

**STUDY OF PHYSIOCHEMICAL PROPERTIES OF
COMMERCIAL SAMPLES OF ISOPROPHYLDICYCLOHEXYL
AND DIETHYLCYCLOHEXANE**

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NOVEMBER 1960

Materials Central
Contract No. AF 33(616)-5587
Project No. 3048

WRIGHT AIR DEVELOPMENT DIVISION
AIR RESEARCH AND DEVELOPMENT COMMAND
UNITED STATES AIR FORCE
WRIGHT-PATTERSON AIR FORCE BASE, OHIO

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FORWORD

This report was prepared by the Inglewood Laboratory, Aircraft System Division of Thompson Products, Indiana under USAF Contract No. AF 33(616)-5587. The contract was initiated under Project No. 3048, "Aviation Fuels", Task No. 30178, "Effect of Fuel Properties on Fuel Systems". It was administered under the direction of the Propulsion Laboratory and Materials Central, Directorate of Advanced Systems Technology, Wright Air Development Division, with Lt. T. L. Gossage acting as project engineer.

This report covers the work performed during the period February 1958 to December 1958.

L. A. Schlagel was the project manager for Thompson Products, Inc., and E. Findl, H. Brande and H. Edwards conducted all the experimental work for this project at the Inglewood Laboratory, Inglewood, California.

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ABSTRACT

The purpose of this program was to determine certain physical and thermodynamic properties of commercial samples of isopropyldicyclohexyl (IDH) and diethylcyclohexane (DCH).

Each of the program objectives was accomplished. Isopropyldicyclohexyl (IDH) is quite similar to fuels meeting the RJ-1 specification in most of its thermodynamic properties. Its distillation range is considerably less for DCH than a JP-6H fuel.

Included for additional information are data on gross heats of combustion of the two fuels.

PUBLICATION REVIEW

This report has been reviewed and is approved.

FOR THE COMMANDER:



M. P. DUNNAM
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Applications Laboratory
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SYMBOLS

C	-	specific heat or heat capacity
$\underline{C(T)}$	-	total heat capacity of vessel at temperature (T)
C_p	-	specific heat at constant pressure
C_p°	-	specific heat at one atmosphere
C_v	-	specific heat at constant volume
H	-	enthalpy
J	-	work-heat equivalent
\underline{J}	-	flow of enthalpy into vessel
P	-	pressure
P°	-	atmospheric pressure
R	-	gas constant
S	-	entropy
T	-	temperature
V	-	volume
V	-	molar volume
W	-	weight

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- Z - compressibility factor
- α - residual volume
- ρ - density

SUBSCRIPTS

- A - vessel A
- B - vessel B
- L - liquid
- T - total
- V - vapor

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INTRODUCTION

The purpose of this program was to determine certain physical thermodynamic properties of commercial samples of isopropyldicyclohexyl (IDH) and diethylcyclohexane (DCH).

Specific experimental properties to be evaluated included:

1. Density - temperature relationships over the range 0° - 500°F.
2. Liquid specific heats over the range 100° - 500°F.
3. Heats of vaporization.
4. Vapor pressure - temperature relationships.

Utilizing this experimental information, entropy temperature relationships were to be computed.

Manuscript released by author September 1960 for publication as a WADD Technical Report.

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TEST EQUIPMENT AND PROCEDURE

Density-temperature measurements are made using a specific volume technique. The device utilized is shown schematically in Figure No. 1. It was developed originally for simultaneous measurement of viscosity, equilibrium solubility and density. Its major components are two concentric glass tubes, invar end caps, an agitation system, a constant temperature bath and a pump. The inner glass tube is a piece of truebore tubing in which the fuel sample is placed. A clear heat transfer fluid, Ondina Oil, is circulated from the constant temperature bath through the annular space between the tubes.

A weighed quantity of fuel is measured into the cell at ambient temperature prior to the final assembly of one end cap. The volume of fuel charged is adjusted such that the initial vapor-liquid volume ratio is approximately 1:2. This value is chosen because past experience has shown that hydrocarbons expand roughly 1/3 in the range of ambient to 500°F.

The cell then is closed and the liquid level is noted. The bath is brought to desired temperature and the circulation of the Ondina Oil is begun.

Cell temperatures are measured by iron-constantan thermocouples. The temperature drop along the test cell is kept smaller than 1°C. Temperature equalization between the fuel and heat transfer oil is accomplished rapidly by rocking the cell. When thermal equilibrium is reached, the agitator is stopped, the cell placed in a vertical position and the scale read. This procedure is continued over the desired temperature range. The change in internal volume per linear unit level change is known. Therefore, since the mass of fuel has not changed, the density can be computed. The accuracy of this device is estimated at $\pm 1\%$.

Liquid specific heats are determined in a comparison calorimeter, (Figure No. 2). It is a modified version of the device used by N. H. Spear (Ref. 1). The modification consists of eliminating the magnetic stirrers and liquid heat transfer bath. Substituted for these items are a mechanical vibrator and an oven using heated air alone as the transfer medium. In addition, the cells are not vented. This prevents evaporation losses which must be considered in this application because the liquids are not pure. Specific heats are determined by comparing the temperature rise rates of a material whose specific heat is known and one whose specific heat is desired.

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A weighed quantity (100cc) of fuel and reference fluid is charged into the fuel cells at ambient temperature. Both cells are then dropped into the air bath oven, the air agitator is turned on and an electric timer is started. The fuel temperature is measured by means of iron-constantan thermocouples. The elapsed time for each of the fuels to reach a specific temperature is noted. The temperature rise rates are then computed and the specific heat determined.

Heats of vaporization are determined in the calorimeter shown in Figure No. 3. This unit contains a spherical fuel cell with an electric heater, a vacuum chamber and associated electrical power and instrumentation equipment. Heats of vaporization are determined by measuring the quantity of electrical energy required to evaporate a measured quantity of fuel. Radiation, convection and conduction losses are very nearly eliminated by maintaining a vacuum of less than (1.0 mm Hg) around the fuel cell, keeping the bath temperature at the same temperature as the test fluids and using thin stainless steel tubing for flow lines.

Approximately 100 cc of fuel is charged into the fuel cell, sufficient to completely immerse the heater and fill the cell approximately 60%. The fuel heater is turned on and the bath heater controlled so that bath and fuel temperatures are equalized. The auxiliary heater is maintained a few degrees hotter than the fuel cell to prevent condensation and refluxing.

Approximately 20 cc of fuel is first boiled off to allow the system to come to a steady state. At this time a condensate collector is inserted in the condensate line and an electric timer started. The condensate is collected for a period of 20 to 30 minutes depending upon the quantity of fuel evolved. This quantity of fuel is then weighed. Knowledge of weight of fuel vaporized and the heater power permits the calculation of the heat of vaporization.

Temperatures are measured by iron-constantan thermocouples. Electrical energy to the fuel heater is measured by utilizing a calibrated shunt and potentiometer for current and a calibrated resistance network and potentiometer for voltage measurement (See Figure No. 4). Regulated, rectified power is supplied by a 110 volt power regulator, 0-18volt D.C. rectifier and a 12 volt storage battery used as a filter. A-C modulation of the D-C output is extremely small, $< 0.1\%$. The accuracy of the device is estimated at $\pm 2\%$.

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ASTM distillations were performed on each of the fuels as a matter of standard practice. Method D 158-54 or D 86-54 was used.

Vapor pressures are measured in the device shown in Figure No. 5. Fuel is charged into the cell and deaerated by one of two methods. For petroleum mixtures such as the JP fuels, the air is removed by means of a vacuum pump and a cold trap. For pure high boiling compounds, deaeration is simply accomplished by slowly bringing the fuel up to boiling while vigorously agitating.

Once the fuel has been deaerated, the cell is sealed. The heat input is then controlled so that the fuel cell walls and fuel attain some desired temperature. Once liquid-vapor equilibrium has been attained, pressure measurements are made by means of strain gauge type pressure transducers and potentiometer read out instruments.

A Burrell model K-2 gas chromatography unit was used to obtain chromatographic separation of the fuels. Helium was used as the carrier gas and the column material was celite and silicon oil. The initial column temperature was approximately 120°C. Charging was accomplished by means of a micrometer syringe. After charge, the temperature was increased to obtain optimum, rapid separation.

Heats of combustion were measured in a Parr adiabatic calorimeter using standard techniques.

EXPERIMENTAL DATA

The experimentally determined density-temperature relationships are shown on Figure Nos. 6, 7 and Table I. Mathematical expressions $\pm 1\%$ for the data in the 0-500° F range are as follows,

where ρ is in cc/gram and T in °F:

1. For IDH $\rho = 0.908 - 3.661 \times 10^{-4} T$

2. For DCH $\rho = 0.831 - 2.555 \times 10^{-4} T - 3.927 \times 10^{-7} T^2$

Figure Nos. 8, 9 and Table II show the liquid specific heat values obtained. It is to be noted that the specific heat values are neither C_P nor C_V values as such, but simply the ratio of the heat absorbed by the fuels to the increase in temperature of the fuel at the conditions in the fuel cell. For all practical purposes however, they can be utilized as C_P° values inasmuch as $(\partial C_P / \partial P)_T = -T(\partial^2 V / \partial T^2)_P$

and this quantity is well within the experimental accuracy of the calorimeter (See discussion). The reference fluid used in the specific heat determinations was a commercial petroleum product called Shell UMF (Grade C). Dr. F. Littman of the Stanford Research Institute obtained the specific heat-temperature relationships of this fuel for us using enthalpy measurements from a drop calorimeter.

