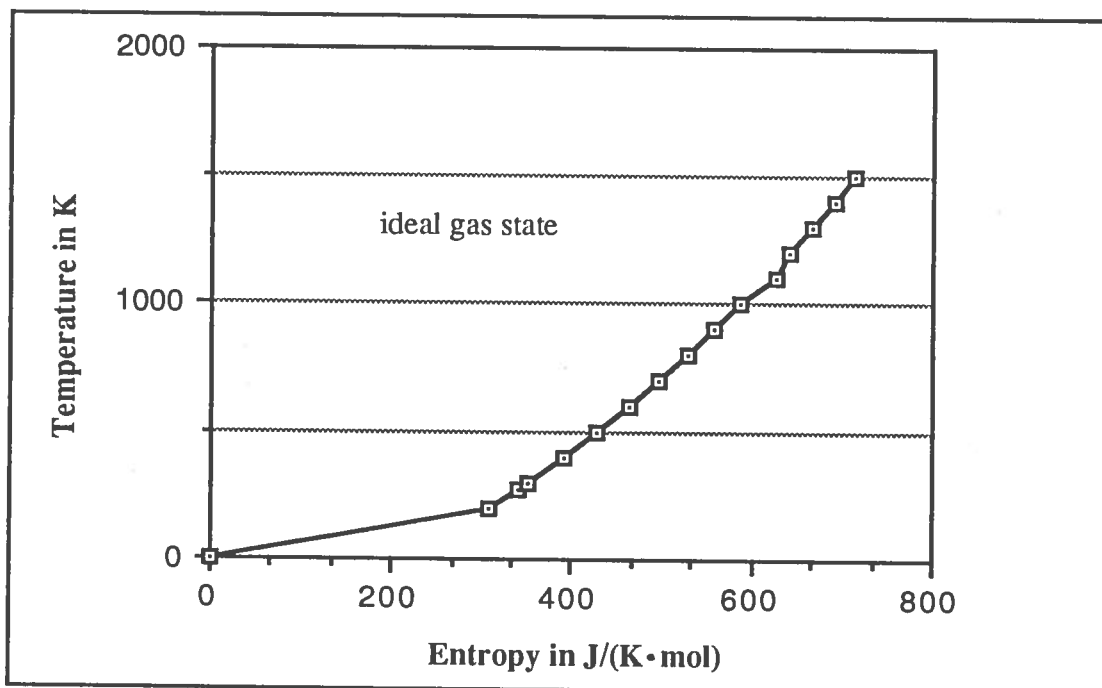
K	0	200	273.15	298.15	300	400	500	600
S	0	307.59	339.35	349.56	350.31	389.35	426.67	462.44
K	700	800	900	1000	1100	1200	1300	1400
S	496.33	528.55	559.09	587.96	624.78	641.10	666.20	689.63
K	1500							
S	712.23							

$$\{S^\circ(T)-S^\circ(0)\} \text{ (at 1 bar)} = \{S^\circ(T)-S^\circ(0)\} \text{ (at 1 atm)} + 0.109 \text{ J/(K} \cdot \text{mol)}$$

$$1 \text{ bar} = 10^5 \text{ N m}^{-2}$$

K = Temperature in K

S = Entropy in J/(K · mol)



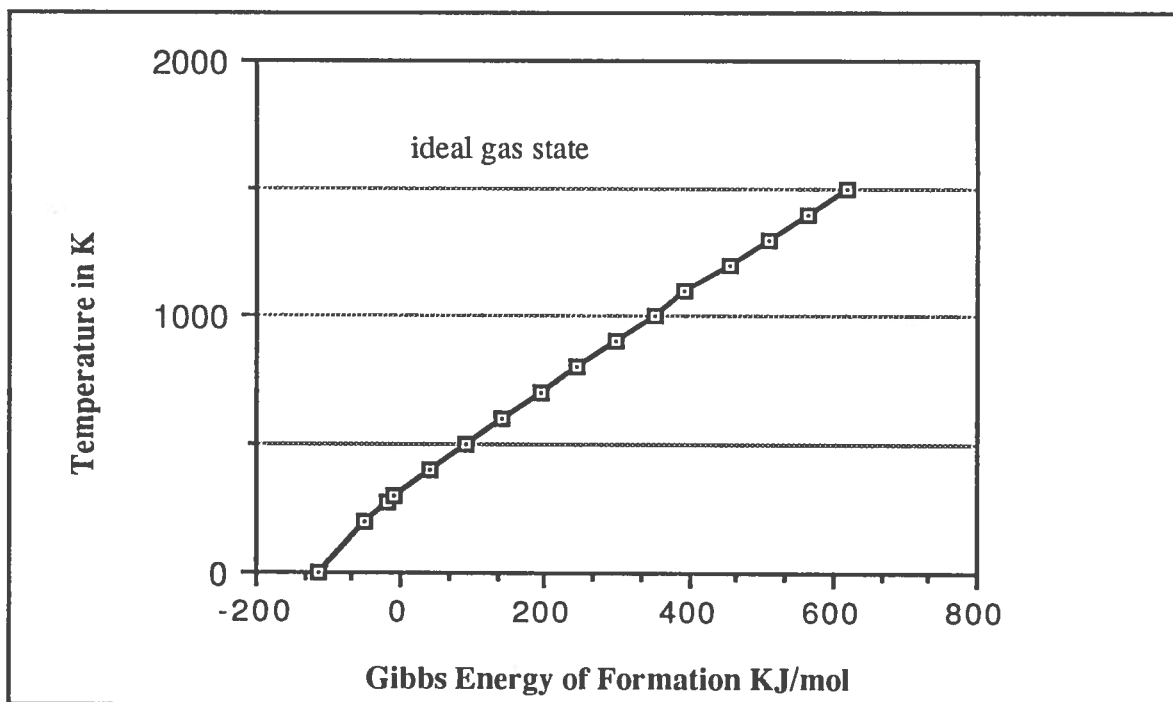
GIBBS ENERGY OF FORMATION, " $\Delta_f G^\circ(T)$ ", FOR THE N-PENTANE IDEAL GAS STATE, AT 1 BAR.

K	0	200	273.15	298.15	300	400	500	600
G	-114.89	-52.35	-20.12	-8.65	-7.81	+39.99	89.78	140.92
K	700	800	900	1000	1100	1200	1300	1400
G	193.00	245.46	298.37	351.68	394.20	458.31	511.08	564.35
K	1500							
G	617.23							

$$\Delta_f G^\circ(T, 1\text{bar}) = \Delta_f G^\circ(T, 1\text{atm}) + 0.0008755 \times T \text{ KJ/mol}$$

K = Temperature in K

G = Gibbs Energy of Formation, in KJ/mol



GIBBS ENERGY FUNCTION $-\{G^\circ(T)-H^\circ(0)\}/T$, FOR THE N-PENTANE IDEAL GAS STATE, AT 1 BAR.

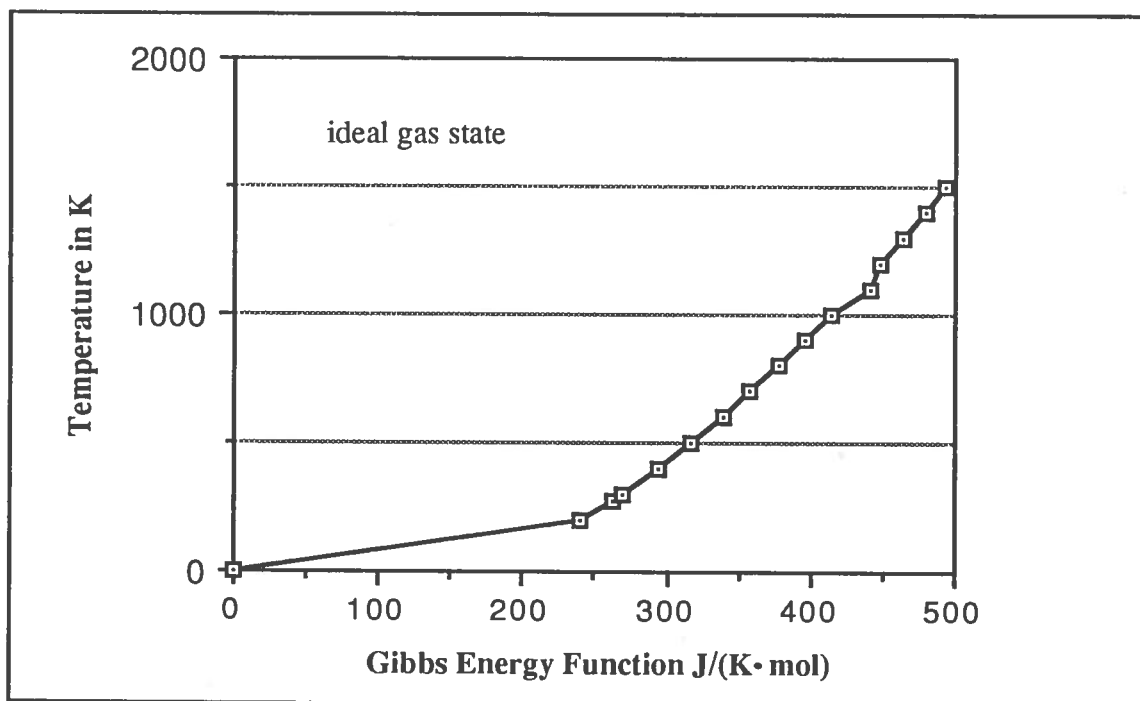
K	0	200	273.15	298.15	300	400	500	600
G	0	238.74	261.49	268.45	269.00	294.16	317.05	338.39
K	700	800	900	1000	1100	1200	1300	1400
G	358.50	377.92	396.38	413.91	440.68	447.24	463.44	478.64
K	1500							
G	493.54							

$$-\{G^\circ(T)-H^\circ(0)\}/T \text{ (at 1 bar)} = -\{G^\circ(T)-H^\circ(0)\}/T \text{ (at 1 atm)} - 0.109 \text{ J/(K} \cdot \text{mol)}$$

$$1 \text{ bar} = 10^5 \text{ N} \cdot \text{m}^{-2}$$

K = Temperature in K

G = Gibbs Energy Function in J/(K · mol)



SECOND VIRIAL COEFFICIENT, "B", FOR THE N-PENTANE GAS.

T/T ^c	0.50	0.55	0.60	0.65	0.70	0.75	0.80	0,85
B	-2620.0	-1910.0	-1470.0	1172.0	-961.0	-804.0	-684.0	-589
T/T ^c	0.90	0.95	1.00	1.10	1.20	1.30	1.40	1,60
B	-512.0	-450.0	-397.0	-314.0	-252.0	-204.0	-165.0	108,0
T/T ^c	1.8	2.0	2.5	3.0	3.5	4.0	4.5	5,0
B	-68.0	-38.0	+11.0	40.0	60.0	73.0	84.0	91,0

B = Second Virial Coefficient, in cm³/mol

T/T^c = Reduced Temperature;

K = Temperature in K

Values of the second virial coefficient B, are calculated from the following constants :

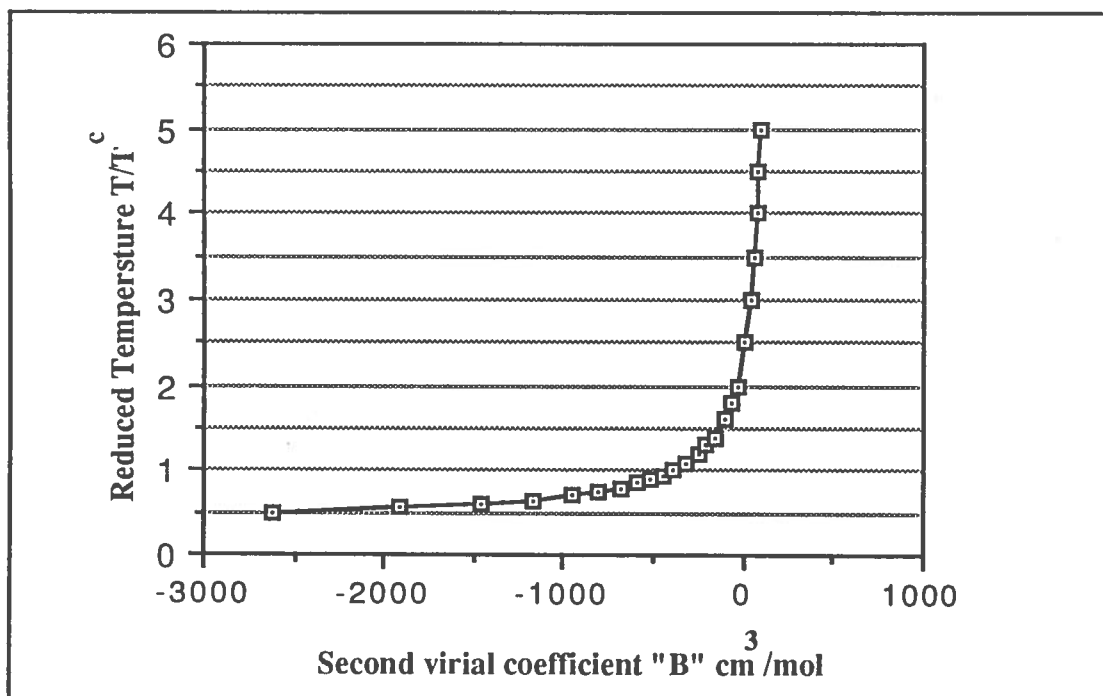
T^c = 469.6 K

u/K = -945.9 K

V* = 110.4 cm³/mol

R₁ = 110.4; R₂ = 0.680; R₃ = 4.511

and the equation :

$$B = 2V^*[R_1 - (1 - R_1)[\exp(\bar{u}/KT) - 1] - (R_2 - 1)[\exp(-\bar{u}/KT) - 1] - (R_3 - R_2)[\exp(-0.21\bar{u}/KT) - 1]$$


These values are drawn from the TRC Thermodynamic Tables-Hydrocarbons

**N-HEXANE, LOW VAPOR PRESSURES AND BOILING POINT,
AT 0.0010 TO 10 mmHg**

State	P	0.0010	0.0020	0.0040	0.0060	0.0080	0.010	0.020
c	T	-105.000	-102.000	-99.000	-97.000	-95.400		
liq	T						-92.000	-87.000
	P	0.0400	0.0600	0.0800	0.1000	0.2000	0.4000	0.6000
liq	C	-82.300	-79.300	-77.000	-75.300	-69.500	-63.100	-59.200
	P	0.8000	1.0000	2.0000	3.0000	4.0000	5.0000	6.0000
liq	C	-56.300	-53.900	-46.200	-41.300	-37.7000	-34.8000	-32.3300
	P	7.0000	8.0000	10.0000				
liq	C	-30.2100	-28.3200	-25.0900				

K = Temperature in °C

P = Vapor Pressure in mmHg

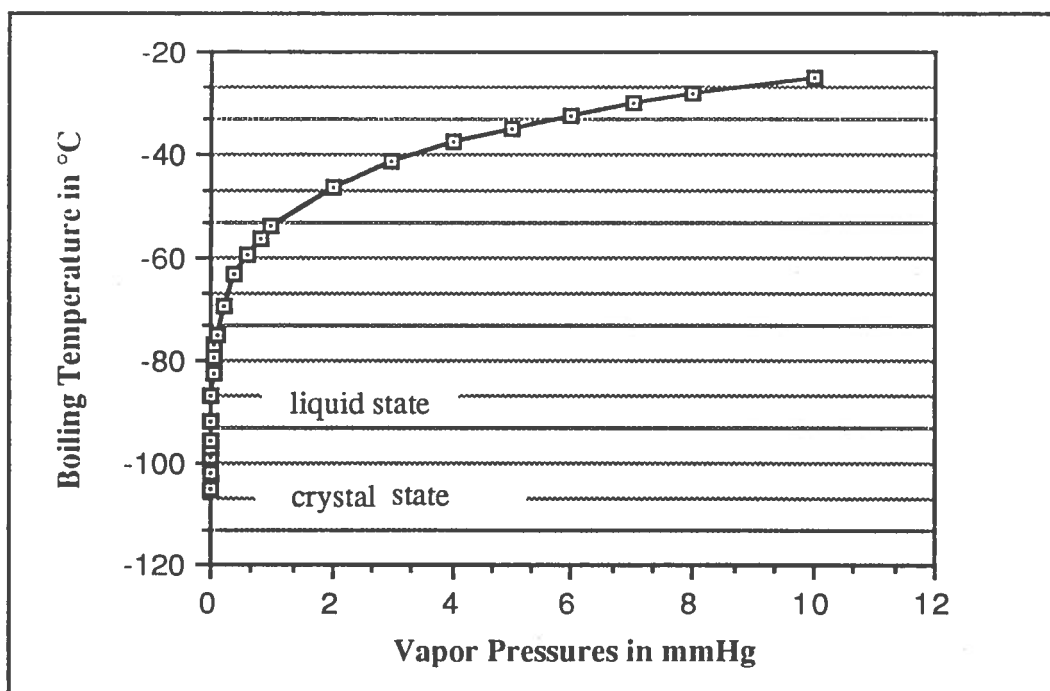
c = n-Hexane crystal state; liq = n-Hexane liquid state

Values of the vapor pressure are calculated from the following constants :

A = 11.4354; B = 2092.7; C = 250.0

and the Antoine equation :

$\log_{10}P = A - B / (C + T)$; $T = B / (A - \log_{10}P) - C$; (P in mmHg; T in °C)



N-HEXANE, VAPOR PRESSURES AND BOILING POINT, AT 10 TO 1500 mmHg.