Mathematical expressions ($\pm 3\%$) for the specific heats of the test fuels are as follows,

where specific heat is in BTU/lb. and temperature in °F:

1. For IDH $C = 0.372 + 6.0 \times 10^{-4} T$

2. For DCH $C = 0.415 + 4.8 \times 10^{-4} T$

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Vapor pressures for the fuels are given in Figure Nos. 10, 11, 12 and Table III. Mathematical expressions ($\pm 2\%$) for these vapor pressures are as follows,

where P is in Psia and Temperature in $^{\circ}\text{R}$

1. For IDH $\log_{10} P = \frac{4,478}{T} + 0.594 \log_{10} T + 3.898$

2. For DCH $\log_{10} P = \frac{3676}{T} + 5.745$

Heats of vaporization ($\pm 2\%$) for each of the test fuels at atmospheric pressure are as follows:

1. IDH - 104.1 BTU/lb.
2. DCH-- 121.2 BTU/lb.

ASTM distillation results are shown on Figure Nos. 13 and 14

Gross heats of combustion for each of the test fuels are as follows:

1. IDH 19,093 BTU/lb.
2. DCH 19,624 BTU/lb.

Figure Nos. 15 and 16 are tracings of the separation results obtained on a Burrell Kromotog Model K-2. The IDH chromatogram shows but one peak. This compound has numerous isomeric possibilities but apparently the column material used did not separate them.

The DCH chromatogram also appears to be relatively simple. Other runs (not shown) at higher sensitivity settings show two minor peaks at the leading edge. This fuel also has numerous isomeric possibilities.

CALCULATION OF ENTHALPY AND ENTROPY

In addition to the physio chemical data given in the preceding, temperature-enthalpy and temperature entropy diagrams for each of the fuels was computed. This was accomplished utilizing standard thermodynamic relationships, certain correlations, and the experimental data.

The experimentally determined specific heat curve was used to obtain the saturated liquid line on an enthalpy-temperature diagram by utilizing the enthalpy-specific heat relationship.

$$\int_{H_1}^{H_2} dH = \int_{T_1}^{T_2} C_P dT$$

An arbitrary datum of $H = 0$ at 0°F was chosen for convenience. Critical constants were computed using correlations of L. C. Roess (Reference 2) and W. C. Edmister and D. H. Pollock (Reference 3).

To the saturated liquid line was added the heats of vaporization as obtained from experimental information and the correlation of K. M. Watson (Reference 4). Interpolation between the points so determined, completed the phase envelope on an H-T chart.

Vapor specific heats at constant pressure then were calculated. The reasonable assumption was made that at pressure below atmospheric, the vapor specific heat is not pressure dependent. Therefore, the saturated vapor line below atmospheric pressure on the H-T chart, represents the specific heat of the saturated vapor or,

$$C_P^\circ = \left(\frac{\partial H}{\partial T} \right)_{P(0-14.7)} \quad (2)$$

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The $C_{P^{\circ}}$ values thus obtained were extrapolated to higher temperatures.

In order to compute C_P values in the regions above 1 atmosphere, of Deming and Shupe (Reference 5) was used.

$$C_P = C_{P^{\circ}} - \frac{T}{J} \int_{P^{\circ}}^P \left(\frac{\partial^2 V}{\partial T^2} \right)_P \cdot dP \quad (3)$$

$$\alpha = \frac{RT}{P} - V \quad (4)$$

$$Z = \frac{PV}{RT} \quad (5)$$

$$\alpha = \frac{RT}{P} (1-Z) \quad (6)$$

$$\left(\frac{\partial^2 V}{\partial T^2} \right)_P = - \left(\frac{\partial^2 \alpha}{\partial T^2} \right)_P \quad (7)$$

$$C_P = C_{P^{\circ}} + \frac{T}{J} \int_{P^{\circ}}^P \left(\frac{\partial^2 \alpha}{\partial T^2} \right)_P \cdot dP \quad (8)$$

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The compressibility factor of (6) was determined using the generalized P-V-T relationships for hydrocarbons of J. B. Maxwell (Reference 7). The second derivative of (8) was evaluated by graphical methods. Values of C_p thus obtained are shown on Figure Nos. 17 and 18.

Superheat enthalpies were computed by (1). This completed the H-T diagram.

Entropy was calculated by using the basic relationship.

$$dS = \frac{dH}{T} = \frac{C_p dT}{T} \quad (9)$$

Values obtained from the H-T charts were used for this purpose. Figure Nos. 19 and 20 are the enthalpy-temperature diagrams and Figure Nos. 21 and 22 are the entropy-temperature diagrams, which were calculated in this manner.

DISCUSSION

It was mentioned in the test equipment and procedure section that the use of specific heats as obtained in the method described are satisfactory for use as C_P° values since pressure has but a minor effect on specific heat at least in the range covered by the experimentation. This fact can be demonstrated quite readily numerically by using the experimental data determined for vapor pressure and density

$$\left(\frac{\partial C_P}{\partial P}\right)_T = -T \left(\frac{\partial^2 v}{\partial T^2}\right)_P \quad (10)$$

$$\left(\frac{\partial^2 v}{\partial T^2}\right)_P = \left(\frac{\partial^2 (1/\rho)}{\partial T^2}\right)_P \quad (11)$$

Utilizing the series the series function to define the variation of density with temperature, i. e., $\rho = A + BT + CT^2 + \dots$, the second derivative of (1) can be obtained. For example,

$$\left(\frac{\partial^2 (1/\rho)}{\partial T^2}\right)_P = \frac{(B + 2CT)}{(A + BT + CT^2)^2} - \frac{C}{(A + BT + CT^2)^3} \quad (12)$$

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$$\left(\frac{\partial C_P}{\partial P}\right)_T = \frac{2T C(A + BT + CT^2) - (B+2CT)^2}{(A + BT + CT^2)^3} \quad (13)$$

Substituting the values for DCH results in a variation of specific heat with pressure at a temperature of $8.07 \cdot 10^{-5}$ BTU/lb \cdot $^{\circ}$ R \cdot atmosphere. This value is well within the experimental error, since ΔP is less than 6 atmospheres at this temperature.

The comparison calorimeter method used to obtain the data presented herein is based upon the following assumption. That the heat transfer rate into a vessel containing a liquid whose specific heat is known is the same as the heat transfer rate into an identical vessel containing a liquid whose specific heat is unknown. This assumption is reasonable if the liquid-metal film heat transfer coefficients and the thermal conductivities of the liquids are nearly identical. Agitation can reduce the effects of these properties so that for all practical purposes the assumption is valid. The device used by N. H. Spear (Reference 1) permitted evaporation of the fluids. We felt that the correction factor this involved was of such a magnitude that the desired experimental accuracy ($\pm 3\%$) could not be attained, especially for petroleum distillates. It therefore became necessary to investigate the effect of pressure on the calorimeter calculations. A mathematical analysis of the corrections is given below:

The basic assumption in this method is that the flow of enthalpy into Vessel A when it is at temperature T is the same as the flow of enthalpy into vessel B when it is this same temperature, T. For either vessel we may write,

$$\underline{J} = \underline{C}(T) \frac{dT}{dt}$$

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where

\underline{J} is the flow of enthalpy into the vessel, enthalpy/unit time.

t is the time

$\underline{C}(T)$ is the total heat capacity of the vessel at the temperature T .

Then,

$$\underline{C}_A(T) \left(\frac{dT}{dt} \right)_A = \underline{C}_B(T) \left(\frac{dT}{dt} \right)_B$$

and if we plot $T(t)$ for A and for B and compare the slopes at any particular temperature, T , we have

$$\underline{C}_A(T) = \underline{C}_B(T) \left(\frac{\text{Slope B}}{\text{Slope A}} \right)_T$$

The problem which remains is to relate the total heat capacity of each vessel to the C_P of its liquid contents.

For the vessel, A, at the temperature, T , we have,

$$\underline{C}_A(T) = W_A \left(C_{PA} + \frac{\partial H_A}{\partial P} \cdot \frac{dP}{dT} \right) + W_L \left(C_{PL} + \frac{\partial H_L}{\partial P} \cdot \frac{dP}{dT} \right) + W_V \left(C_{PV} + \frac{\partial H_V}{\partial P} \cdot \frac{dP}{dT} \right) + (H_V - H_L) \frac{dW_V}{dT}$$

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where

$$W_A = \text{Wt of vessel A}$$

$$W_L = \text{Wt of liquid in vessel A}$$

$$W_V = \text{Wt of vapor in vessel A}$$

$$C_P = \text{Heat capacity per unit wt at constant P (Tilde: per mole)}$$

$$H = \text{Enthalpy per unit wt}$$

$$P = \text{Pressure within vessel}$$

$$W_T = W_L + W_V, \text{ the total wt. of the cell contents, assumed to be constant during an experiment}$$

It appears that within the desired accuracy, ($\pm 3\%$ in C_{PL})

$$\underline{C}_A(T) = W_A C_{PA} + W_L C_{PL}$$

This may be demonstrated by showing that the remaining terms are negligible even at the highest temperature of the experiments where dP/dT and dW_V/dT have their largest values. As an example, DCH at 500°F (533°K) will be examined. In this case (partly from the

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properties of DCH, partly assumed as reasonable parameters:

$$W_L = 81 \text{ g}$$

$$W_L C_{PL} = 53 \text{ cal/}^\circ\text{K}$$

$$W_A = 140 \text{ g}$$

$$V_A = 127 \text{ cm}^3 / \text{g}$$

$$W_T = 221$$

$$\text{Total Volume} : V_T = 167 \text{ ml}$$

$$\text{Liquid Density} : L = 0.61 \text{ g/ml}$$

$$: V_L = 1.64 \text{ ml/g}$$

$$\text{Molec. Wt.} : M = 140 \text{ g/mole}$$

$$: P = 83 \text{ Psia} = 5.65 \text{ Atm.}$$

$$\text{Molar Volume of Vapor} : \widetilde{V}_V = \frac{RT}{P} = 7.75 \times 1/\text{mole}$$

(Z assumed = 1)

$$V_V = 55.3 \text{ ml/g}$$

$$\text{Molar Volume of Liquid} : \widetilde{V}_L = M/L = 0.230 \text{ l/mole}$$

$$: \widetilde{\Delta V} = 7.52 \text{ l/mole}$$

$$: \Delta H_V = H_V - H_L = 100 \text{ Btu/lb;}$$

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$$\begin{aligned}\widetilde{\Delta H}_V &= 321 \text{ l. Atm/mole} \\ &= 55.6 \text{ cal/g} \\ \frac{dP}{dT} &= \frac{\widetilde{\Delta H}}{T\widetilde{\Delta V}} = 8.01 \times 10^{-2} \text{ atm/}^\circ\text{K}\end{aligned}$$

We use the general relation,

$$\frac{\partial H_A}{\partial P} = + T \frac{\partial S_A}{\partial P} + V_A = - T \frac{\partial V_A}{\partial T} + V_A$$

$$\frac{d \ln V_A}{dT} = 3.55 \times 10^{-5} / ^\circ\text{K}$$

(This thermodynamic equation is not strictly applicable in this case because the vessel is not subject to the same pressure inside and out, However, it is assumed that it gives at least the order of magnitude of H/P even in this case.) Inserting numerical values it is found,

$$V_A - T \frac{\partial V_A}{\partial T} = 0.130 \text{ ml/g}$$

and therefore for the first correction term,

$$W_A \cdot \frac{\partial H_A}{\partial P} \cdot \frac{dP}{dT} = 2.8 \times 10^{-2} \text{ cal/}^\circ\text{K.}$$

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Also,

$$\frac{\partial H_L}{\partial P} = -T \frac{\partial V_L}{\partial T} + V_L = 0.61 \text{ ml/g},$$

and therefore the second correction term is

$$W_L \cdot \frac{\partial H_L}{\partial P} \cdot \frac{dP}{T} = 0.096 \text{ cal/}^\circ\text{K}.$$

The weight of vapor is given approximately by the equation

$$W_V = \frac{MP}{RT} \left(V_T - \frac{W_L}{\rho_L} \right) = 0.34 \text{ g}$$

Using $C_{PV} = 0.5 \text{ cal/g } ^\circ\text{K}$ the next correction term is

$$W_V C_{PV} = 0.17 \text{ cal/}^\circ\text{K}.$$

Since this term is small compared to $W_L C_{PL}$ the following correction term is certainly also negligible.

For the final term we differentiate the equation for W_V to obtain

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$$\frac{d W_V}{dT} = \frac{M}{RT} \cdot \left[(V_T - V_L) \left(\frac{\partial P}{\partial T} + \frac{P}{T} \right) - P \frac{\partial V_L}{\partial T} \right] = 9.5 \cdot 10^{-3} \text{ g/}^\circ\text{K}$$

This gives for the final correction term.

$$\Delta H_V \cdot \frac{d W_V}{dT} = 0.53 \text{ cal/}^\circ\text{K.}$$

$$W_L \cdot C_{PL} = 53.5 \text{ }^\circ\text{K}$$

The sum of all of the correction terms is about 1.5% of $W_L C_{PL}$.

Neglecting these terms will produce a smaller error than 1.5% because there will be similar effects in the reference vessel. If the correction terms are taken into account for the 'unknown' liquid, they must be used for the reference liquid as well.

The effect of pressure on liquid specific does become significant in the critical region. Corrections to the entropy-temperature charts in this region due to liquid specific heat variation have not been made. The reason for omitting these corrections was that the critical constants are estimates and the specific heat data is extrapolated to this region. Therefore, it would seem that the corrections are not meaningful.

CONCLUSIONS

Presented in this report are the data completed on two tentative aviation fuels. A great deal of effort was spent in a literature survey for information relating to these fuels. A few references (References 7 through 16) in which information pertinent to the properties being investigated were located. The information reported in these references is given in Tables I and II. Information supplied by the manufacturers of the fuels is given on Tables IV and V. A recent report has been issued by the Monsanto Chemical Company (Reference 15) giving certain properties of the fuels reported herein. This report was received too late for data comparison and inclusion into this report.

1. Spear, N. H., Analytical Chemistry, Volume 24, No. 6, pp 938-941, June, 1952.
2. Roess, L. C., Journal of the Institute of Petroleum Technology, Volume 22, p 665, 1936.
3. Edmister, W. C., Pollack, D. H., Chemical Engineering Progress, Volume 44, No. 12, 1905, 1948.
4. Watson, K. M., Industrial and Engineering Chemistry, Volume 35, p 398, 1943.
5. Deming, W. E., Shupe, L. E., The Physical Review, Volume 38, pp 2245-2264, 1931, Volume 40, pp 848-859, 1932.
6. Maxwell, J. B., Data Book on Hydrocarbons, First Edition, D. Van Nostrand Co., Inc, Princeton, N. J., March, 1951.
7. Egeloff, E., "Physical Constants of Hydrocarbons", Volume 2, Reinhold Publishing Corp., New York, N. Y.
8. Dice, J. R., Loveless, L. E., Cote, H. L., Jr., Journal American Chemical Society Volume 71, 11 3546-8, 1949.
9. Schmerling, L., U. S. Patent 2,481, 160, Sept. 6, 1949.
10. Schmerling L., Journal American Chemical Society, Volume 71, pp 698-701, 1949.
11. Signargo, F. K., Cramer, P. L., Journal American Chemical Society, Volume 55, p 3326, 1933.
12. Stratford, R., Annales Combustibles Liquides, Volume 4, p 83, 1929.
13. Zelinsky, N. D., Rudervitsch, W., Berichte, Volume 28, p 1341, 1894.
14. Whitley, J. M., Lynch, C. S., U. S. Patent 2,433,079, Dec. 23, 1947.
15. Morris, H. E., Director, Research and Engineering Division, Monsanto Chemical Company, Private Communication.
16. Kennedy, E. R., Market Development Department Shell Chemical Company, Private Communication.