State	P 10	20	30	40	50	60	80
liq	T -25.090	-14.330	-7.480	-2.340	+1.820	5.330	11.100
	P 100	150	200	250	400	500	600
liq	T 15.782	24.781	31.586	37.126	49.617	55.975	61.392
	P 700	720	740	750	760	770	780
liq	T 66.139	67.024	67.889	68.315	68.736	69.154	69.566
	P 800	900	1000	1200	1500		
liq	T 70.380	74.225	77.750	84.050	92.130		

P = Vapor pressures in mmHg

T = Boiling points in °C

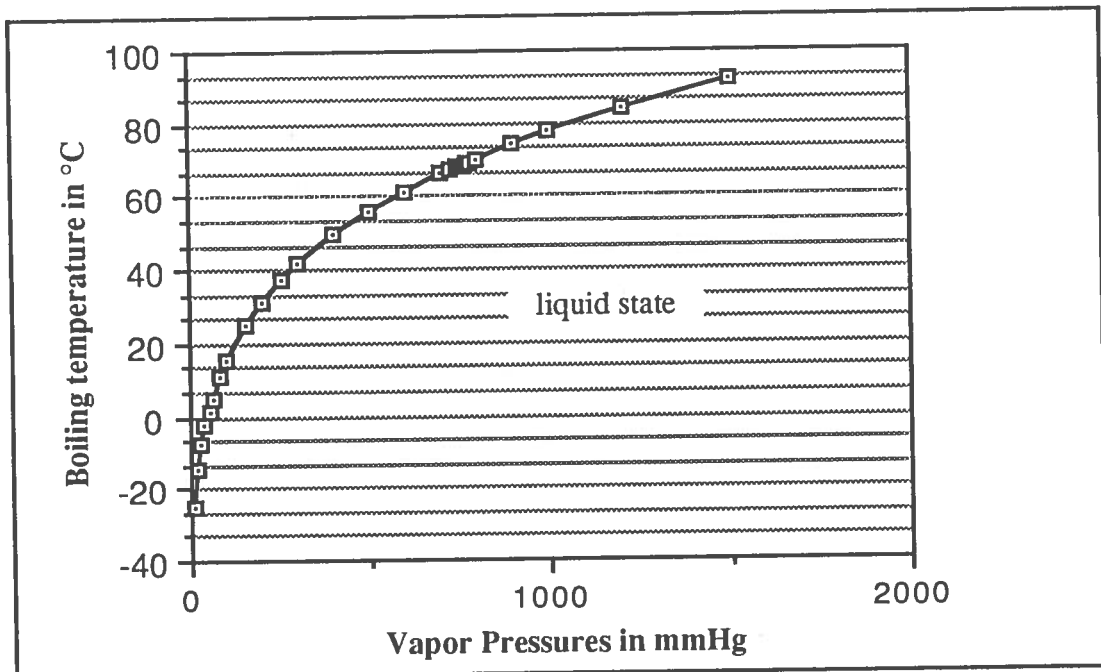
liq = n-Hexane liquid state

Values of the vapor pressure are calculated from the following constants :

A = 6.87601; B = 1171.17; C = 224.408

and the Antoine equation :

$\log_{10}P = A - B/(C+T)$; $T = B/(A - \log_{10}P) - C$; (P in mmHg; T in °C)



N-HEXANE, HIGH VAPOR PRESSURES (atm) AND BOILING POINTS (°C), FOR THE LIQUID PHASE ABOVE 1 ATM.

t-t _s	5	10	15	20	25	30	35	40
P	1.6219	1.8631	2.1308	2.4271	2.7537	3.1126	3.5057	3.9351
t-t _s	45	50	55	60	65	70	80	90
P	4.4030	4.9110	5.4610	6.0560	6.6980	7.3880	8.9250	10.6900
t-t _s	100	110	120	130	140	150	154.15	
P	12.69	14.98	17.57	20.53	23.93	27.88	29.71a	

t-t_s = temperature in °C; t_s is a fiducial temperature below t₀

P = vapor pressure in atm

a) Critical point;

1 atm = 1.01325 x 10⁵ Pa

Values of the saturated vapor pressure P/atm are calculated from the following constants :

A = 6.87601; B = 1171.17; C = 224.408

T^c = 507.30 K; t₀ = 78 °C; t_s = 80 °C

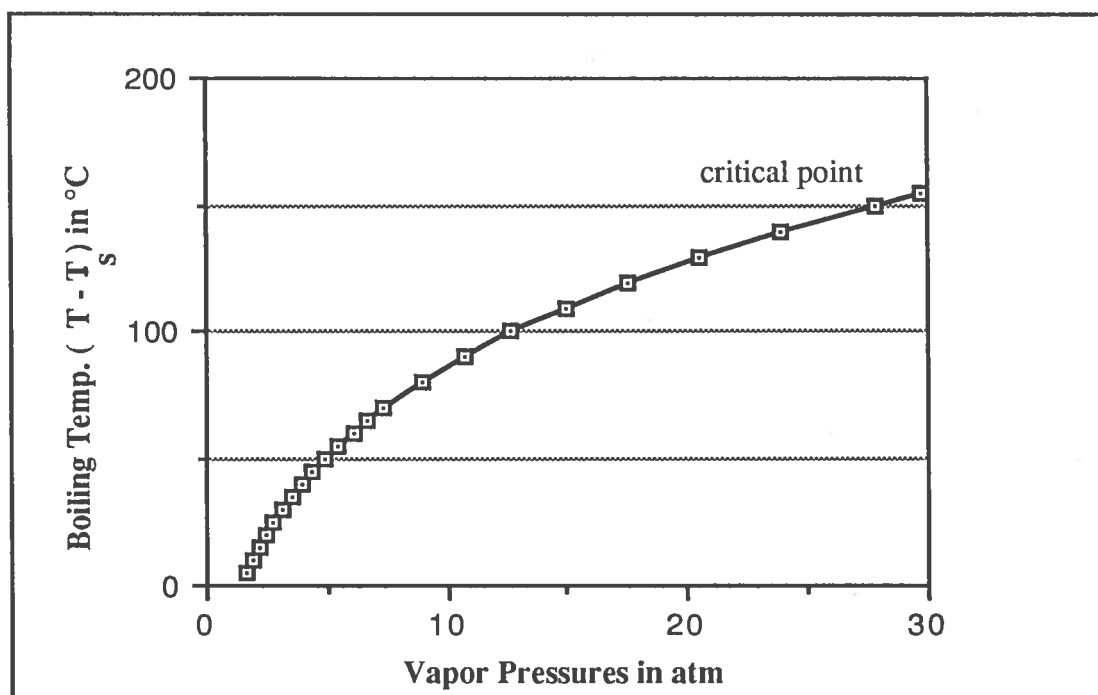
E = 274.59 ; F = -4838.2; n = 2.96881

and the equation for temperatures t > t₀ :

$$\log_{10}P = (A-2.88081)-B/(C+t)+D[(t-t_0)/T^c]^n+E[(t-t_0)/T^c]^8+F[(t-t_0)/T^c]^{12},$$

where D = log₁₀ e = 0.434294

For t < t₀ set D = E = F = 0



**N-HEXANE, DENSITY FOR THE CONDENSED PHASES
AT ONE ATMOSPHERE OR AT EQUILIBRIUM VAPOR PRESSURE
ABOVE THE BOILING POINT.**

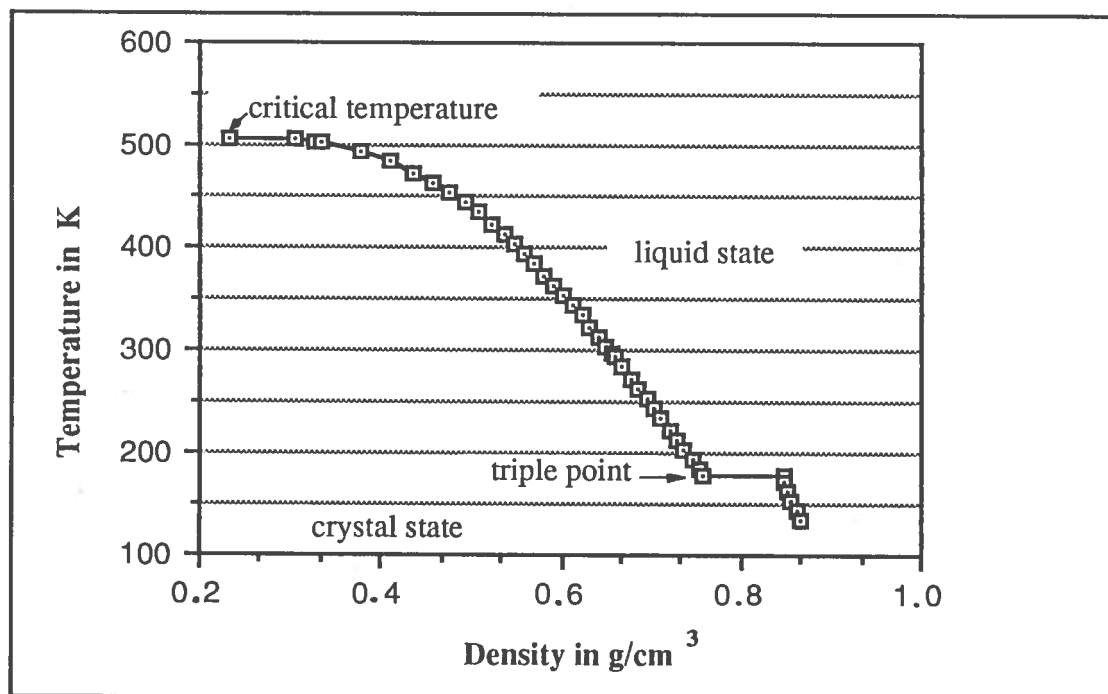
State	K	-140.00	-130.00	-120.00	-110.00	-100.00	-95.29	-80.00
c	D	0.86500	0.86100	0.85700	0.85300	0.84900	0.84700 ^a	
liq	D						0.75850	0.74580
K	-70.00	-60.00	-50.00	-40.00	-30.00	-20.00	-10.00	
liq	D	0.73740	0.72890	0.72050	0.71190	0.70330	0.69470	0.68600
K	0.00	10.00	20.00	25.00	30.00	40.00	50.00	
liq	D	0.67710	0.66820	0.65925	0.65471	0.65015	0.64090	0.63150
K	60.00	70.00	80.00	90.00	100.00	110.00	120.00	
liq	D	0.62200	0.61230	0.60240	0.59220	0.58170	0.57080	0.55940
K	130.00	140.00	150.00	160.00	170.00	180.00	190.00	
liq	D	0.54750	0.53490	0.52170	0.50750	0.49230	0.47570	0.45730
K	200.00	210.00	220.00	229.20	230.00	232.20	234.20	
liq	D	0.43640	0.41100	0.37900	0.33300	0.32700	0.30600	0.2330 ^b

K = Temperature in K

D = Density in g/cm³

c = n-Hexane, crystal state; liq = n-Hexane liquid state

a) At the triple point; b) At the critical temperature



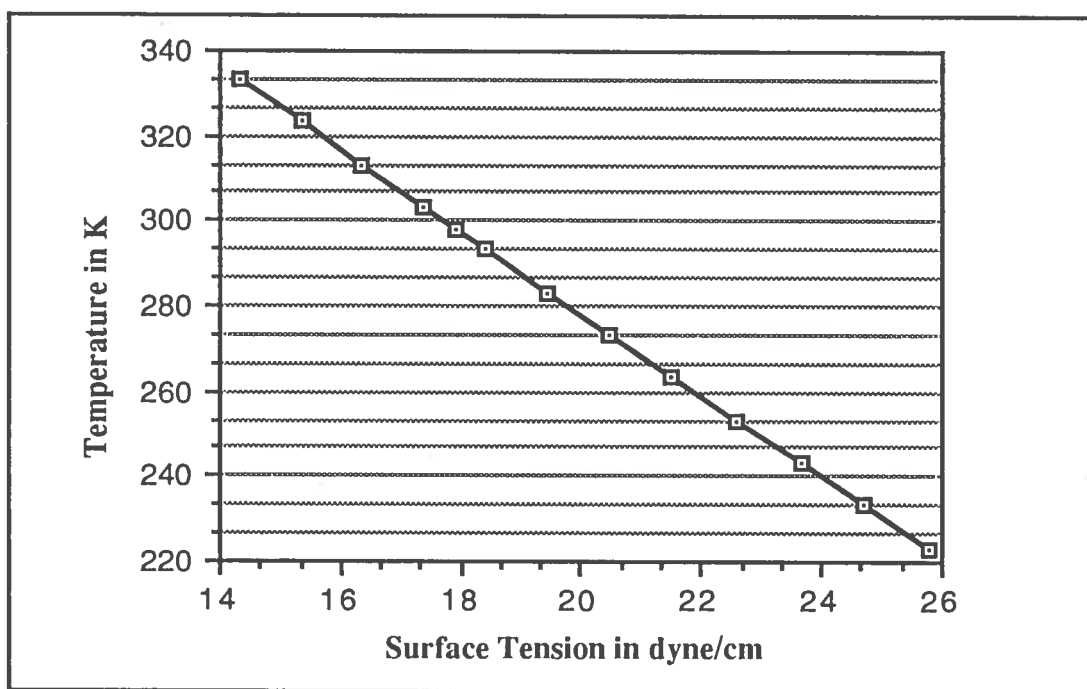
These values are drawn from the TRC Thermodynamic Tables-Hydrocarbons

**SURFACE TENSION, FOR THE N-HEXANE NORMAL LIQUID RANGE,
AT ATMOSPHERIC PRESSURE.**

K	223.15	233.15	243.15	253.25	263.15	273.15	283.15	293.15
S.T.	25.80	24.70	23.64	22.57	21.51	20.46	19.42	18.42
K	298.15	303.15	313.15	323.15	333.15			
S.T.	17.90	17.38	16.36	15.36	14.33			

T = Temperature in K

S.T. = Surface Tension in Dyne/cm



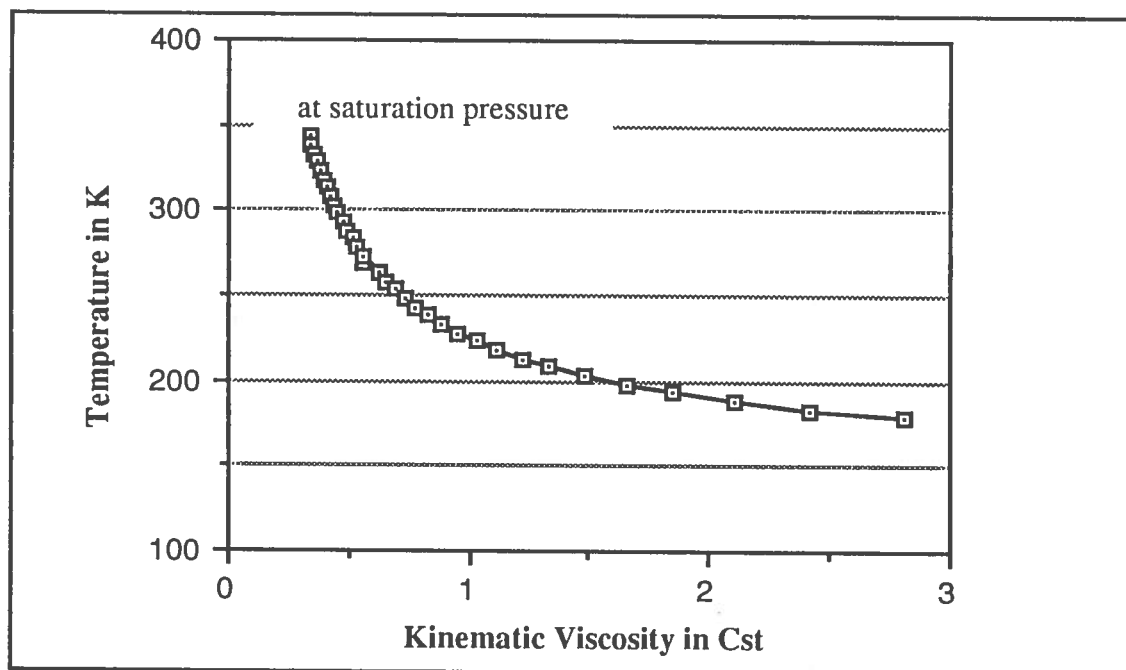
N-HEXANE, KINEMATIC VISCOSITY FOR THE NORMAL LIQUID RANGE, AT ATMOSPHERIC PRESSURE.

K	178.15	183.15	188.15	193.15	198.15	203.15	208.15	213.15
V	2.8100	2.4200	2.1000	-1.8400	1.6500	1.4800	1.3310	1.2150
K	218.15	223.15	228.15	233.15	238.15	243.15	248.15	253.15
V	1.1140	1.0260	0.9510	0.8850	0.8280	0.7760	0.7290	0.6890
K	258.15	263.15	268.15	273.15	278.15	283.15	288.15	293.15
V	0.6510	0.6190	0.5880	0.5612	0.5360	0.5129	0.4920	0.4727
K	298.15	303.15	308.15	313.15	318.15	323.15	328.15	333.15
V	0.4545	0.4376	0.4218	0.4073	0.3936	0.3806	0.3566	0.3455
K	343.15							
V	0.3350a							

a) At saturation pressure

K = Temperature in K

V = Kinematic Viscosity in Centistokes



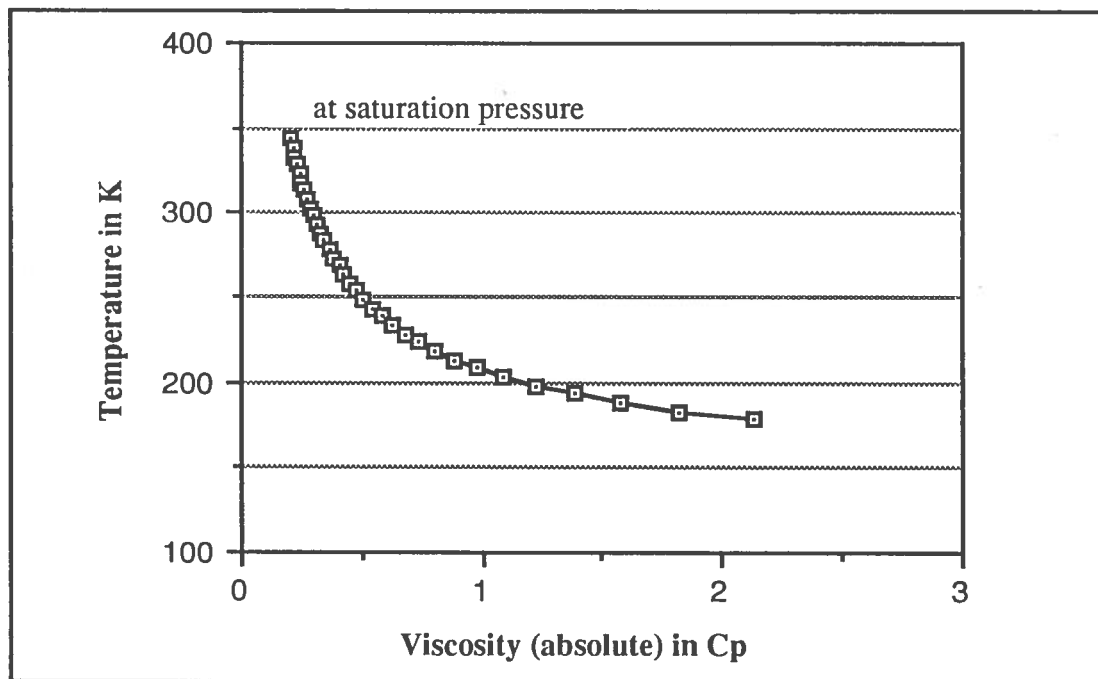
N-HEXANE, VISCOSITY (ABSOLUTE), FOR THE NORMAL LIQUID RANGE, AT ATMOSPHERIC PRESSURE.

K	178.15	183.15	188.15	193.15	198.15	203.15	208.15	213.15
V	2.1300	1.8200	1.5800	1.3800	1.2200	1.0900	0.9750	0.8850
K	218.15	223.15	228.15	233.15	238.15	243.15	248.15	253.15
V	0.8070	0.7390	0.6810	0.6300	0.5850	0.5450	0.5090	0.4790
K	258.15	263.15	268.15	273.15	278.15	283.15	288.15	293.15
V	0.4500	0.4250	0.4010	0.3799	0.3604	0.3426	0.3265	0.3117
K	298.15	303.15	308.15	313.15	318.15	323.15	328.15	333.15
V	0.2976	0.2845	0.2724	0.2611	0.2504	0.2404	0.2307	0.2216
K	338.15	343.15						
V	0.2128	0.2044a						

a) At saturation pressure

K = Temperature in K

V = Absolute Viscosity in Centipoises



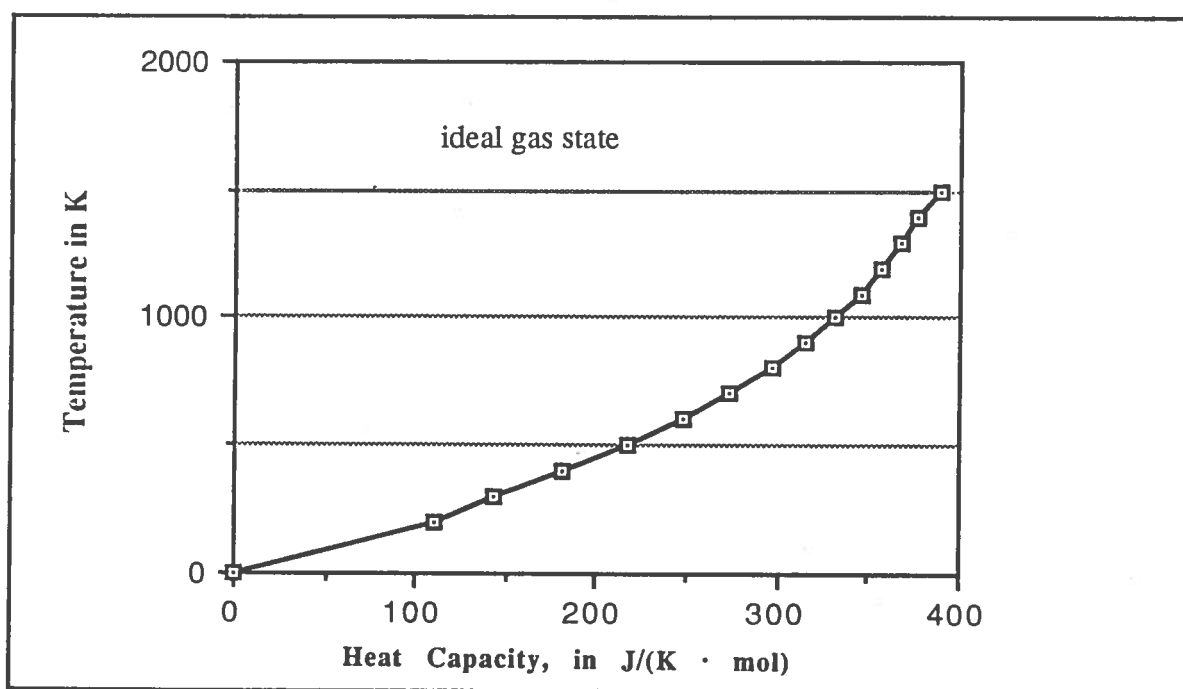
HEAT CAPACITY, " $C_p^\circ(T)$ ", FOR THE N-HEXANE IDEAL GAS STATE.

K	0	200	298.15	300	400	500	600	700
C	0	110.58	142.59	143.26	181.54	217.28	248.11	274.05
K	800	900	1000	1100	1200	1300	1400	1500
C	292.23	315.06	331.37	345.18	357.31	368.19	376.56	389.11

K = Temperature in K

C = Heat Capacity in J/(K · mol)

$C_p^\circ(T)$ is independent of pressure



HEAT CAPACITY, "C_s", FOR THE N-HEXANE CRYSTAL AND LIQUID STATES.

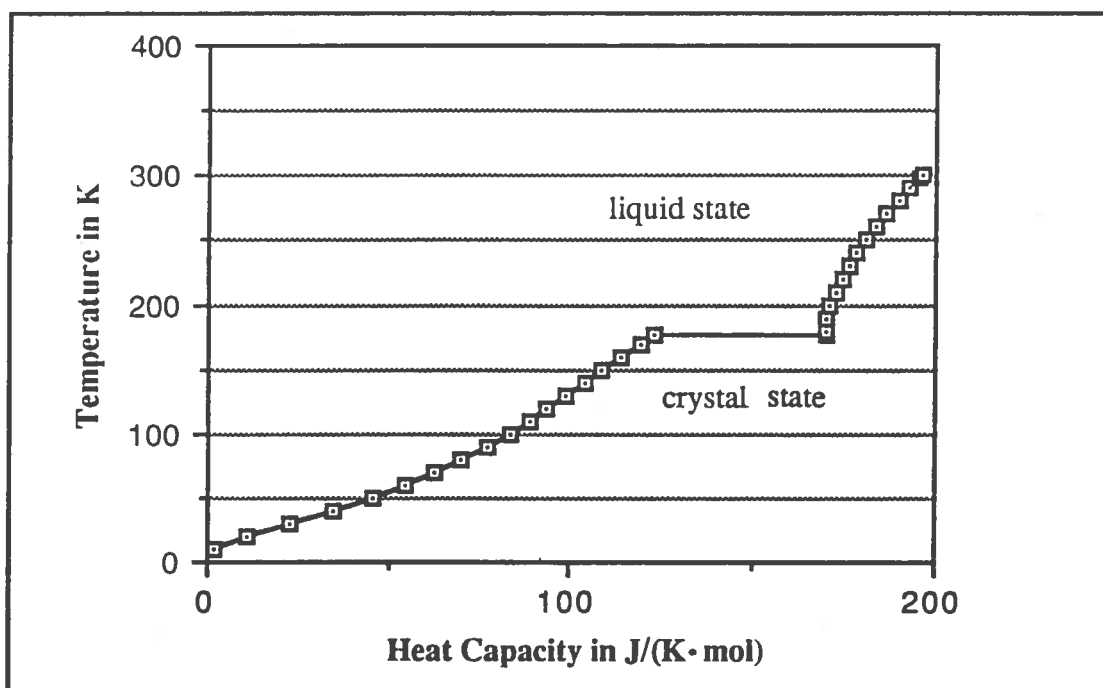
State	K	10	20	30	40	50	60	70
c	Cs	1.715	10.830	22.920	34.380	45.160	54.570	62.650
	K	80	90	100	110	120	130	140
c	Cs	70.080	76.720	82.830	88.400	93.630	98.76	103.780
	K	150	160	170	177.86	180	190	200
c	Cs	108.880	113.970	119.050	123.030			
liq	Cs				169.84	169.93	170.480	171.410
	K	210	220	230	240	250	260	270
liq	Cs	172.660	174.240	176.200	178.590	181.150	183.830	186.660
	K	280	290	298.15	300			
liq	Cs	189.660	192.810	195.480	196.100			

K = Temperature in K

Cs = Heat Capacity in J/(K · mol)

c = n-Hexane, Crystal state

liq = n-Hexane, Liquid state



These values are drawn from the TRC Thermodynamic Tables-Hydrocarbons

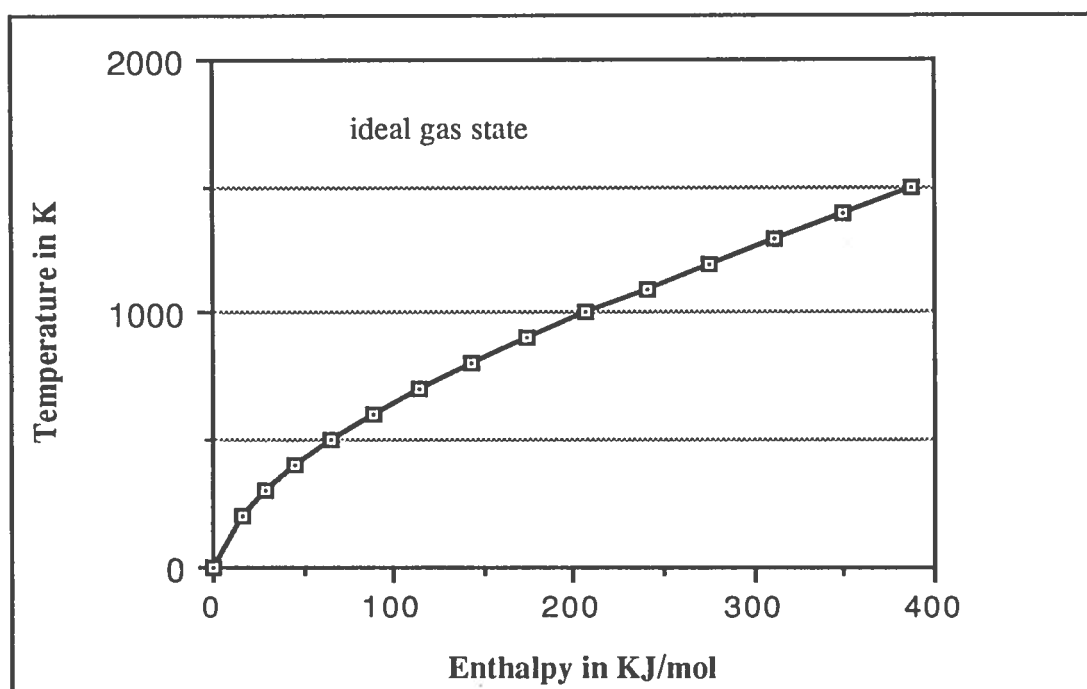
ENTHALPY, " $H^\circ(T)-H^\circ(0)$ ", FOR THE N-HEXANE IDEAL GAS STATE.

K	0	200	298.15	300	400	500	600	700
H	0	16.364	28.702	28.953	45.190	65.190	88.490	114.640
K	800	900	1000	1100	1200	1300	1400	1500
H	143.090	173.640	206.270	240.160	275.310	311.290	348.950	387.020

$H^\circ(T)-H^\circ(0)$ is independent of pressure

K = Temperature in K

H = Enthalpy, in KJ/mol



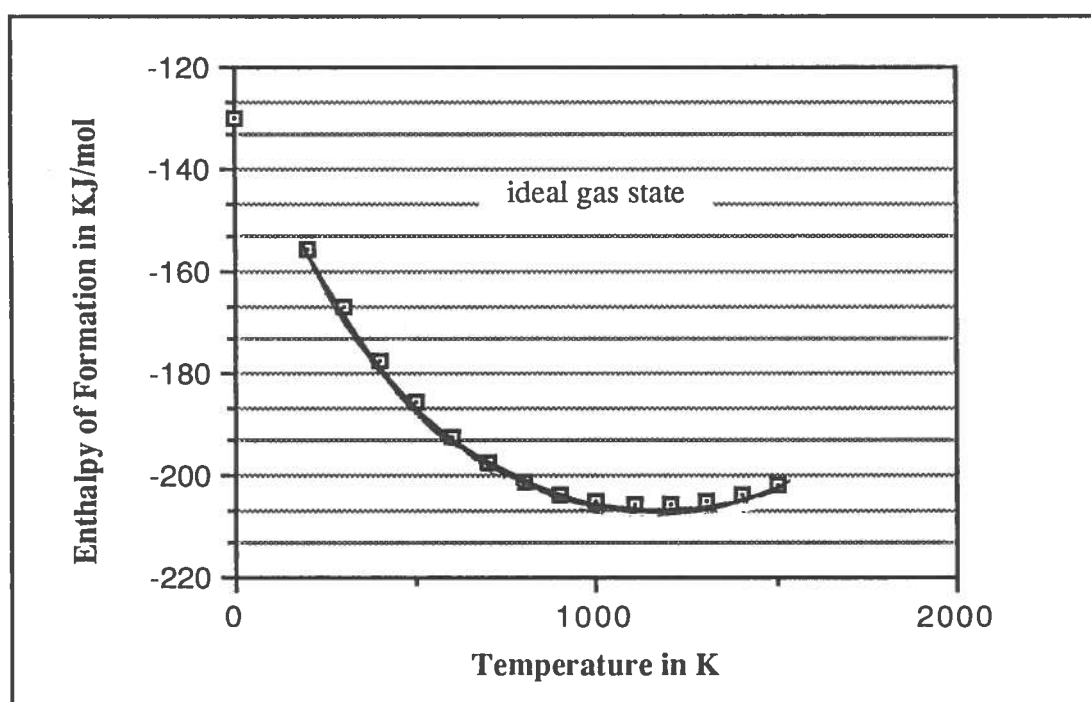
ENTHALPY OF FORMATION, " $\Delta_f H^\circ(T)$ ", FOR THE N-HEXANE IDEAL GAS STATE.