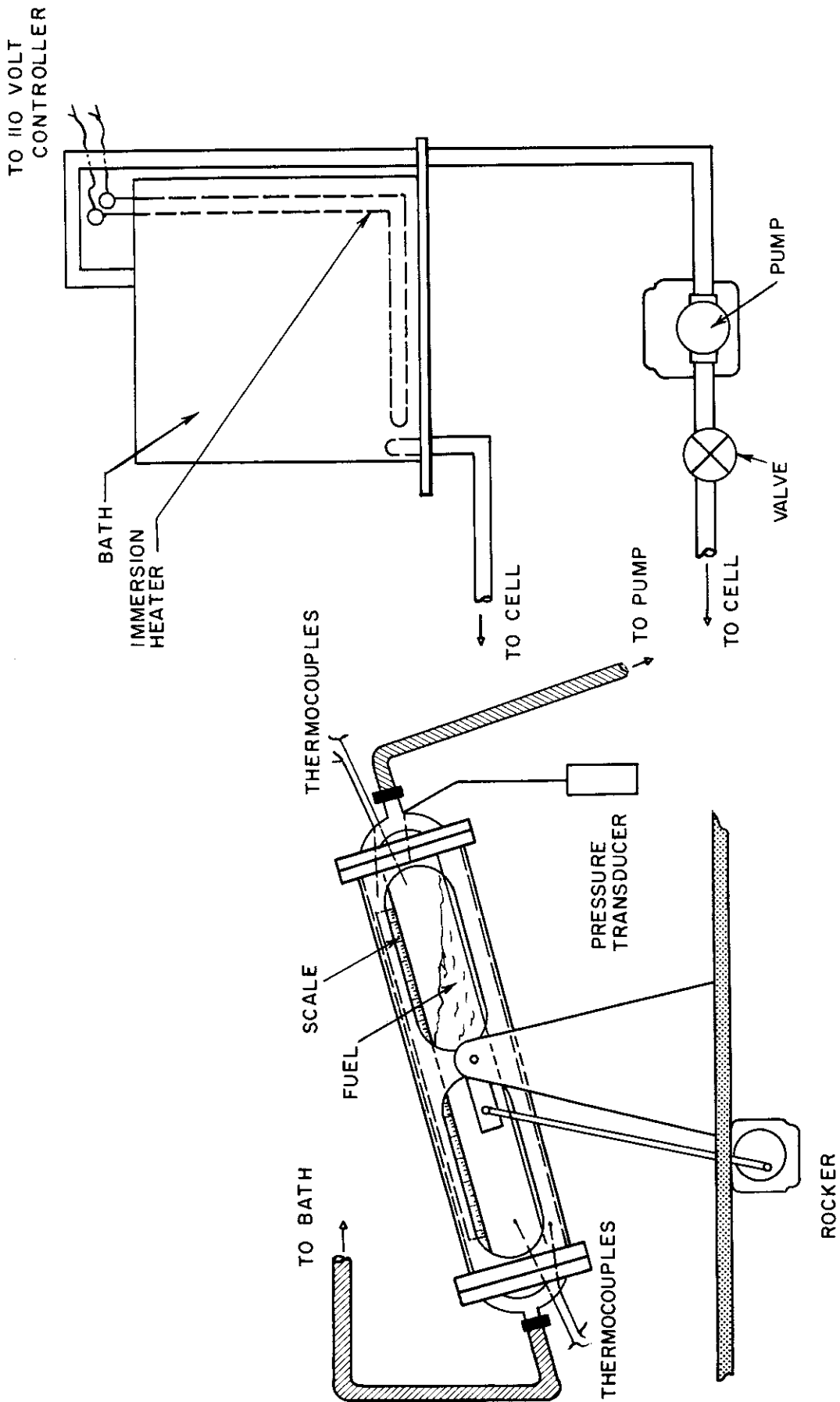


FIGURE 1. SPECIFIC VOLUME TEST APPARATUS

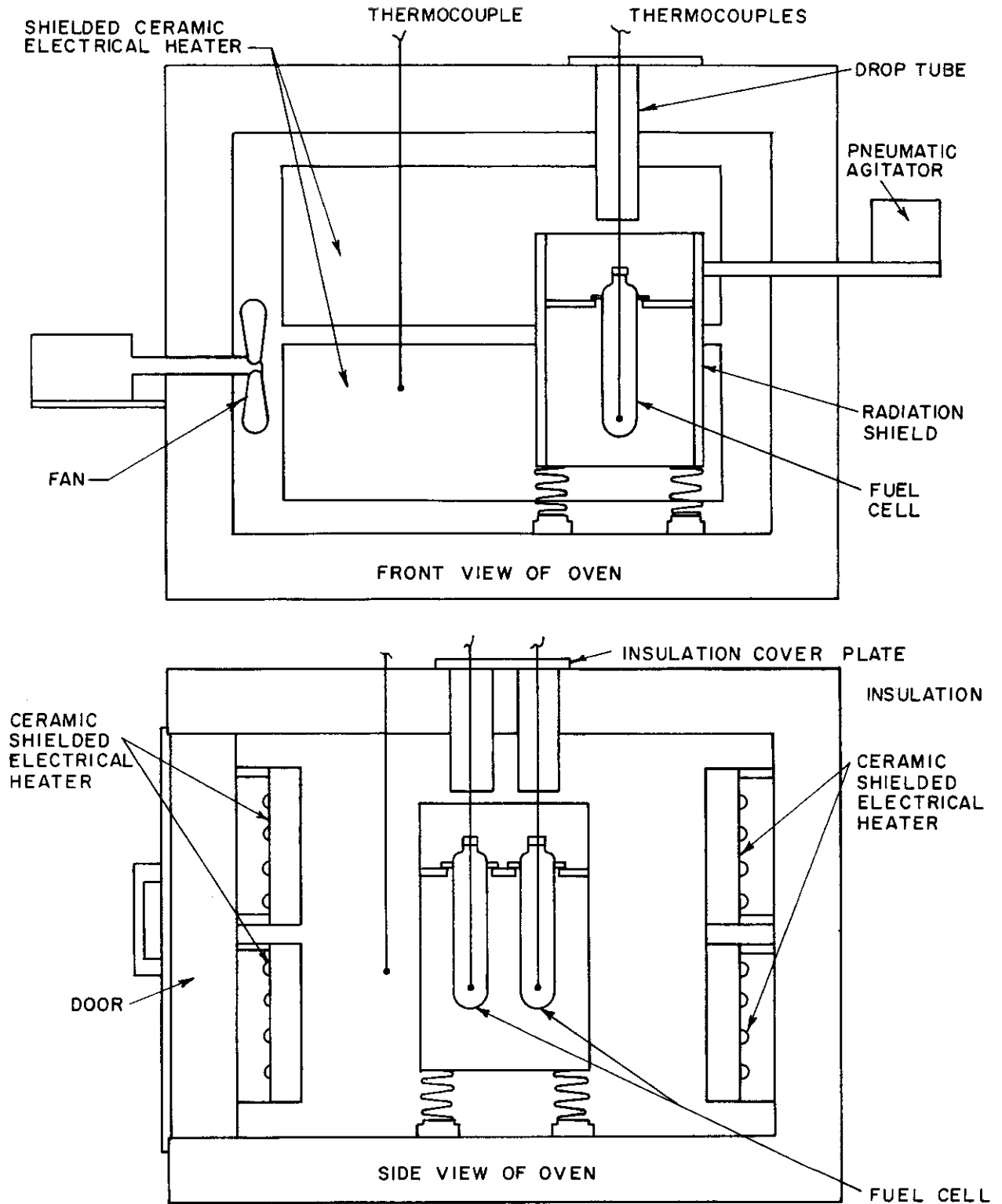
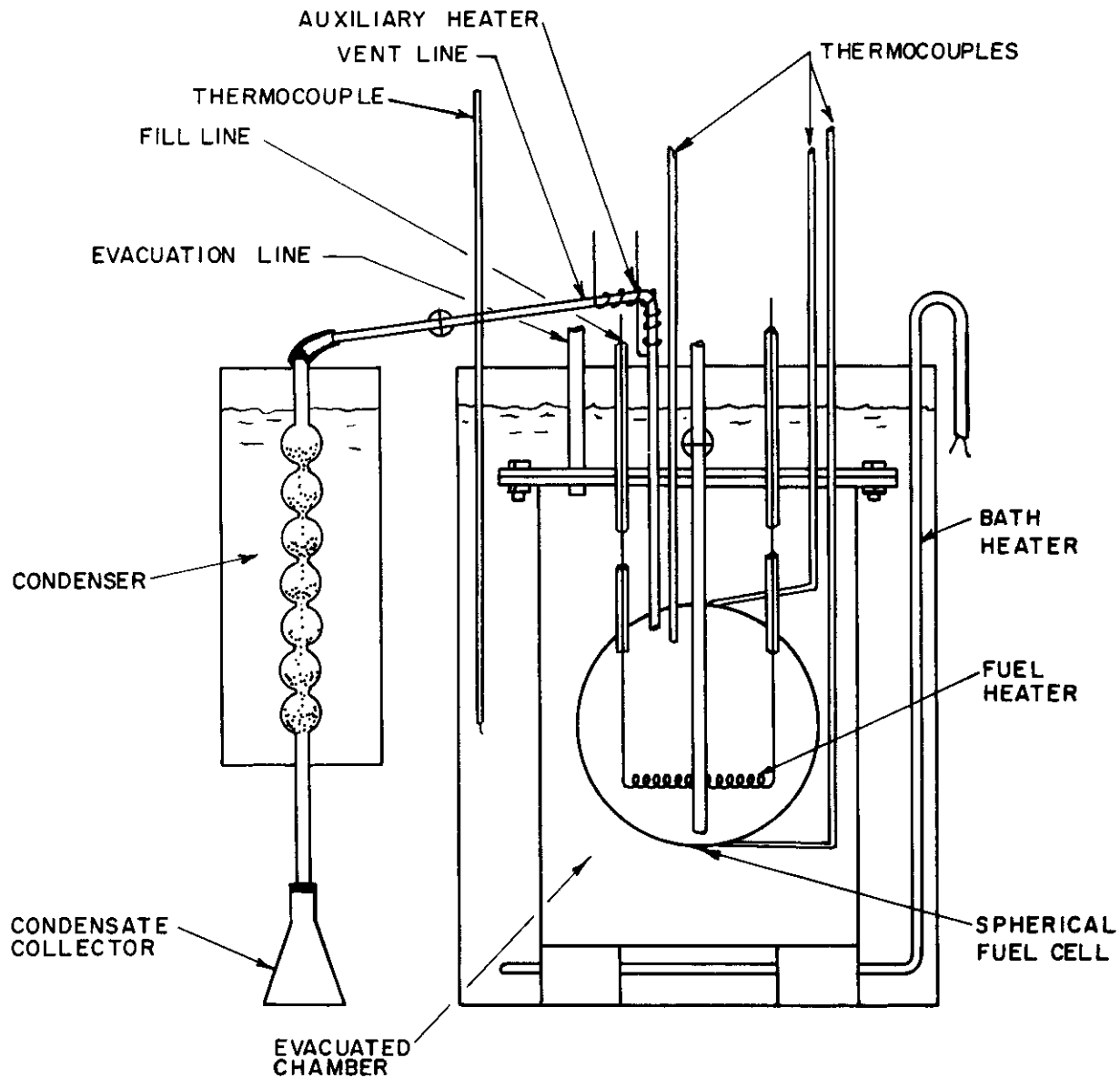


FIGURE 2. SCHEMATIC OF SPECIFIC HEAT RIG



NOTE: BATH AGITATOR NOT SHOWN

FIGURE 3. SCHEMATIC OF HEAT OF VAPORIZATION TEST APPARATUS

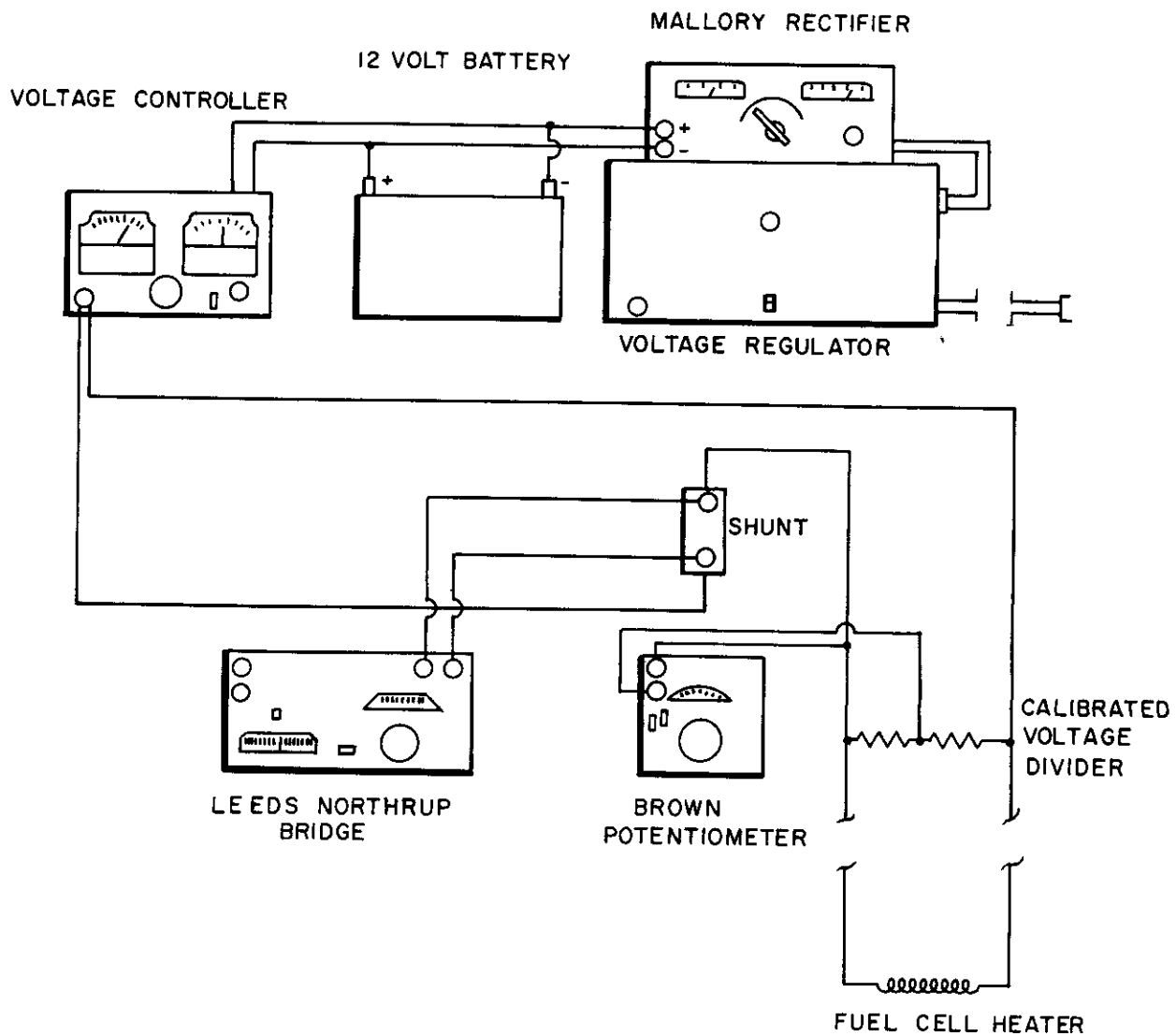


FIGURE 4. HEAT OF VAPORIZATION ELECTRICAL INSTRUMENTATION

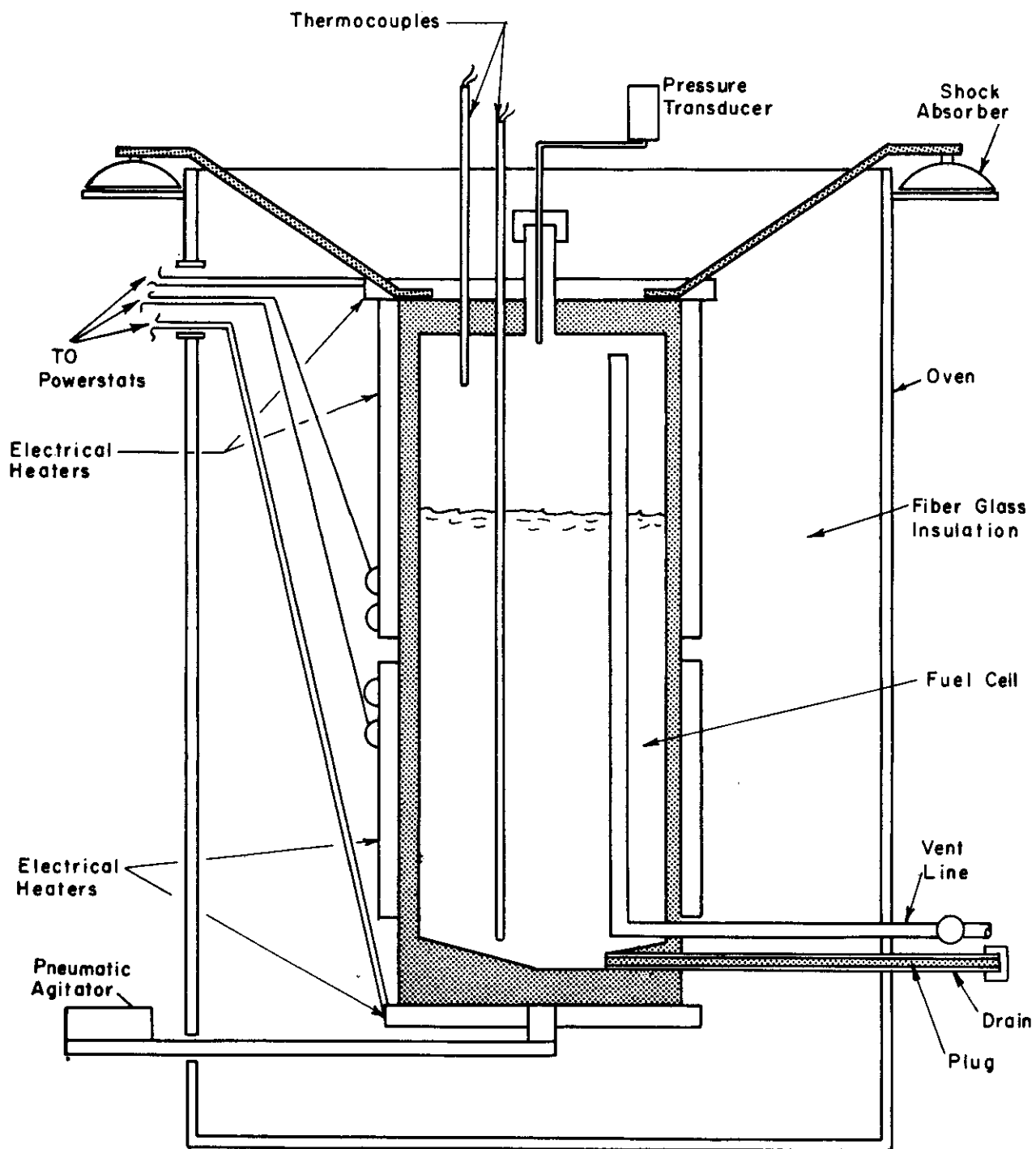


FIGURE 5. VAPOR PRESSURE TEST CELL

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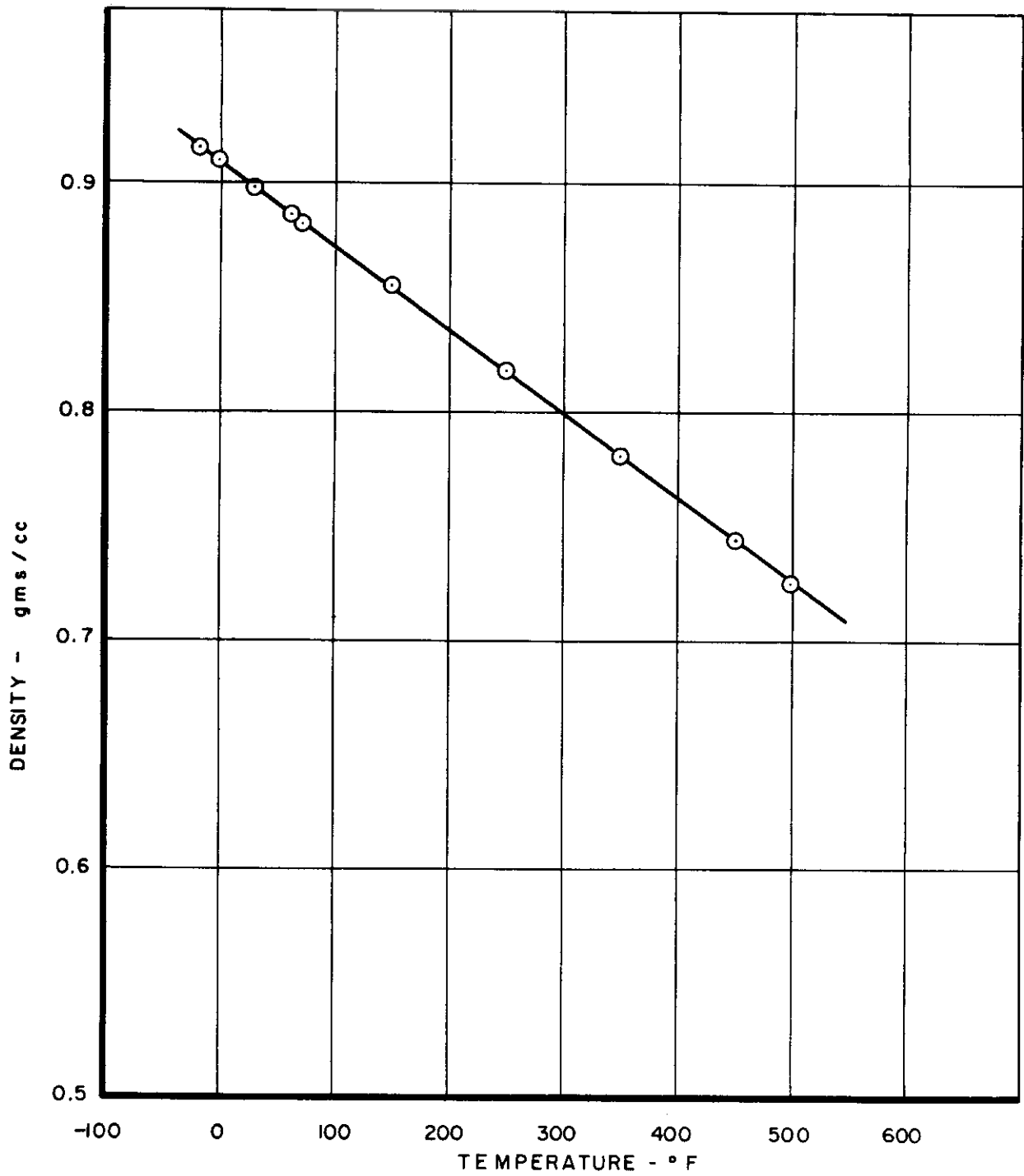