K	0	200	298.15	300	400	500	600	700
H	-130.05	-155.85	-166.92	-167.14	-177.38	-185.80	-192.47	-197.52
K	800	900	1000	1100	1200	1300	1400	1500
H	-201.26	-203.74	-204.88	-205.43	-205.33	-204.99	-203.52	-202.15

$\Delta_f H^\circ(T)$ is independent of pressure

K = Temperature in K

H = Enthalpy of Formation, in KJ/mol



ENTHALPY, " $(H_s - H^0)$ ", FOR THE N-HEXANE CRYSTAL AND LIQUID STATES.

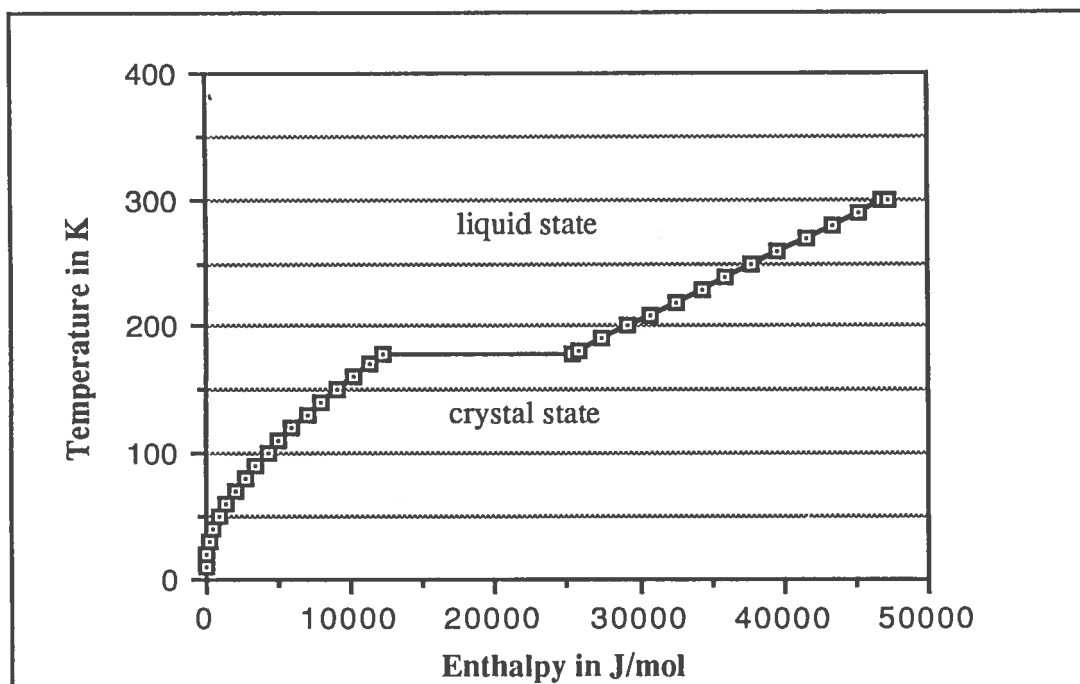
State	K	10	20	30	40	50	60	70
c	H	4.28	62.20	230.00	518.00	918.00	1418.00	2004.00
c	K	80	90	100	110	120	130	140
c	H	2669.00	3403.00	4202.00	5059.00	5968.00	6930.00	7943.00
c	K	150	160	170	177.86	180	190	200
c	H	9006.00	10120.00	11280.00	12240.00			
liq	H				25310.00	25680.00	273809.00	29090.0
liq	K	210	220	230	240	250	260	270
liq	H	30809.00	32540.00	34300.00	36070.00	37870.00	39690.00	41550.0
liq	K	280	290	298.15	300			
liq	H	43430.00	45340.00	46920.00	47280.00			

K = Temperature in K

H = Enthalpy, in J/mol

c = n-Hexane Crystal State

liq = n-Hexane Liquid State



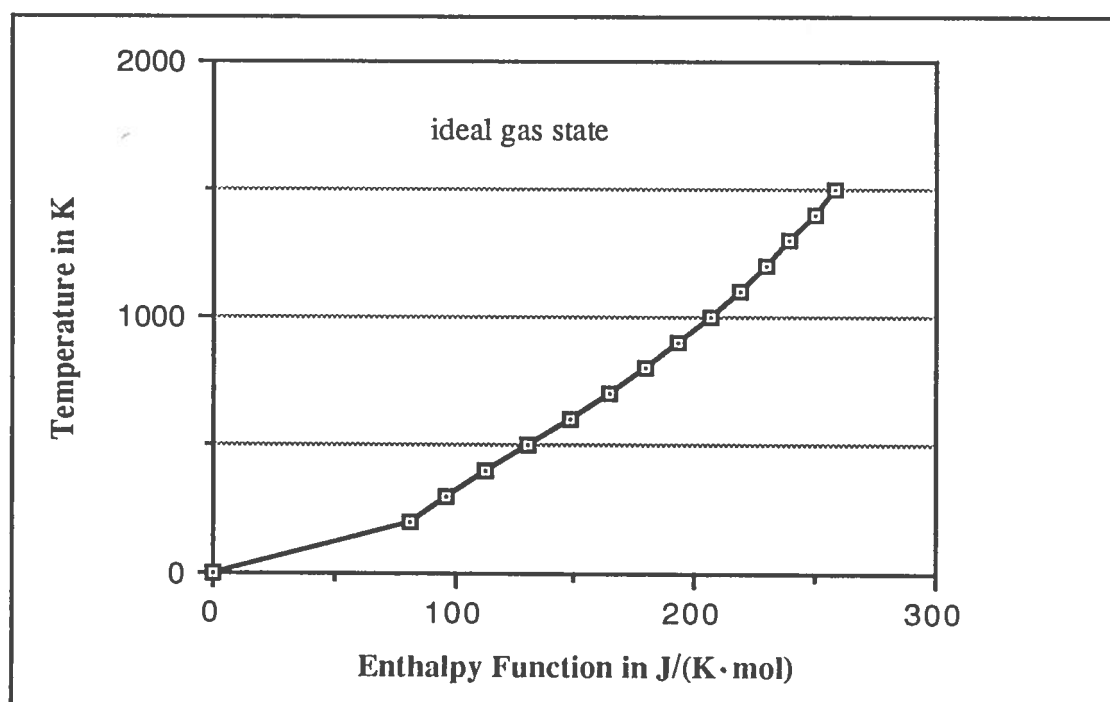
**ENTHALPY FUNCTION, " $\{H^\circ(T)-H^\circ(0)\}/T$ ", FOR N-HEXANE
IDEAL GAS STATE.**

K	0	200	298.15	300	400	500	600	700
H	0	81.82	96.27	96.51	112.97	130.37	147.49	163.77
K	800	900	1000	1100	1200	1300	1400	1500
H	178.86	192.93	206.27	218.33	229.43	239.45	249.25	258.01

$\{H^\circ(T)-H^\circ(0)\}/T$ is independent of pressure

K = Temperature in K

H = Enthalpy function, in J/(K · mol)



ENTROPY, " $S^\circ(T)-S^\circ(0)$ ", FOR THE N-HEXANE IDEAL GAS STATE.

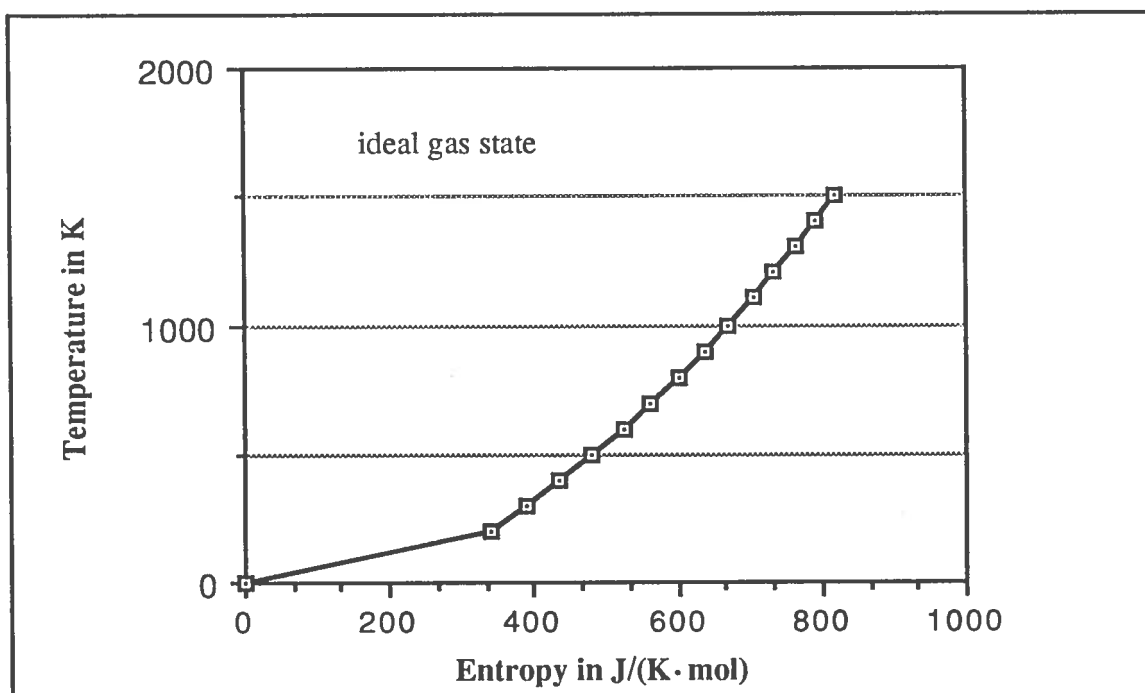
K	0	200	298.15	300	400	500	600	700
S	0	339.06	388.85	389.72	436.17	480.60	523.11	563.28
K	800	900	1000	1100	1200	1300	1400	1500
S	601.35	637.33	671.64	703.86	734.40	763.27	790.89	817.66

$$S^\circ(T)-S^\circ(0) \text{ (at 1 bar)} = S^\circ(T)-S^\circ(0) \text{ (at 1 atm)} + 0,109 \text{ J/(K} \cdot \text{mol)}$$

K = Temperature in K

$$1 \text{ bar} = 10^5 \text{ N m}^{-2}$$

S = Entropy, in J/(K · mol)



ENTROPY, "S_s", FOR THE N-HEXANE CRYSTAL AND LIQUID STATES.

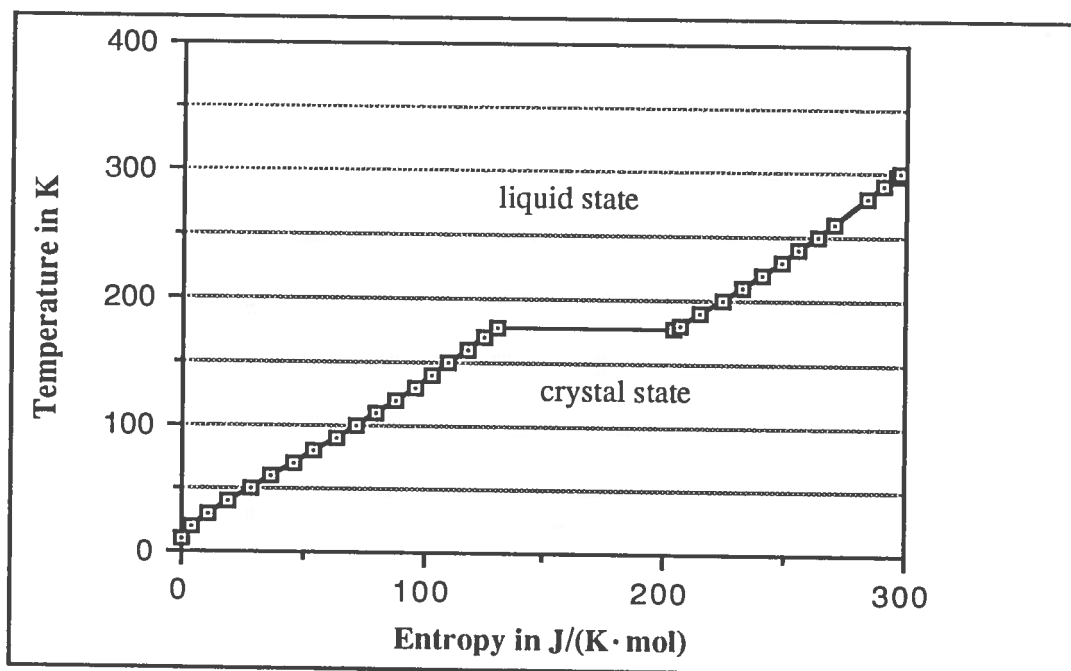
State	K	10	20	30	40	50	60	70
c	S	0.573	4.230	10.880	19.090	27.970	37.050	46.070
c	K	80	90	100	110	120	130	140
c	S	54.940	63.580	71.980	80.150	88.060	95.760	103.260
c	K	150	160	170	177.86	180	190	200
c	S	110.590	117.780	124.840	130.320			
liq	S				203.840	205.860	215.06	223.840
liq	K	210	220	230	240	250	260	270
liq	S	232.250	240.290	248.080	255.650	262.980	270.140	277.130
liq	K	280	290	298.15	300			
liq	S	283.990	290.690	296.090	297.260			

K = Temperature in K

S = Entropy in J/(K · mol)

c = n-Hexane Crystal State

liq = n-Hexane Liquid State



These values are drawn from the TRC Thermodynamic Tables-Hydrocarbons

GIBBS ENERGY OF FORMATION, " $\Delta_f G^\circ(T)$ ", FOR THE N-HEXANE IDEAL GAS STATE.