FIGURE 6. DENSITY TEMPERATURE PLOT - ISOPROPYLDICYCLOHEXYL

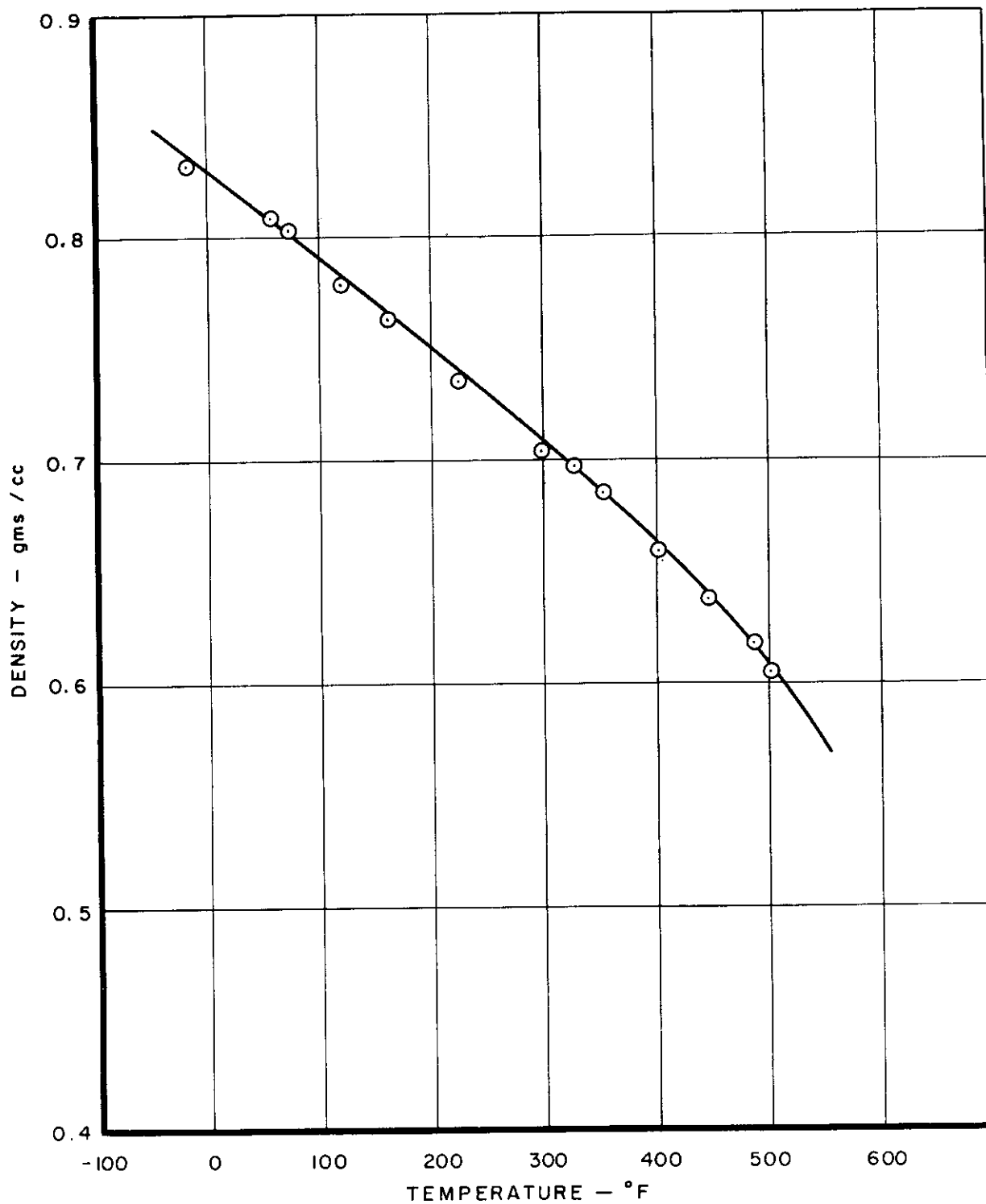


FIGURE 7. DENSITY TEMPERATURE PLOT - DIETHYLCYCLOHEXANE
WADD TR 60-766 26

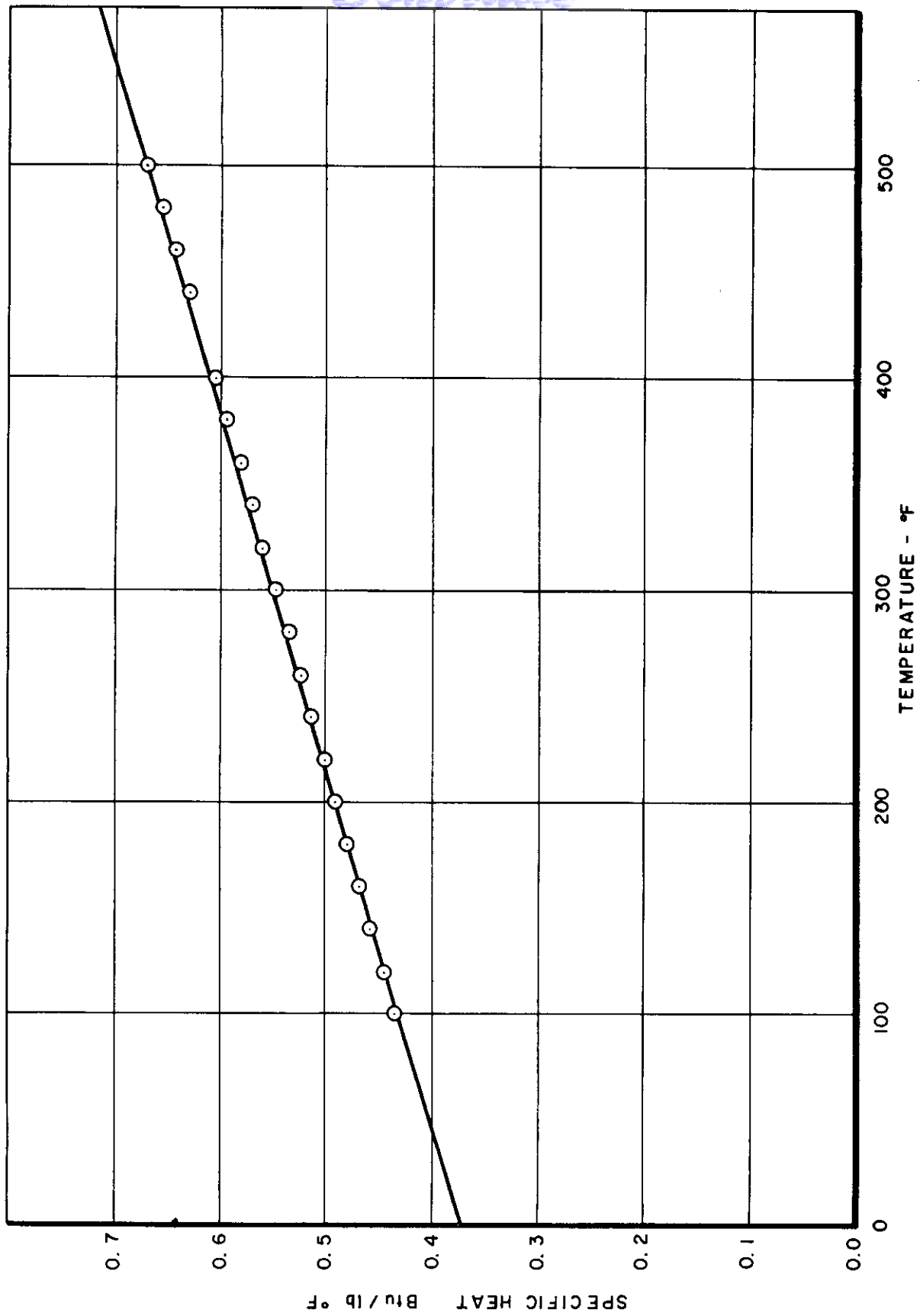


FIGURE 8. SPECIFIC HEAT OF LIQUID ISOPROPYLDICYCLOHEXYL

WADD TR 60-766

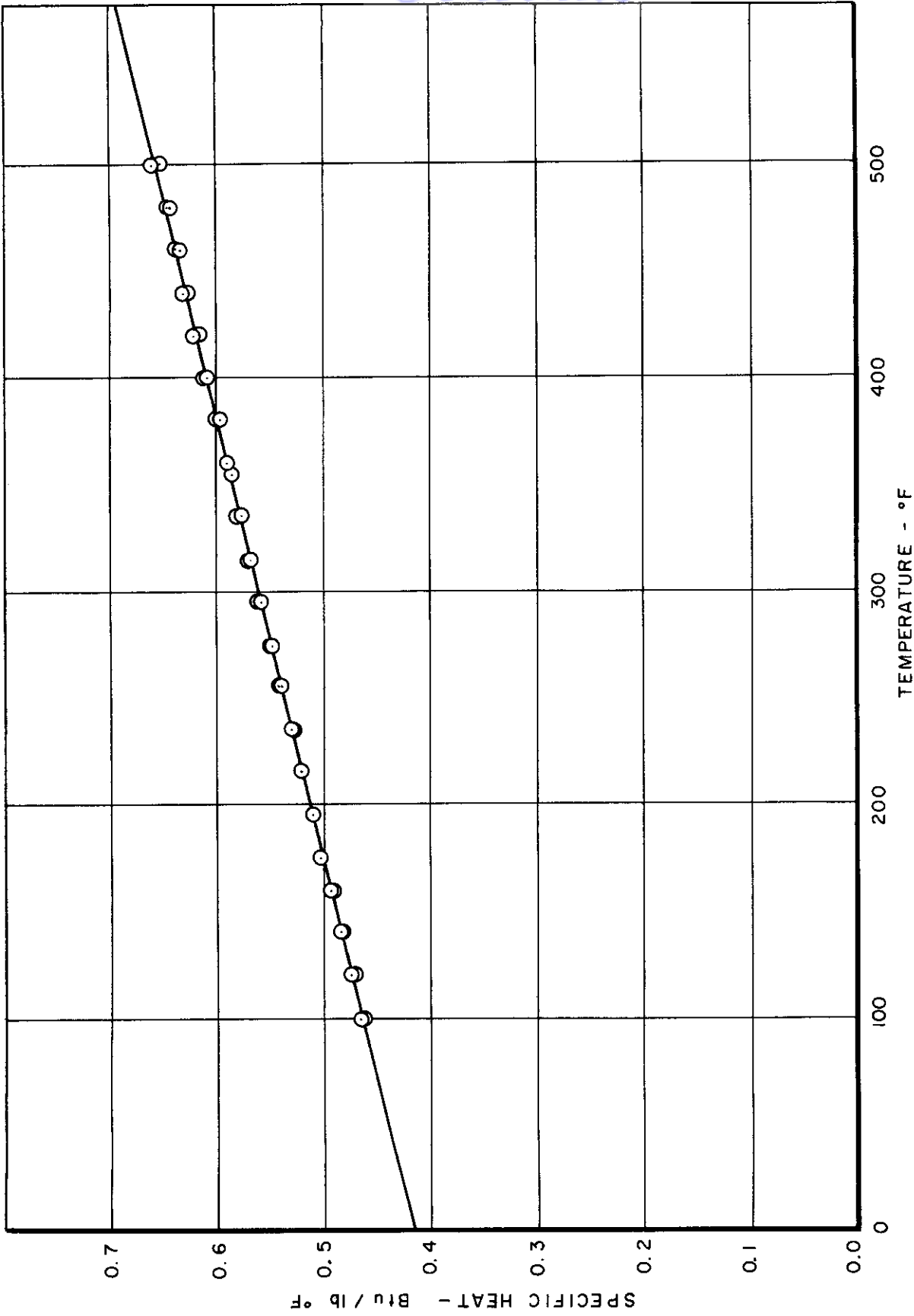


FIGURE 9. SPECIFIC HEAT OF LIQUID DIETHYLCYCLOHEXANE