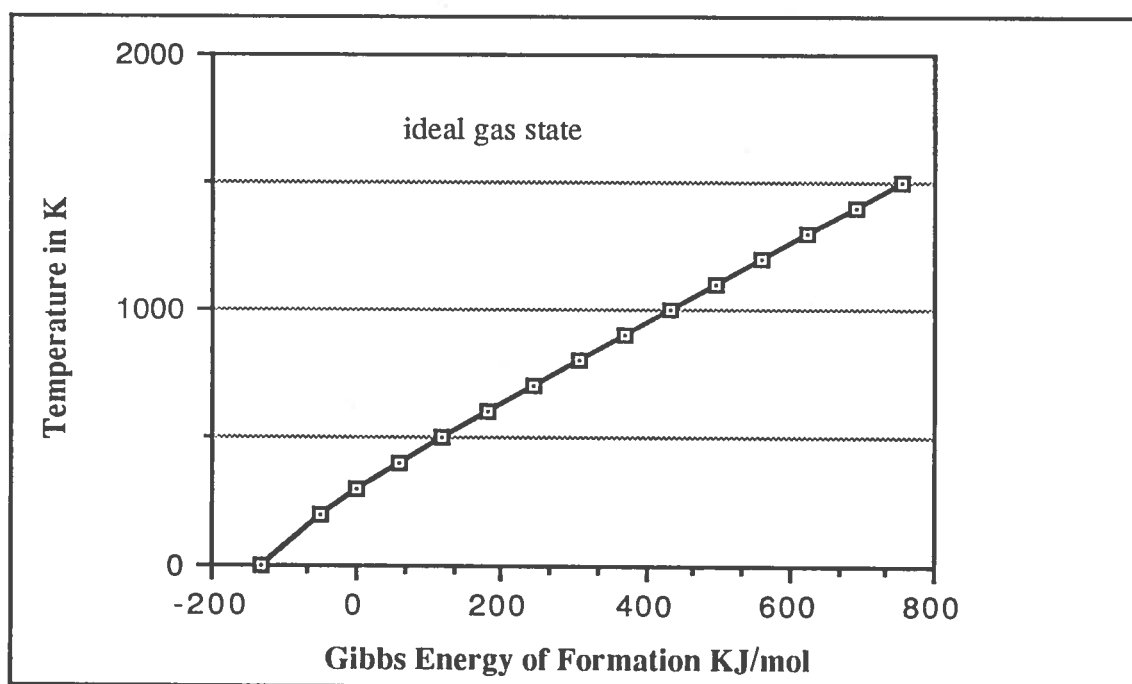
K	0	200	298.15	300	400	500	600	700
G	-130.05	-52.79	+0.15	1.18	58.87	118.96	180.51	243.15
K	800	900	1000	1100	1200	1300	1400	1500
G	306.28	369.87	433.73	497.70	561.67	625.47	689.70	752.70

1 bar = $10^5 \text{ N} \cdot \text{m}^{-2}$

$\Delta_f G^\circ(T, 1 \text{ bar}) = \Delta_f G^\circ(T, 1 \text{ atm}) + 0.0008755 \times T \text{ KJ/mol}$

K = Temperature in K

G = Gibbs Energy of Formation, in KJ/mol



These values are drawn from the TRC Thermodynamic Tables-Hydrocarbons

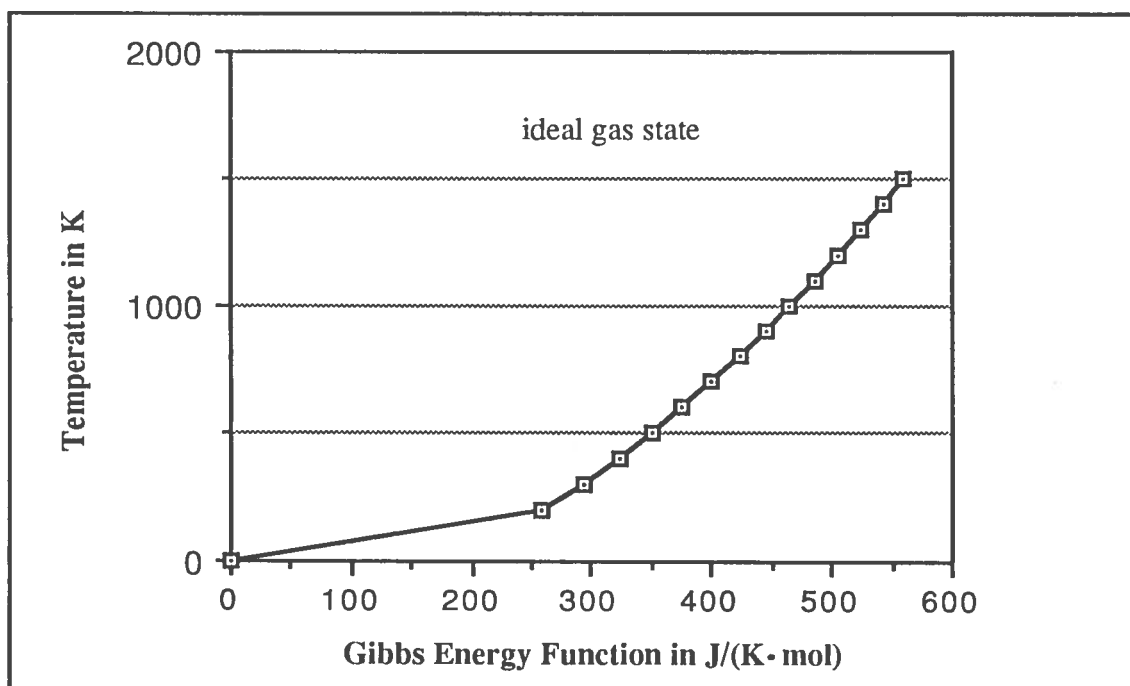
GIBBS ENERGY FUNCTION, " $-\{G^\circ(T)-H^\circ(0)\}/T$ ", FOR THE N-HEXANE IDEAL GAS STATE, AT 1 BAR.

K	0	200	298.15	300	400	500	600	700
G	0	257.24	292.58	293.21	323.20	350.23	375.62	399.51
K	800	900	1000	1100	1200	1300	1400	1500
G	422.49	444.40	465.37	485.53	504.97	523.82	541.64	559.65

$-\{G^\circ(T)-H^\circ(0)\}/T$ (at 1 bar) = $-\{G^\circ(T)-H^\circ(0)\}/T$ (at 1 atm) - 0.109 J/(K · mol)

K = Temperature in K

G = Gibbs Energy Function, in J/(K · mol)



These values are drawn from the TRC Thermodynamic Tables-Hydrocarbons

GIBBS ENERGY FUNCTION, " $(G_s - H^\circ_0)/T$ ", FOR THE N-HEXANE CRYSTAL AND LIQUID STATES.

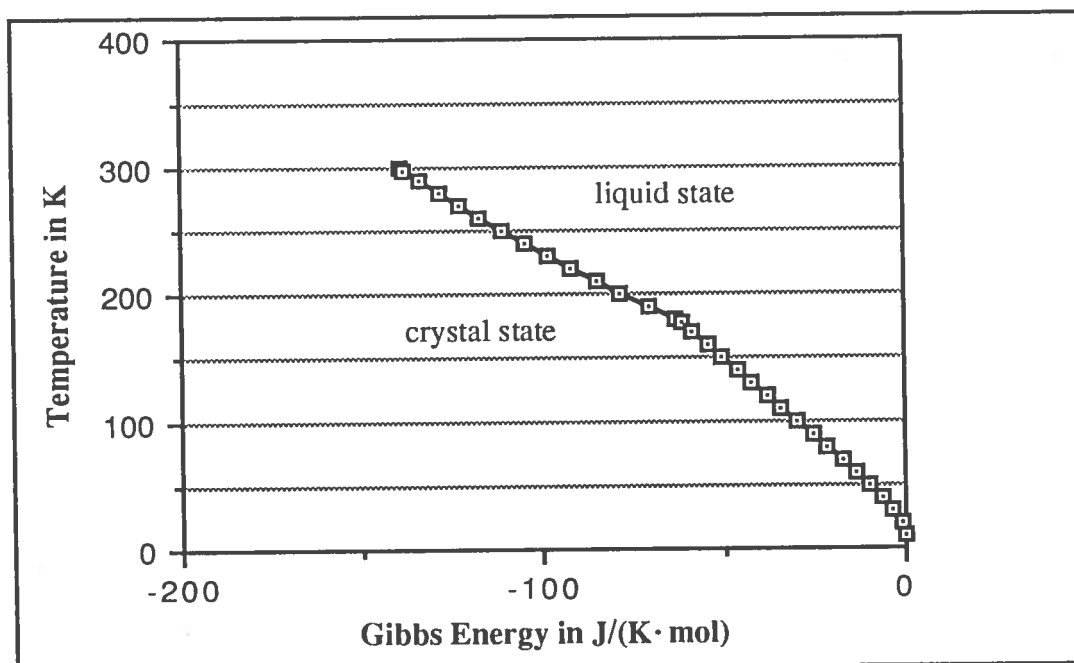
State	K	10	20	30	40	50	60	70
c	G	-0.146	-1.120	-3.210	-6.130	-9.610	-13.420	-17.440
	K	80	90	100	110	120	130	140
c	G	-21.580	-25.760	-29.970	-34.160	-38.320	-42.450	-46.530
	K	150	160	170	177.86	180	190	200
c	G	-50.550	-54.530	-58.460	-61.520			
liq	G				-61.510	-63.210	-70.950	-78.400
	K	210	220	230	240	250	260	270
liq	G	-85.510	-92.370	-98.980	-105.340	-111.490	-117.470	-123.240
	K	280	290	298.15	300			
liq	G	-128.890	-134.330	-138.680	-139.640			

K = Temperature in K

G = Gibbs Energy Function, in J/(K · mol)

c = n-Hexane Crystal State;

liq = n-Hexane Liquid State



SECOND VIRIAL COEFFICIENT, "B" FOR THE N-HEXANE GAS.

T/T ^c	0.50	0.55	0.60	0.65	0.70	0.75	0.80	0.85
B	-3310.0	-2370.0	-1800.0	-1420.0	-1160.0	-961.0	-813.0	-697
T/T ^c	0.90	0.95	1.00	1.10	1.20	1.30	1.4	1.6
B	-603.0	-527.0	-463.0	-363.0	-289.0	-231.0	-186.0	-118
T/T ^c	1.80	2.00	2.50	3.00	3.50	4.00	4.50	5.00
B	-70.0	-35.0	+22.0	57.0	79.0	95.0	107.0	116
T/T ^c	5.0							
B	116.0							

B = Second Virial Coefficient, in cm³/mol

T/T^c = Reduced Temperature

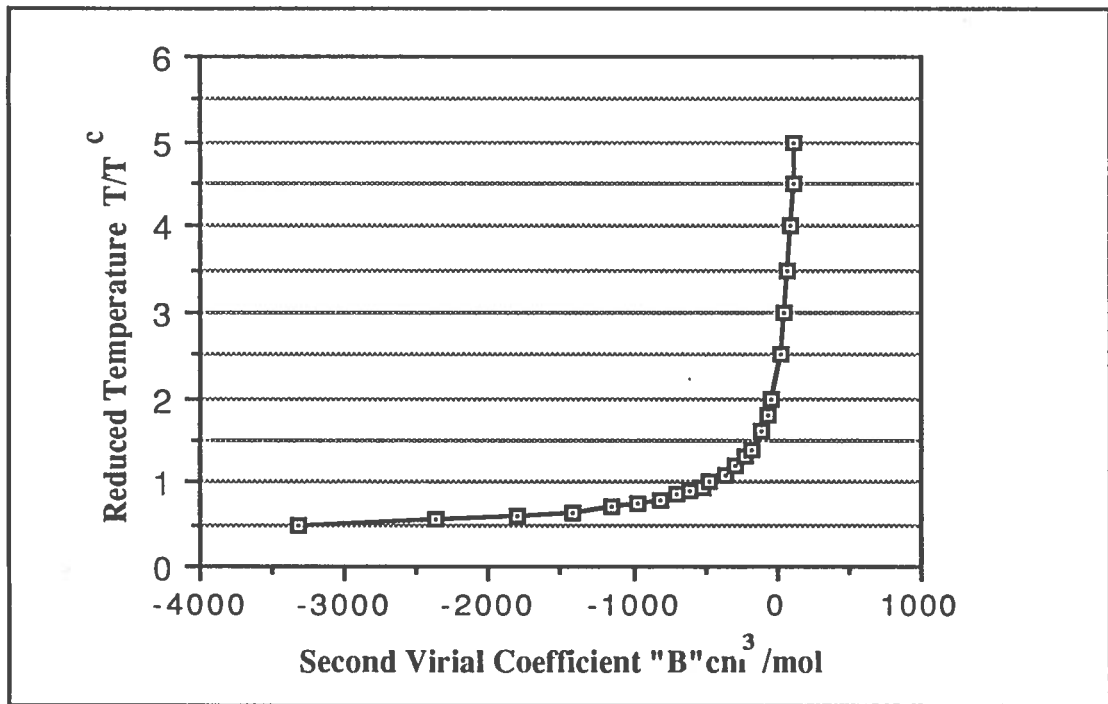
Values of the second virial coefficient B are calculated from the following constants :

T^c = 507.4 K; u/K = - 1087.0 K; V* = 132.8 cm³/mol

R₁ = 0.688; R₂ = 1.124; R₃ = 4.244

and the equation:

$$B = 2V^*\{R_1-(1-R_1)[\exp(\bar{u}/kT)-1]-(R_2-1)[\exp(-\bar{u}/kT)-1]- (R_3-R_2)[\exp(-0.21\bar{u}/kT)-1]\}$$



PSEUDOCUMENE, VAPOR PRESSURES AND BOILING POINTS.

State	P	0.02	0.03	0.04	0.05	0.06	0.08	0.10
liq	T	59.490	67.800	74.020	79.030	83.263	90.197	95.807
	P	0.15	0.20	0.30	0.40	0.50	0.60	0.70
liq	T	106.554	114.650	126.790	135.442	143.442	149.791	155.340
	P	0.80	0.90	0.95	0.99	1.00	1.01135	1.03
liq	T	160.287	164.763	166.854	168.466	168.860	169.378	170.026
	P	1.05	1.10	1.20	1.30	1.60	2.00	
liq	T	170.788	172.644	176.17	179.46	188.28	198.22	

P = Vapor pressure in bar

T = Boiling Point in °C

liq = Pseudocumene liquid phase

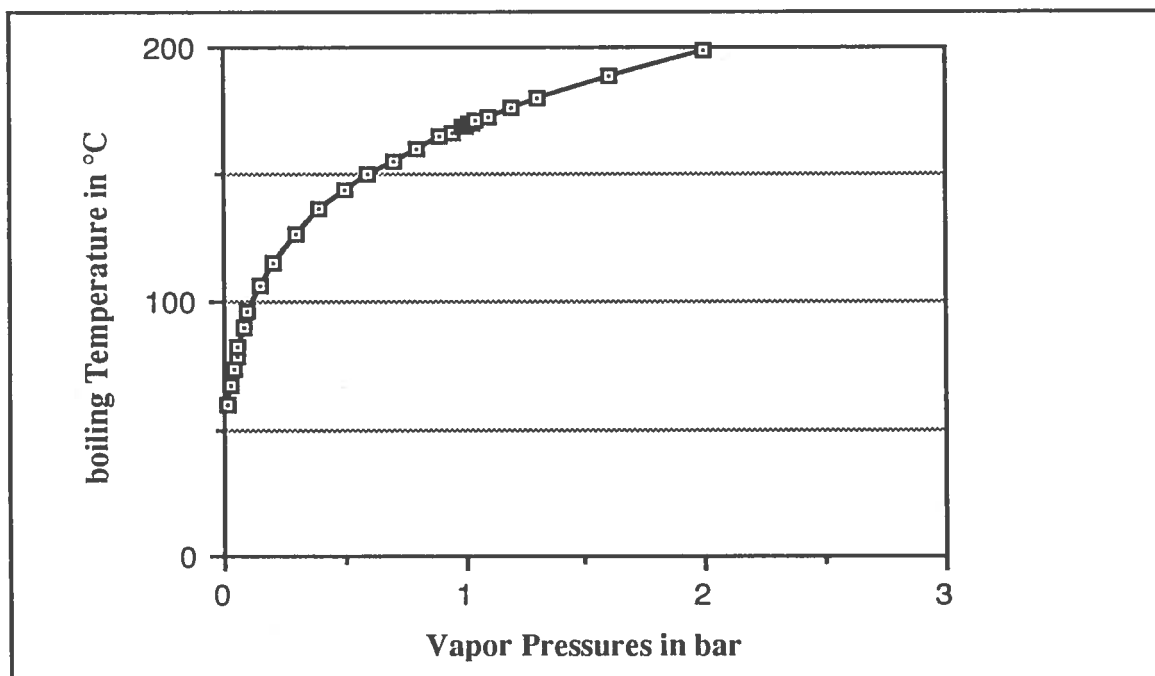
1 bar = 10^5 N m⁻²

Values of the vapor pressure are calculated from the following constants:

A = 4.18422; B = 1584.67; C = 209.865

and the Antoine equation :

$\log_{10}P = A - B / (C + T)$; $T = B / (A - \log_{10}P) - C$; (P in bar; T in °C)



PSEUDOCUMENE, HIGH VAPOR PRESSURES (in Bar) AND BOILING POINT, (in Celsius degrees) ABOVE 1.3 BAR.

T	5	10	15	20	25	30	35	40
P	1.8631	2.0801	2.3163	2.5730	2.8513	3.1530	3.4780	3.8280
T	50	60	70	80	90	100	110	120
P	4.6110	5.5120	6.5410	7.7120	9.0360	10.5300	12.2000	14.0600
T	130	140	150	160	170	180	186.02	
P	16.1300	18.4300	20.9600	23.7500	26.8100	30.1600	32.3200a	

$T = (T - T_s)$ in °C

P = Pressure in bar

a) At the critical point, t_s is a fiducial temperature, for temperature below t_0
 Values of the saturated vapor pressure P/bar are calculated from the following constants :

A = 4.18422; B = 1584.67; C = 209.865

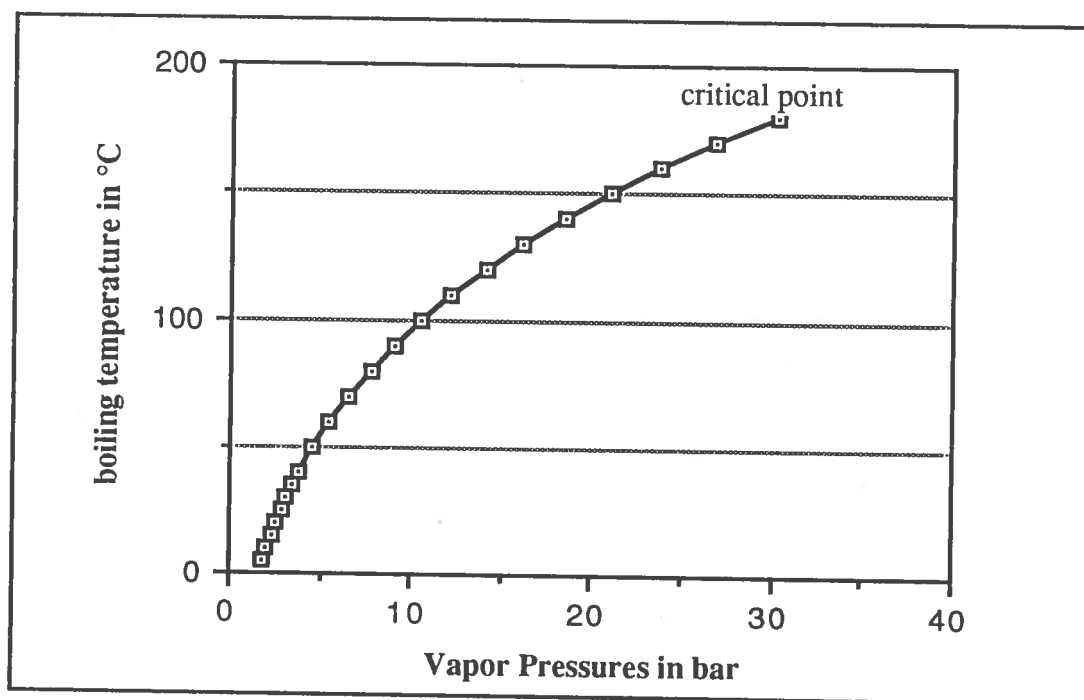
$T^c = 649.17$ K; $T_0 = 180$ °C; $T_s = 190$ °C

E = 0; F = 0; n = 2.2319

and the equation for temperatures $t > t_0$:

$\log_{10}P = (A-B)/(C+t)+D[(t-t_0)/T^c]^n+E[(t-t_0)/T^c]^8+F[(t-t_0)/T^c]^{12}$, where $D = \log_{10}e = 0.434294$

for $t < t_0$, set $D=E=F=0$



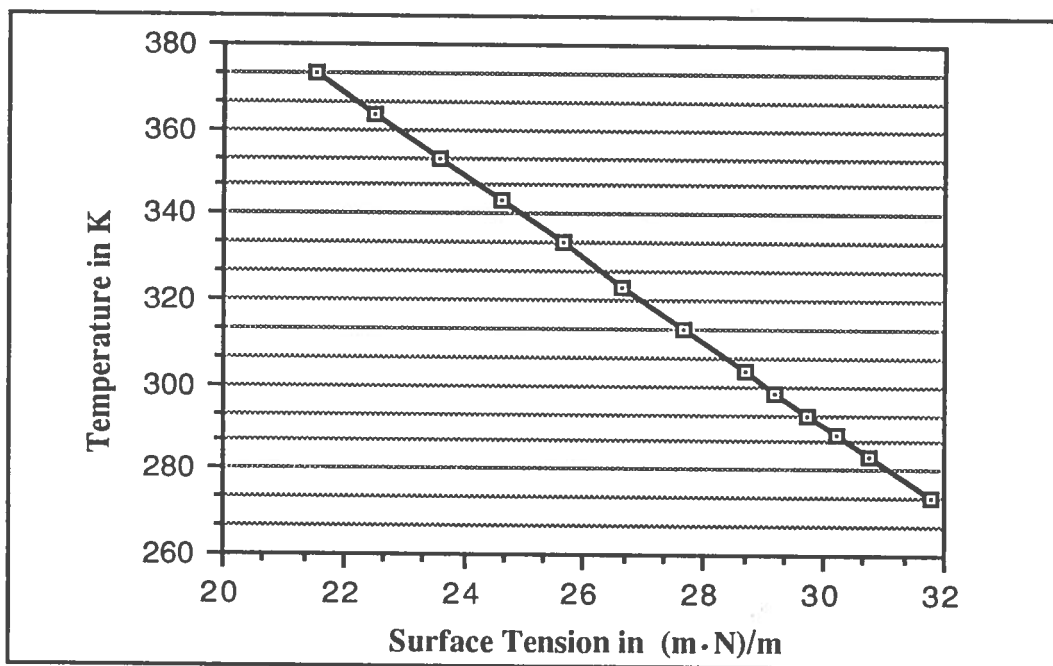
These values are drawn from the TRC Thermodynamic Tables-Hydrocarbons

PSEUDOCUMENE, SURFACE TENSION, FOR THE NORMAL LIQUID RANGE AT ATMOSPHERIC PRESSURE IN AIR.

K	273.15	283.15	288.15	293.15	298.15	303.15	313.15	323.15
S.T.	31.77	30.74	30.23	29.72	29.20	28.69	27.67	26.64
K	333.15	343.15	353.15	363.15	373.15			
S.T.	25.62	24.60	23.60	22.50	21.50			

K = Temperature in K

S.T. = Surface Tension, in mN/m



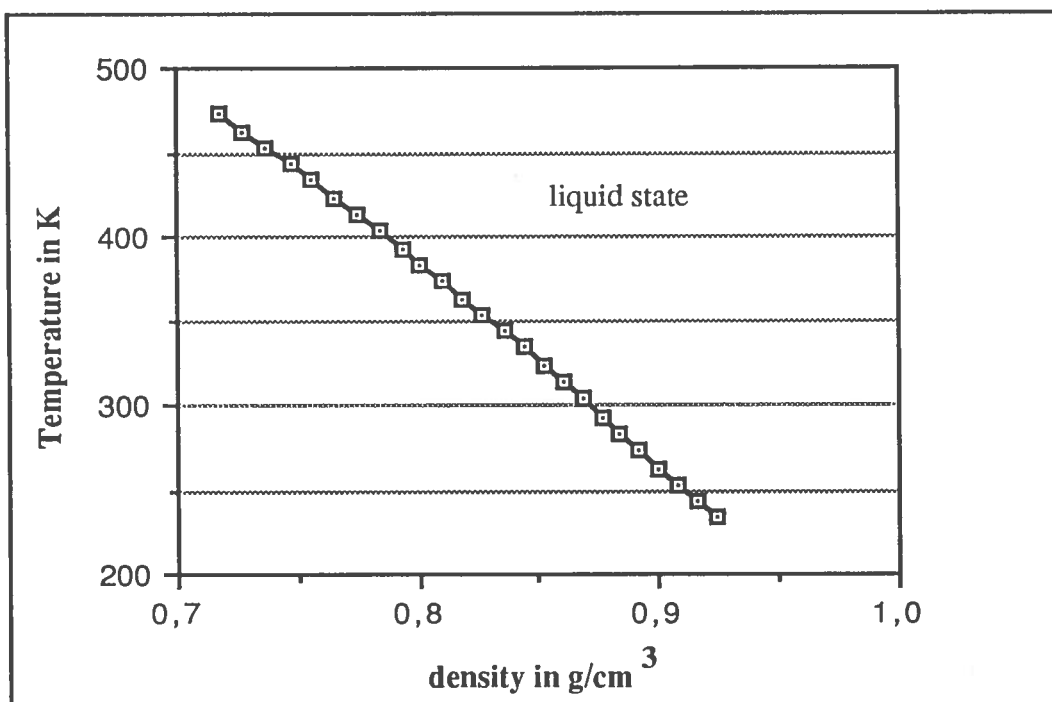
**DENSITY, FOR THE PSEUDOCUMENE CONDENSED PHASE
AT ONE ATMOSPHERE, OR AT EQUILIBRIUM VAPOR PRESSURE
ABOVE THE NORMAL BOILING POINT.**

State	K	233.15	243.15	253.15	263.15	273.15	283.15	293.15
liq	D	0.9238	0.9158	0.9078	0.8998	0.8918	0.8838	0.8758
	K	303.15	313.15	323.15	333.15	343.15	353.15	363.15
liq	D	0.8679	0.8598	0.8517	0.8435	0.8353	0.8269	0.8185
	K	373.15	383.15	393.15	403.15	413.15	423.15	433.15
liq	D	0.8099	0.8010	0.7930	0.7840	0.7750	0.7650	0.7560
	K	443.15	453.15	463.15	473.15			
liq	D	0.7470	0.7370	0.7270	0.7170			

K = Temperature in K

D = Density in g/cm³

Liq = Pseudocumene Liquid Phase



TRC

Page d-3290 table 23-2-(33.1119)-d, page 1

TRC

Page d-3291 table 23-2-(33.1110)-d, page 2

TRC

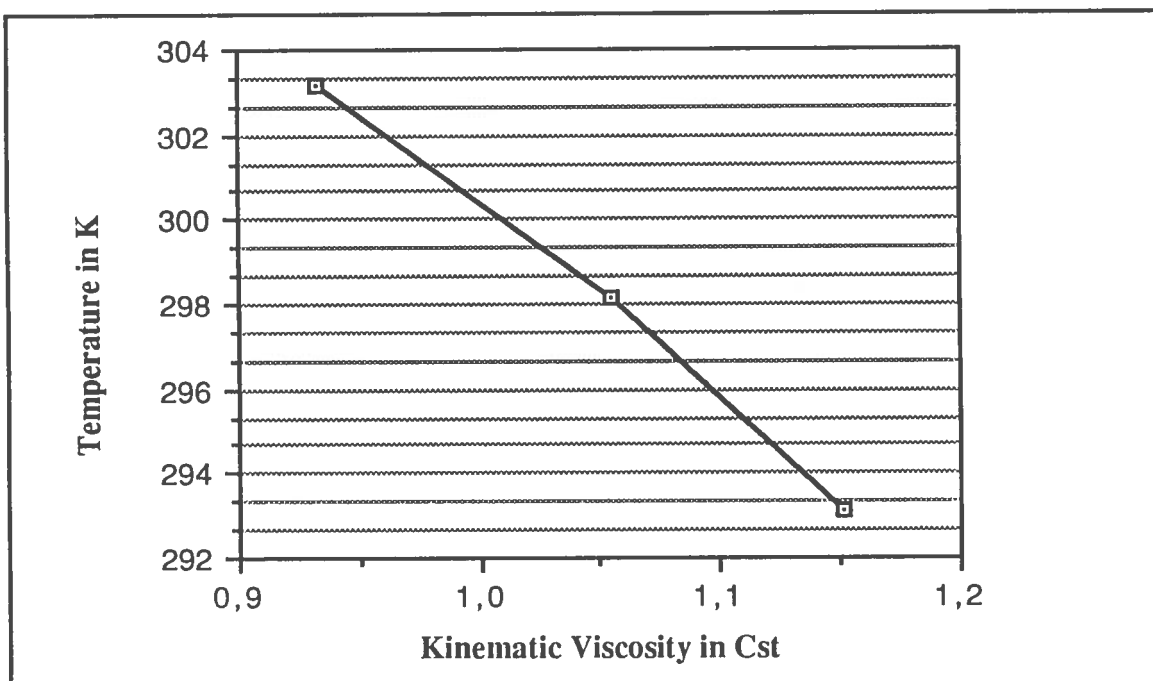
Page d-3292 table 23-2-(33.1110)-d, page 3

These values are drawn from the TRC Thermodynamic Tables-Hydrocarbons

PSEUDOCUMENE, KINEMATIC VISCOSITY, FOR THE NORMAL LIQUID RANGE, AT ATMOSPHERIC PRESSURE.

K	20	25	30
V	1.151	1.055	0.933

K = Temperature in K
V = kinematic Viscosity in Centistokes



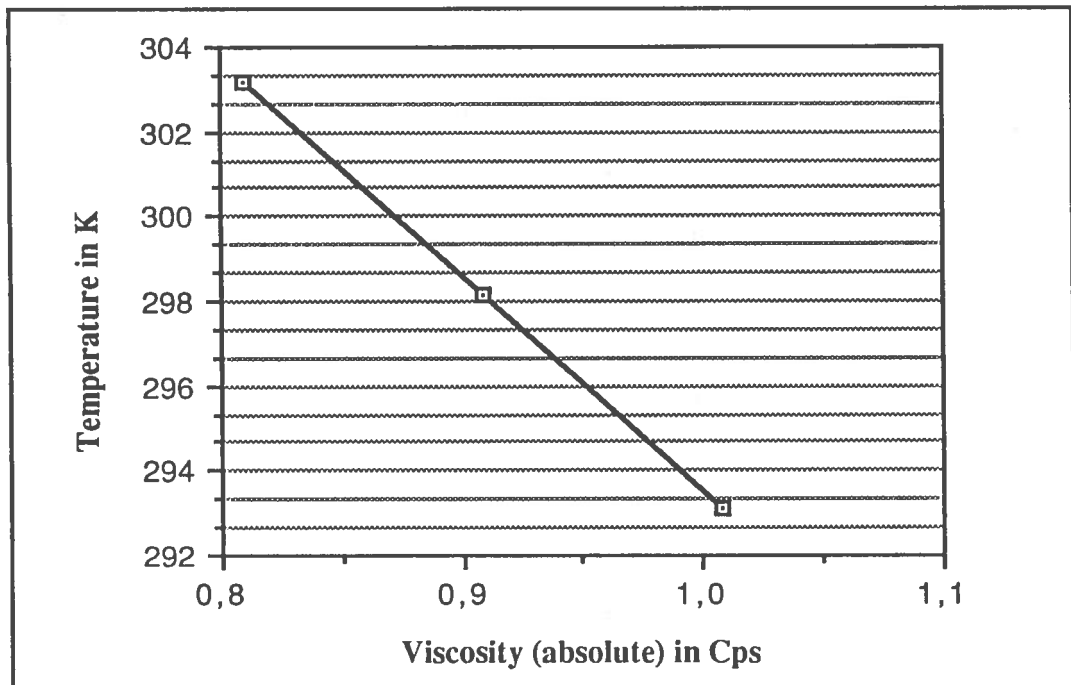
These values are drawn from the TRC Thermodynamic Tables-Hydrocarbons

PSEUDOCUMENE, VISCOSITY (ABSOLUTE), FOR THE NORMAL LIQUID RANGE, AT ATMOSPHERIC PRESSURE.

K	293.15	298.15	303.15
V	1.008	0.9090	0.8100

K = Temperature in K

V = Absolute Viscosity in Centipoises



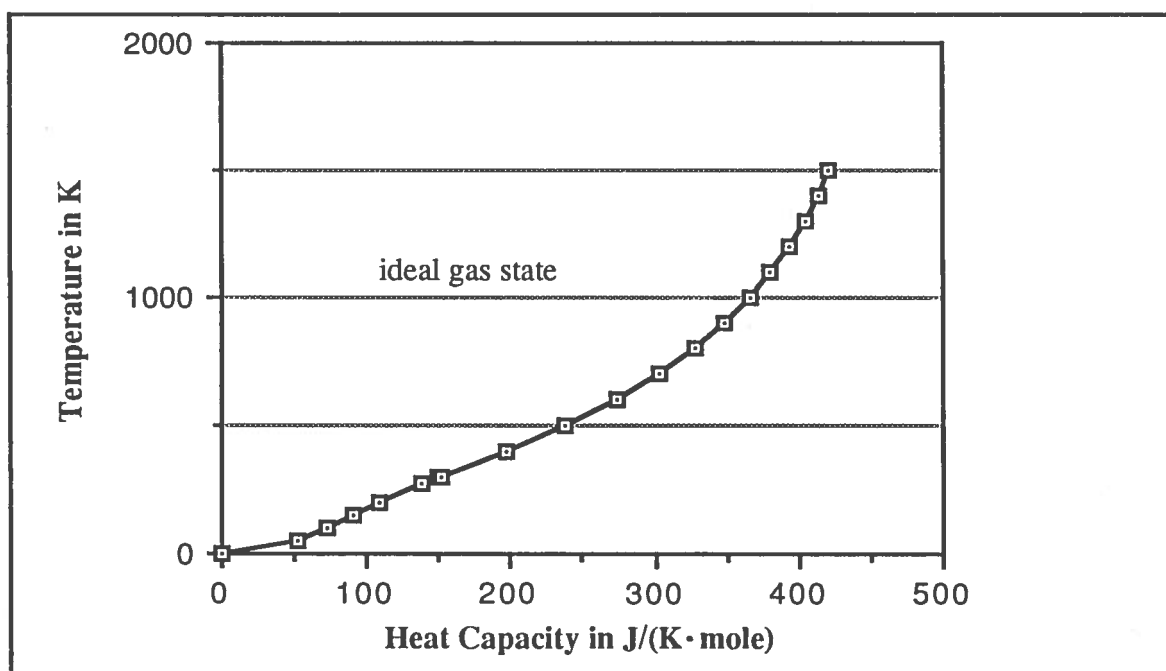
These values are drawn from the TRC Thermodynamic Tables-Hydrocarbons

HEAT CAPACITY, " C_p° ", FOR THE PSEUDOCUMENE IDEAL GAS STATE.