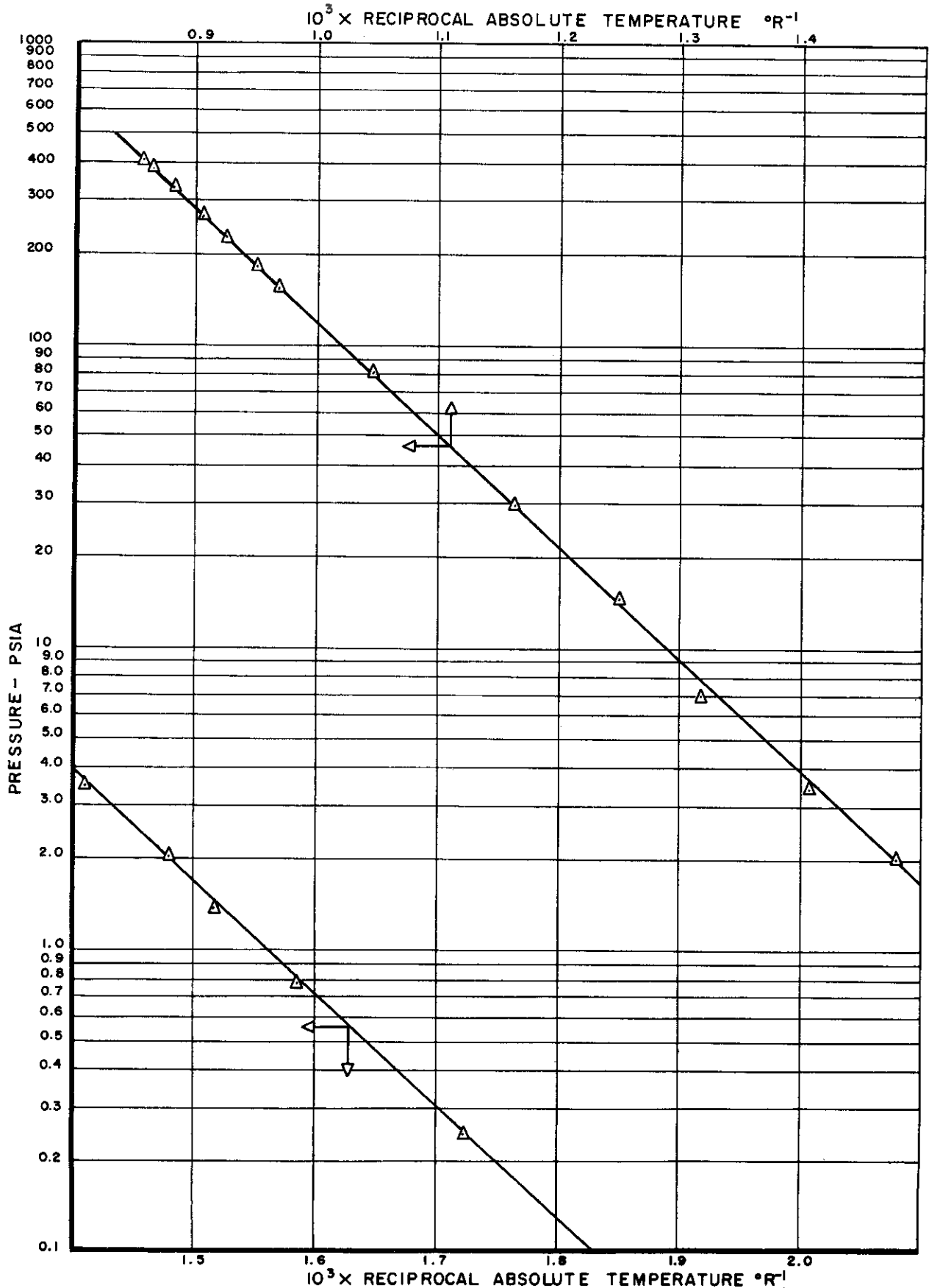


FIGURE 10. VAPOR PRESSURE PLOT - DIETHYLCYCLOHEXANE
WADD TR 60-766 29

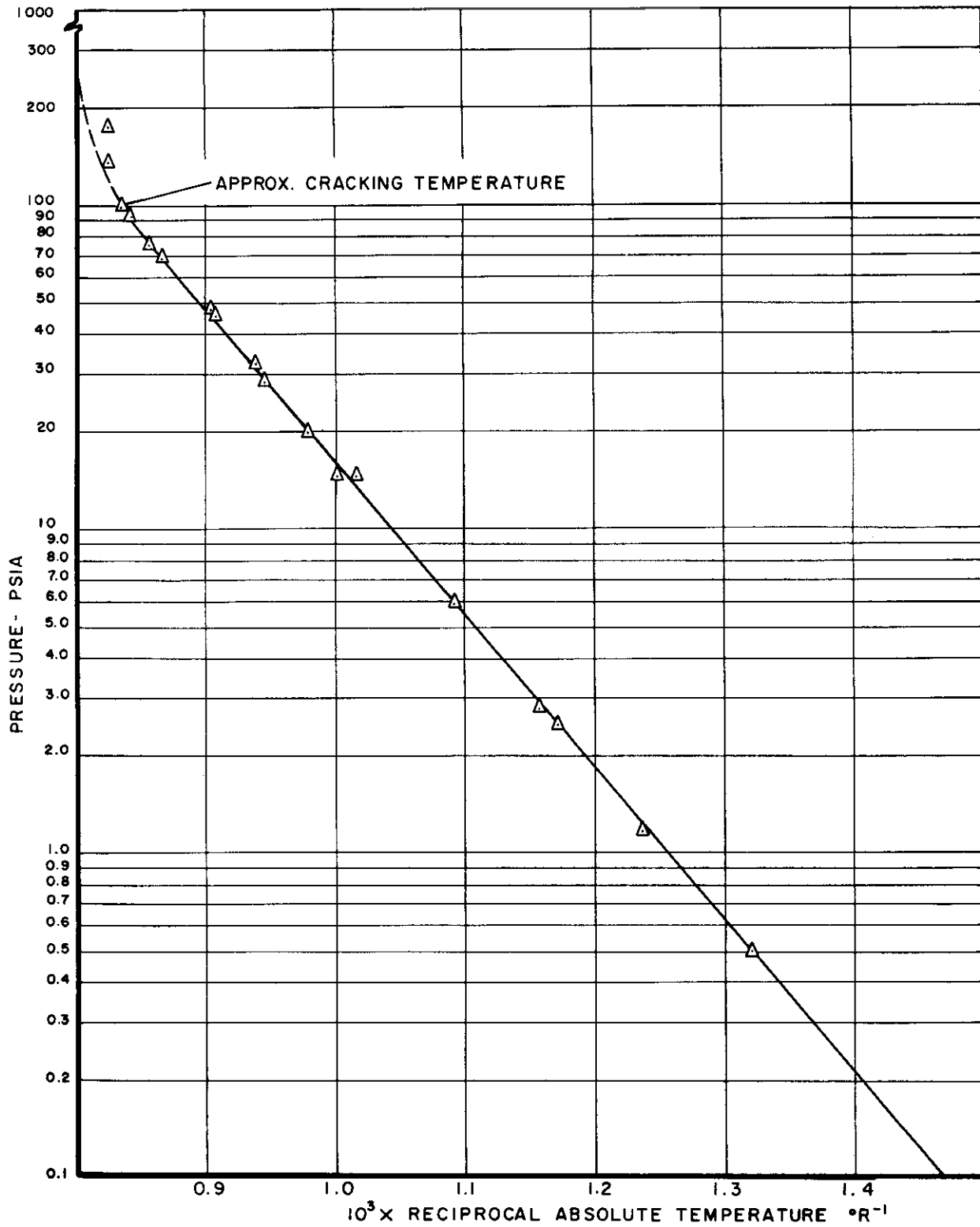


FIGURE II. VAPOR PRESSURE PLOT- ISOPROPYLDICYCLOHEXYL
WADD TR 60-766

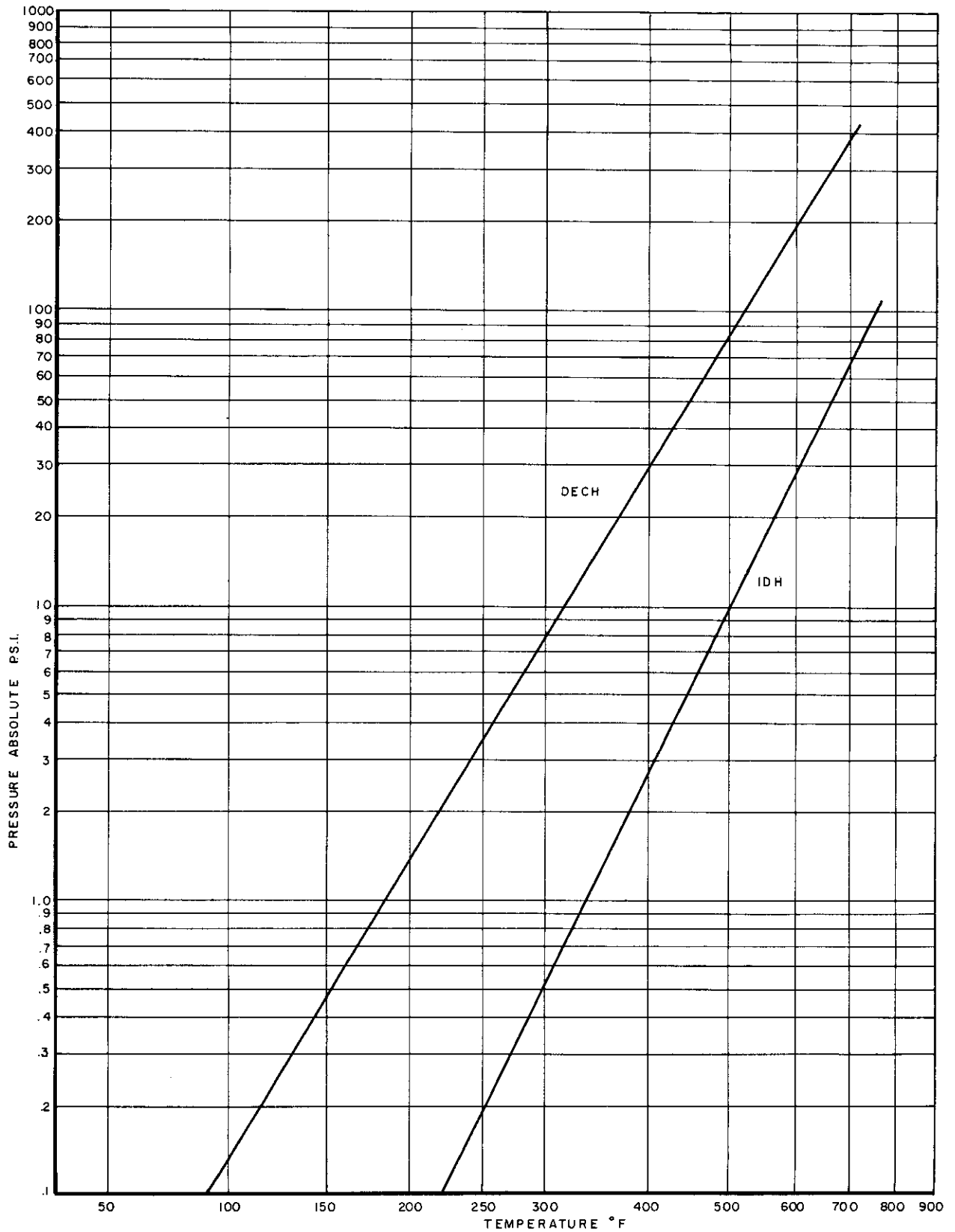


FIGURE 12. VAPOR PRESSURE OF TEST FUELS - IDH & DECH

FUEL	Isopropyl Bicyclo Hexyl
SP. GR @ 60° F	0.891
MOL. WT.	208
DESIG.	Fuel E