K	0	50	100	150	200	273.15	298.15	300
C_p°	0	52.14	72.50	89.69	107.78	138.37	149.71	150.56
K	400	500	600	700	800	900	1000	1100
C_p°	196.40	238.01	273.24	302.62	327.22	347.95	365.52	380.48
K	1200	1300	1400	1500				
C_p°	393.25	404.21	413.64	421.78				

K = Temperature in K

C_p° = Heat Capacity, in J/(K · mol)



HEAT CAPACITY, C_s , FOR THE PSEUDOCUMENE CRYSTAL AND LIQUID STATES.

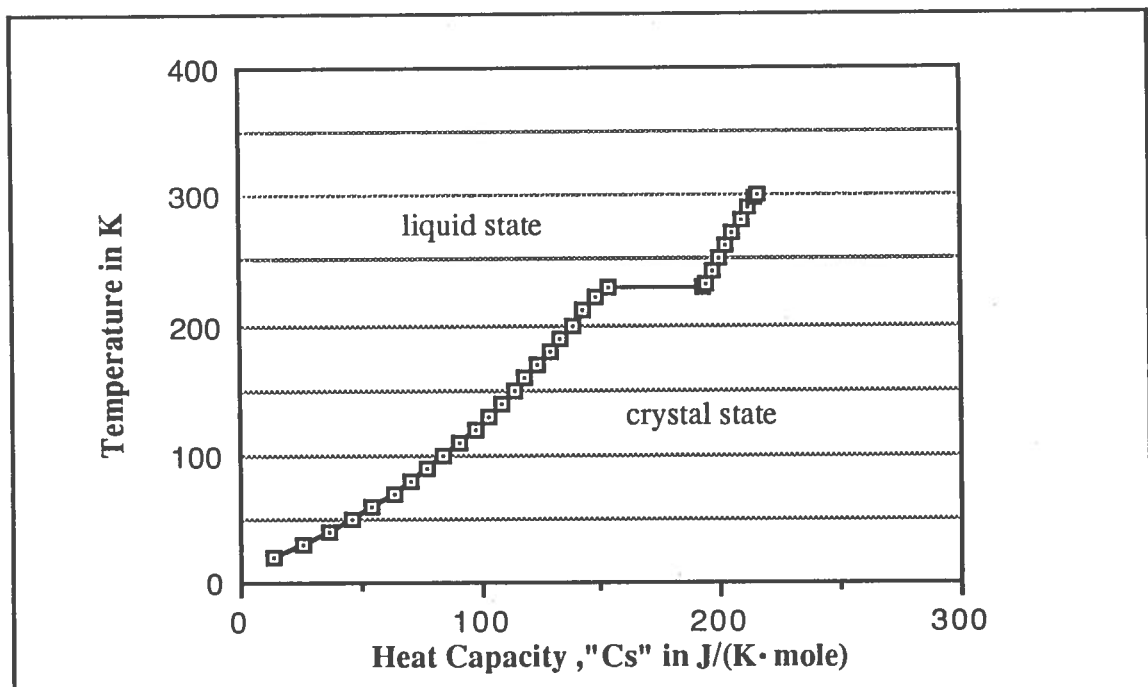
State	K	20	30	40	50	60	70	80
c	Cs	14.153	25.590	36.135	45.860	54.836	63.134	70.825
	K	90	100	110	120	130	140	150
c	Cs	77.999	84.730	91.070	97.970	102.780	108.250	113.530
	K	160	170	180	190	200	210	220
c	Cs	118.670	123.700	128.610	133.470	138.300	143.160	148.090
	K	229.33	230	240	250	260	270	280
c	Cs	152.790	193.370	193.550	196.270	199.120	202.100	205.230
liq	Cs							208.540
	K	290	298.15	300				
liq	Cs	212.030	215.030	215.730				

K = Temperature in K

Cs = Heat Capacity, in J/(K · mol)

c = Pseudocumene Crystal State

liq = Pseudocumene Liquid State



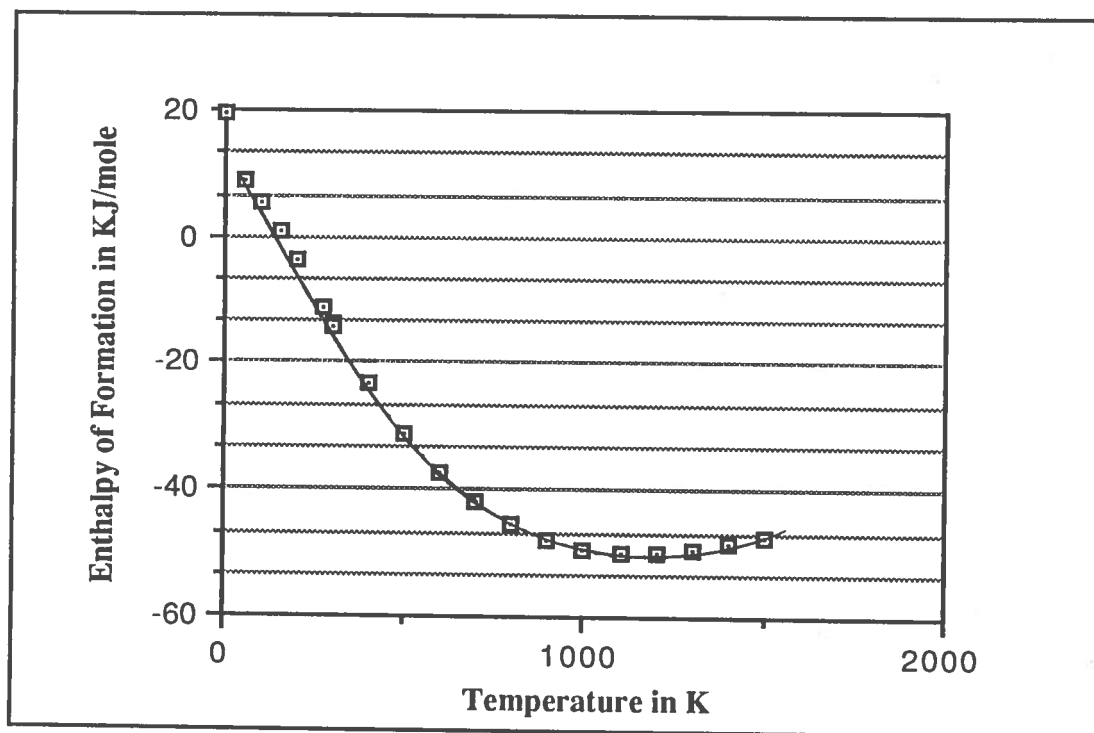
These values are drawn from the TRC Thermodynamic Tables-Hydrocarbons

ENTHALPY OF FORMATION, " $\Delta_f H^\circ$ ", FOR THE PSEUDOCUMENE IDEAL GAS STATE.

K	0	50	100	150	200	273.15	298.15	300
H	19.71	9.07	5.29	1.05	-3.79	-11.31	-13.81	-13.99
K	400	500	600	700	800	900	1000	1100
H	-23.37	-31.14	-37.30	-42.05	-45.56	-47.96	-49.31	-49.84
K	1200	1300	1400	1500				
H	-49.82	-49.36	-48.53	-47.39				

K = Temperature in K

H = Enthalpy of Formation, in KJ/mol



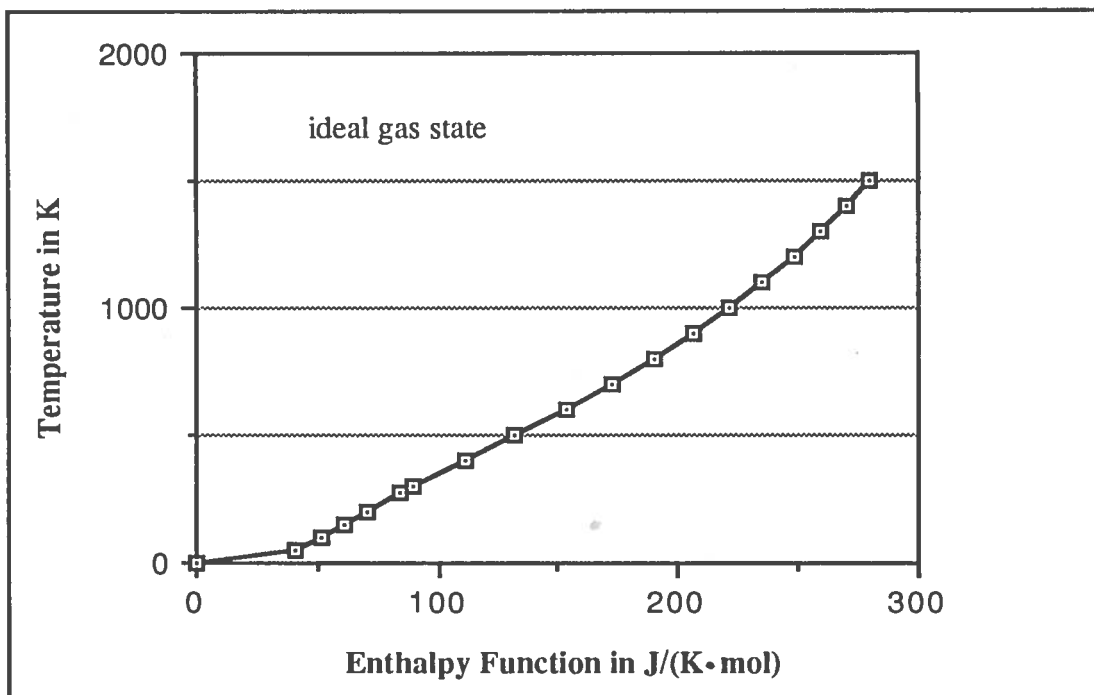
These values are drawn from the TRC Thermodynamic Tables-Hydrocarbons

ENTHALPY FUNCTION, " $(H^\circ - H^\circ_0)/T$ ", FOR THE PSEUDOCUMENE IDEAL GAS STATE.

K	0	50	100	150	200	273.15	298.15	300
H	0	40.84	51.80	61.58	70.83	84.71	89.69	90.06
K	400	500	600	700	800	900	1000	1100
H	110.95	132.30	152.94	172.29	190.16	206.58	221.62	235.40
K	1200	1300	1400	1500				
H	248.03	259.64	270.31	280.24				

K = Temperature in K

H = Enthalpy Function , in J/ (K · mol)

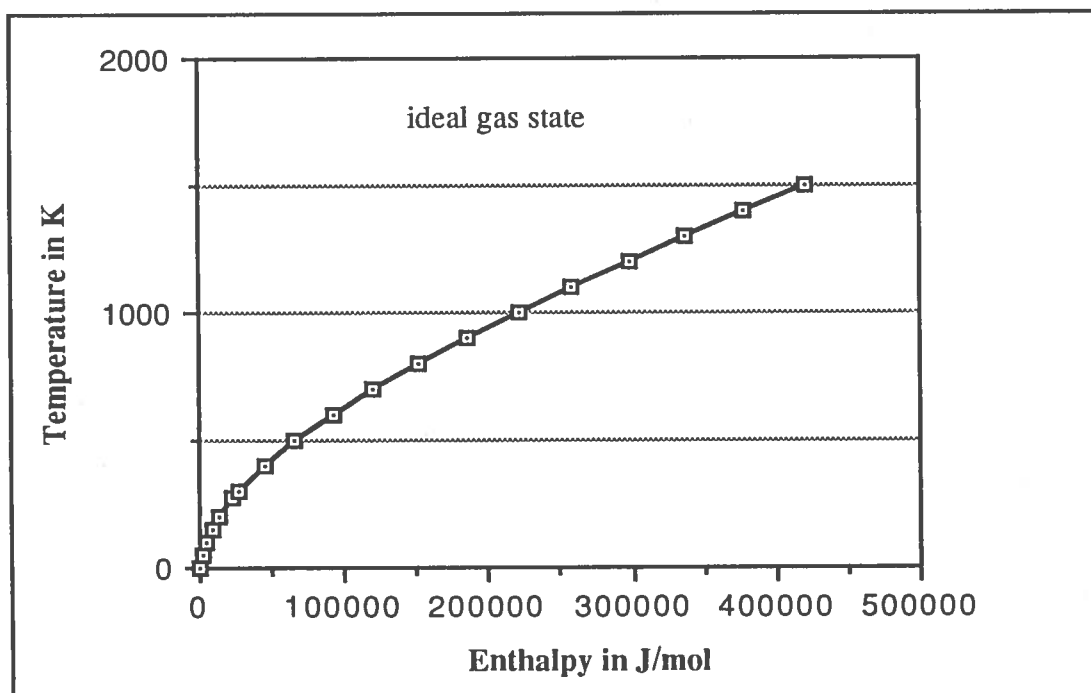


ENTHALPY, " $H^\circ - H^\circ_0$ ", FOR THE PSEUDOCUMENE IDEAL GAS STATE.

K	0	50	100	150	200	273.15	298.15	300
H	0	2042.0	5180.4	9237.8	14166.0	23140.0	26740.0	27018.0
K	400	500	600	700	800	900	1000	1100
H	44379.0	66151.0	91766.0	120600.0	152130.0	185920.0	221620.0	258940.0
K	1200	1300	1400	1500				
H	297640.0	337530.0	378430.0	420210.0				

K = Temperature in K

H = Enthalpy, in J/mol



These values are drawn from the Thermodynamic Tables-Hydrocarbons

ENTHALPY, " $(H_s - H^0)$ ", FOR THE PSEUDOCUMENE CRYSTAL AND LIQUID STATES.

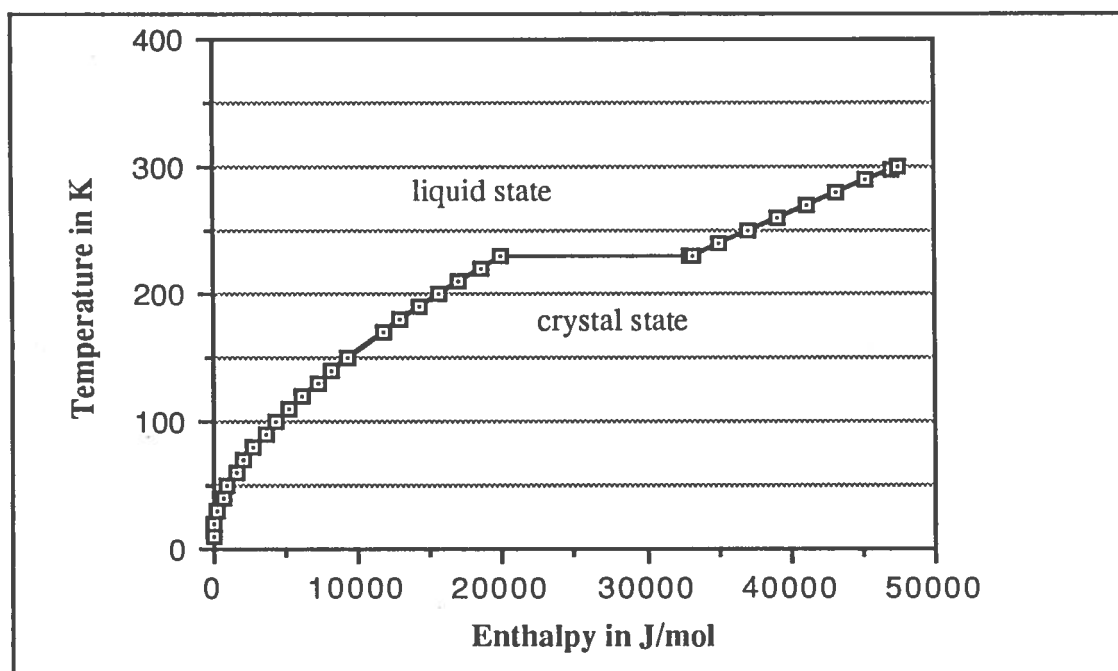
State	K	10	20	30	40	50	60	70
c	H	3.7	91.1	290.6	599.9	1010.5	1514.6	2105.0
	K	80	90	100	110	120	130	140
c	H	2775.3	3519.8	4333.8	5213.1	6154.0	7153.5	8208.
	K	150	160	170	180	190	200	210
c	H	9317.9	10479.0	11691.0	12952.0	14263.0	15622.0	17029.0
	K	220	229.33	230	240	250	260	270
c	H	18485.0	19889.0					
liq	H		33079.0	33208.0	35157.0	37134.0	39140.0	41177.0
	K	280	290	298.15	300			
liq	H	43245.0	45348.0	47088.0	47487.0			

K = Temperature in K

H = Enthalpy, in J/mol

c = Pseudocumene Crystal State

liq = Pseudocumene Liquid State



TRC
TRC
TRC

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Page uc-3292 table 23-2-(33.1110)-uc, page 3

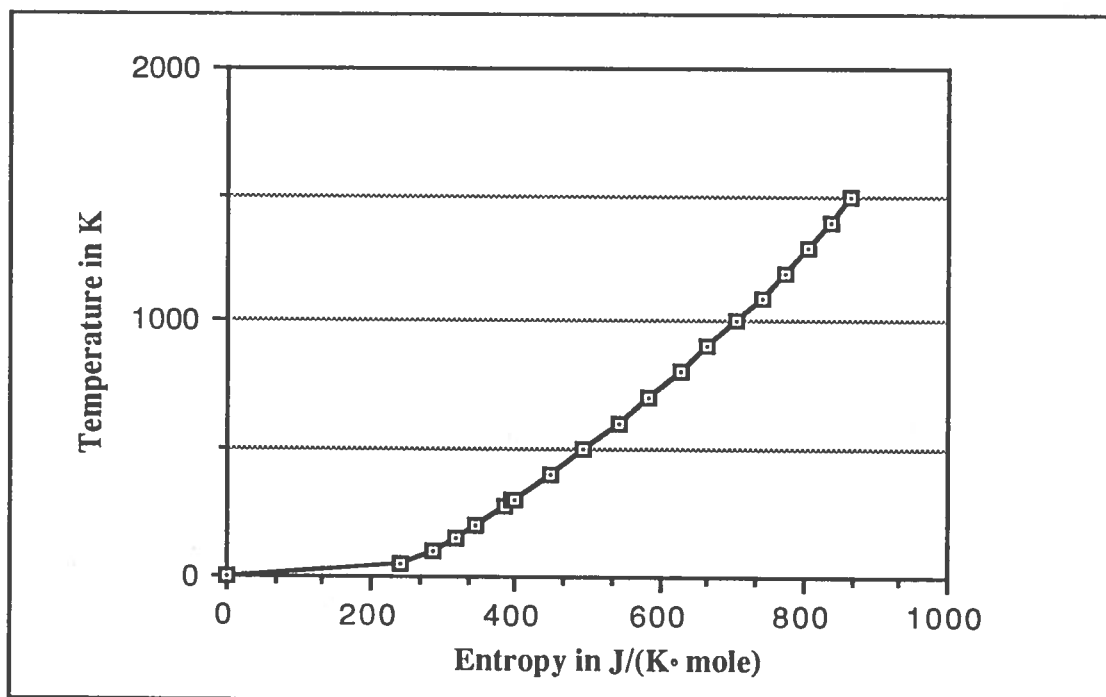
These values are drawn from the TRC Thermodynamic Tables-Hydrocarbons

ENTROPY, "S", FOR THE PSEUDOCUMENE IDEAL GAS STATE.

K	0	50	100	150	200	273.15	298.15	300
S	0	241.01	283.71	316.37	344.61	382.60	395.20	396.13
K	400	500	600	700	800	900	1000	1100
S	445.76	494.17	540.77	585.17	627.23	667.00	704.60	740.16
K	1200	1300	1400	1500				
S	773.82	805.74	836.05	864.88				

K = Temperature in K

S = Entropy, in J/(K · mol)



ENTROPY, S_s , FOR THE PSEUDOCUMENE, CRYSTAL AND LIQUID STATES.

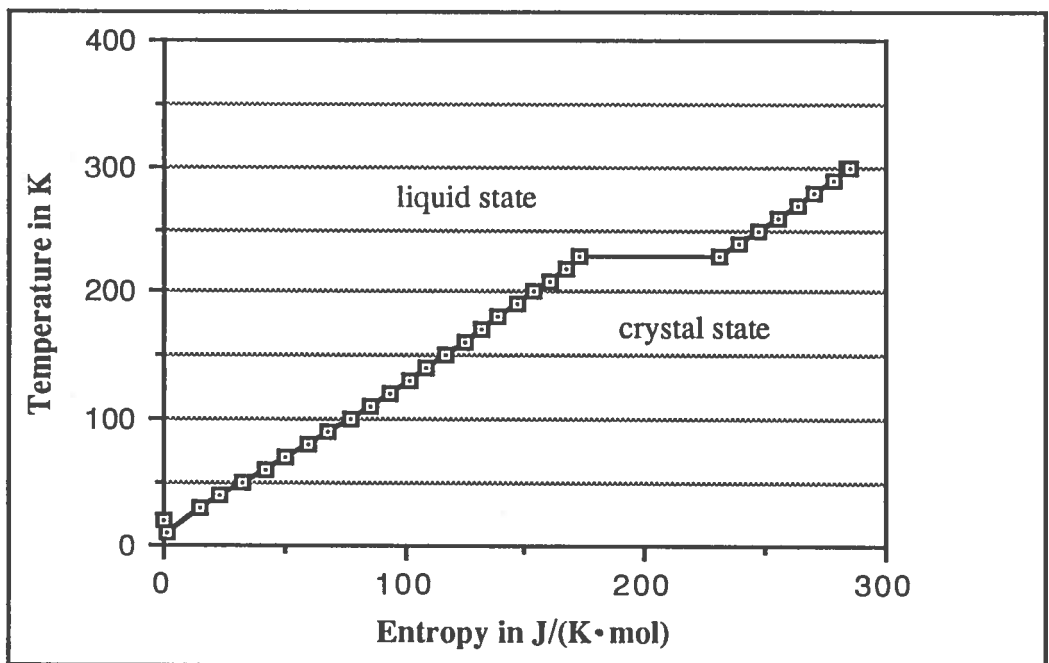
State	K	20	30	40	50	60	70	80
c	S	6.428	14.350	23.176	32.299	41.465	50.549	59.488
	K	90	100	110	120	130	140	150
c	S	68.249	76.819	85.195	93.378	101.380	109.190	116.840
	K	160	170	180	190	200	210	220
c	S	124.340	131.680	138.890	145.970	152.940	159.810	166.580
	K	229.33	230	240	250	260	270	280
c	S	172.330						
liq	S	230.340	230.910	239.200	247.270	255.140	262.820	270.350
	K	290	298.15	300				
liq	S	277.730	283.640	284.980				

K = Temperature in K

S = Entropy, in J/(K · mol)

c = Pseudocumene Crystal State

liq = Pseudocumene Liquid State

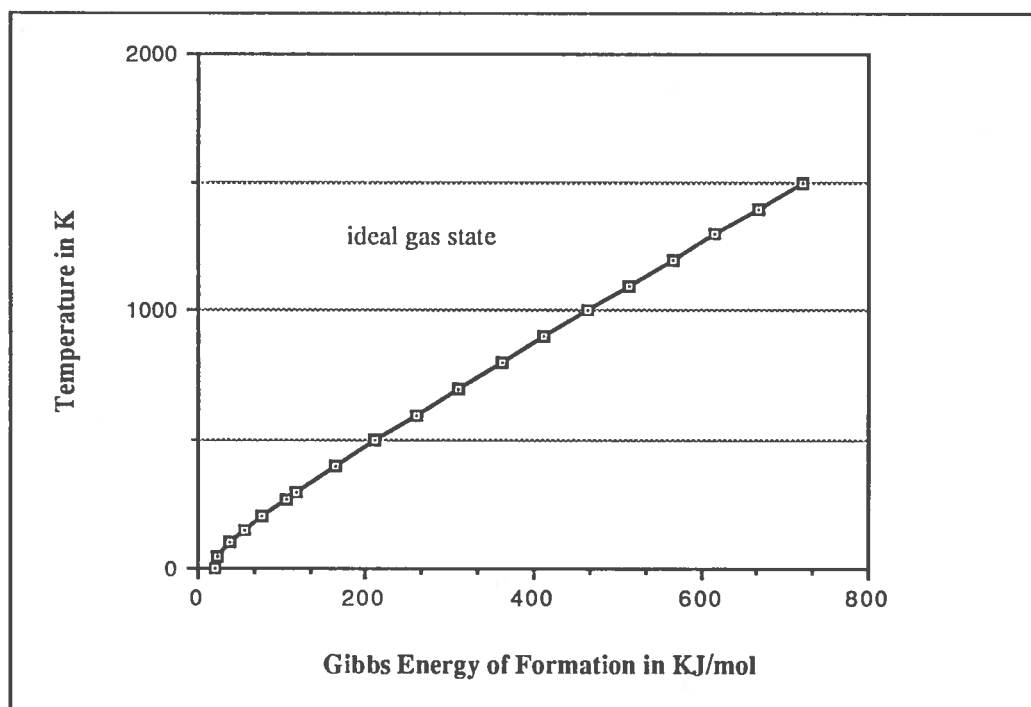


GIBBS ENERGY OF FORMATION, " $\Delta_f G^\circ$ ", FOR THE PSEUDOCUMENE IDEAL GAS STATE.

K	0	50	100	150	200	273.15	298.15	300
G	19.71	23.30	39.00	56.73	76.05	106.37	117.34	118.17
K	400	500	600	700	800	900	1000	1100
G	163.71	211.37	260.46	310.52	361.14	412.15	463.54	514.38
K	1200	1300	1400	1500				
G	566.04	617.27	668.92	719.94				

K = Temperature in K

G = Gibbs Energy of Formation, in KJ/mol

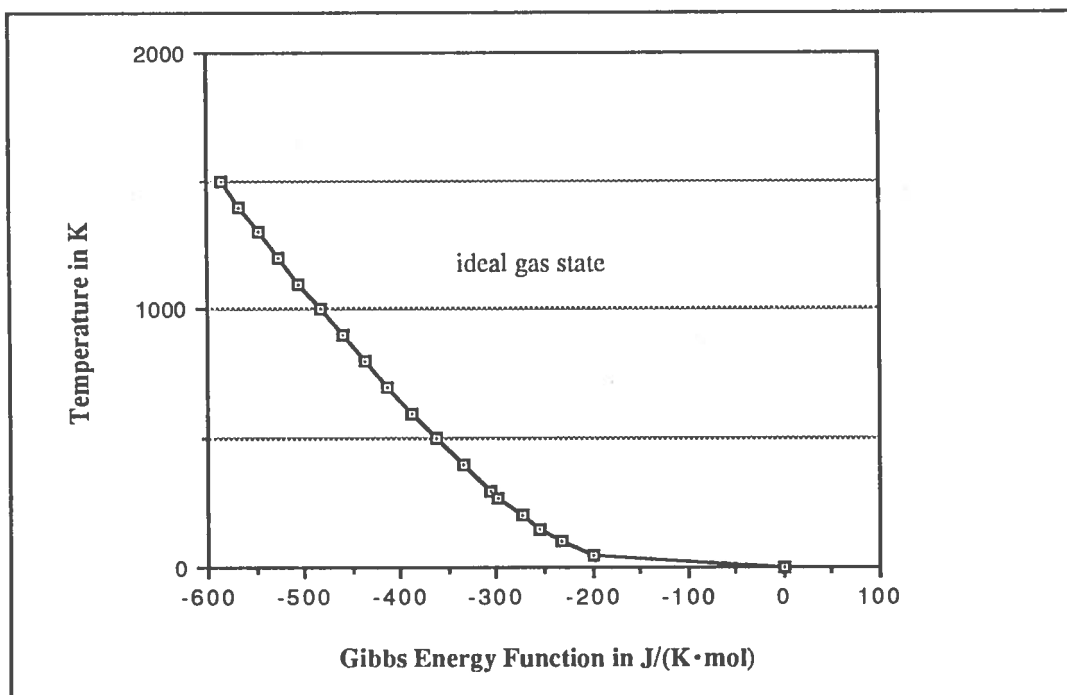


GIBBS ENERGY FUNCTION, $(G^\circ - H_0)/T$, FOR THE PSEUDOCUMENE IDEAL GAS STATE.

K	0	50	100	150	200	273.15	298.15	300
G	0	-200.17	-231.90	-254.79	-273.78	-297.88	-305.52	-306.07
K	400	500	600	700	800	900	1000	1100
G	-334.81	-361.87	-387.83	-412.88	-437.07	-460.43	-482.98	-504.76
K	1200	1300	1400	1500				
G	-525.79	-546.11	-565.75	-584.74				

K = Temperature in K

G = Gibbs Energy Function, in J/(K · mol)



**GIBBS ENERGY FUNCTION, $(G_S - H^0)/T$,
FOR THE PSEUDOCUMENE CRYSTAL AND LIQUID STATES.**

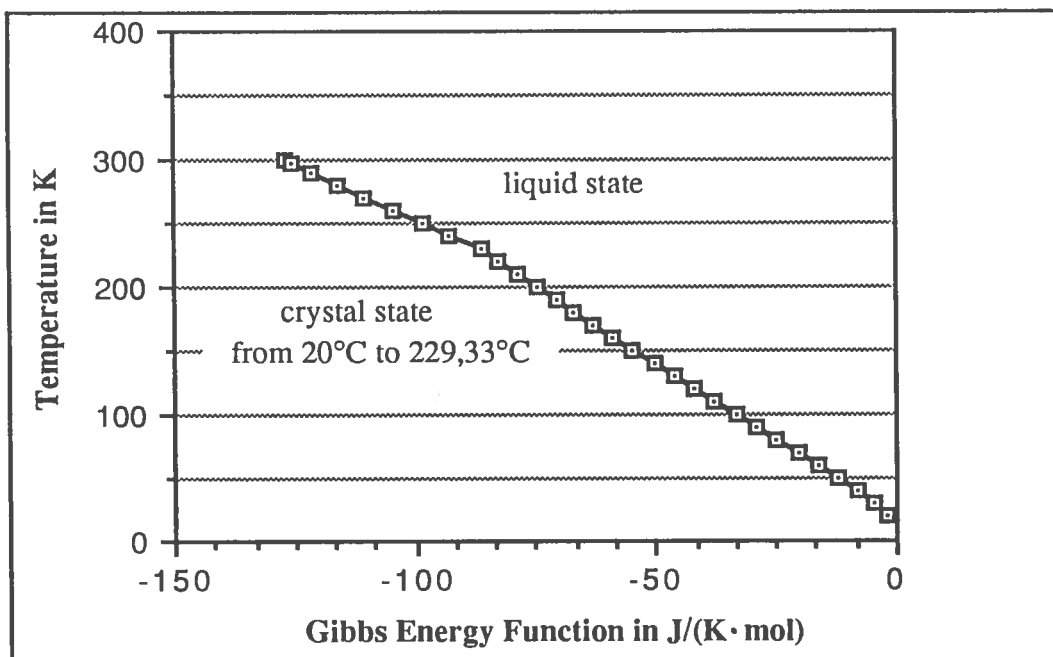
State	K	20	30	40	50	60	70	80
c	G	-1.864	-4.664	-8.179	-12.088	-16.221	-20.478	-24.797
	K	90	100	110	120	130	140	150
c	G	-29.140	-33.481	-37.803	-42.094	-46.348	-50.559	-54.724
	K	160	170	180	190	200	210	220
c	G	-58.841	-62.910	-66.932	-70.906	-74.834	-78.718	-82.558
	K	229.33	230	240	250	260	270	280
c	G	-86.103						
liq	G	-86.103	-86.524	-92.714	-98.736	-104.600	-110.320	-115.900
	K	290	298.15	300				
liq	G	-121.350	-125.710	-126.690				

K = Temperature in K

G = Gibbs Energy Function, in J/(K · mol)

c = Pseudocumene Crystal State

liq = Pseudocumene Liquid State



SECOND VIRIAL COEFFICIENT, "B" , FOR THE PSEUDOCUMENE GAS.

T/T ^c	0.50	0.55	0.60	0.65	0.70	0.75	0.80	0.85
B	-4600	-3200	-2420	-1890	-1520	-1260	-1060	-910
T/T ^c	0.90	0.95	1.00	1.10	1.20	1.30	1.40	1.60
B	-780	-684	-601	-473	-378	-304	-247	-161
T/T ^c	1.80	2.00	2.50	3.00	3.50	4.00	4.50	5.00
B	-102	-58	+14	56	84	104	119	130

B = Second Virial Coefficient, in cm³/mol

T/T^c = Reduced Temperature

Values of the second virial coefficient B are calculated from the following constants :

T^c = 649.05 K; u/K = -1452 K; V* = 151.1 cm³/mol

R₁ = 0.703; R₂ = 1.13; R₃ = 4.25

and the equation :

$$B = 2V^*[R_1 - (1-R_1)[\exp(\bar{u}/kt) - 1] - (R_2 - 1)[\exp(-\bar{u}/kT) - 1] - (R_3 - R_2)[\exp(-0.21\bar{u}/kT) - 1]]$$