DISTILLATION PER	158 - 41
A.S.T.M.	
R.V.P.	
DATE	12-20-58

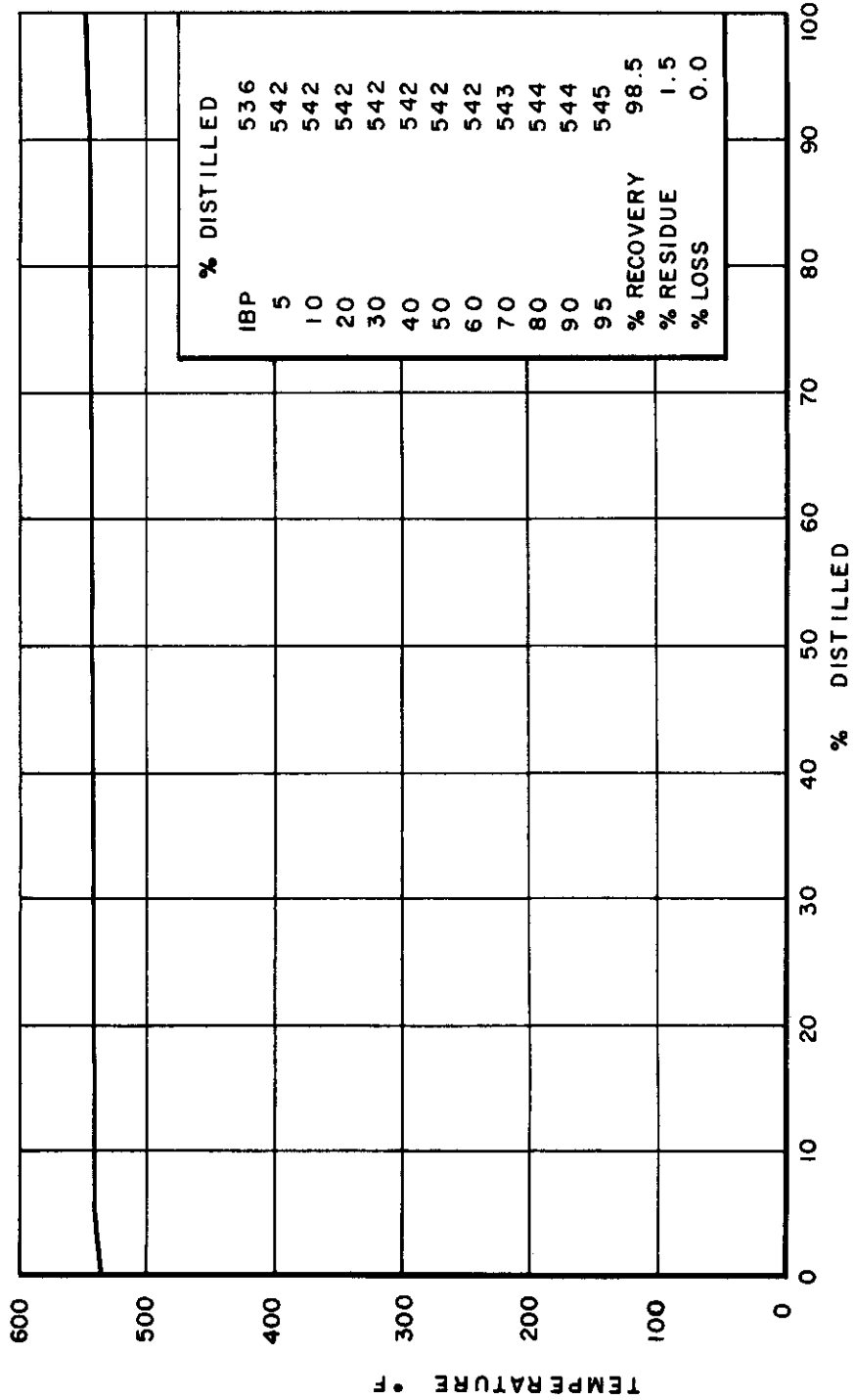


FIGURE 13. DISTILLATION PLOT

FUEL Diethylcyclohexane
 SP GR @ 60° F 0.808
 MOL. WT.
 DESIG. Fuel F
 DISTILLATION PER
 A.S.T.M.
 R.V.P.
 DATE 7-31-58

% DISTILLED	
IBP	337
5	341
10	342
20	342
30	342
40	343
50	344
60	344
70	344
80	344
90	344
95	344
% RECOVERY	99.8
% RESIDUE	0.0
% LOSS	0.2

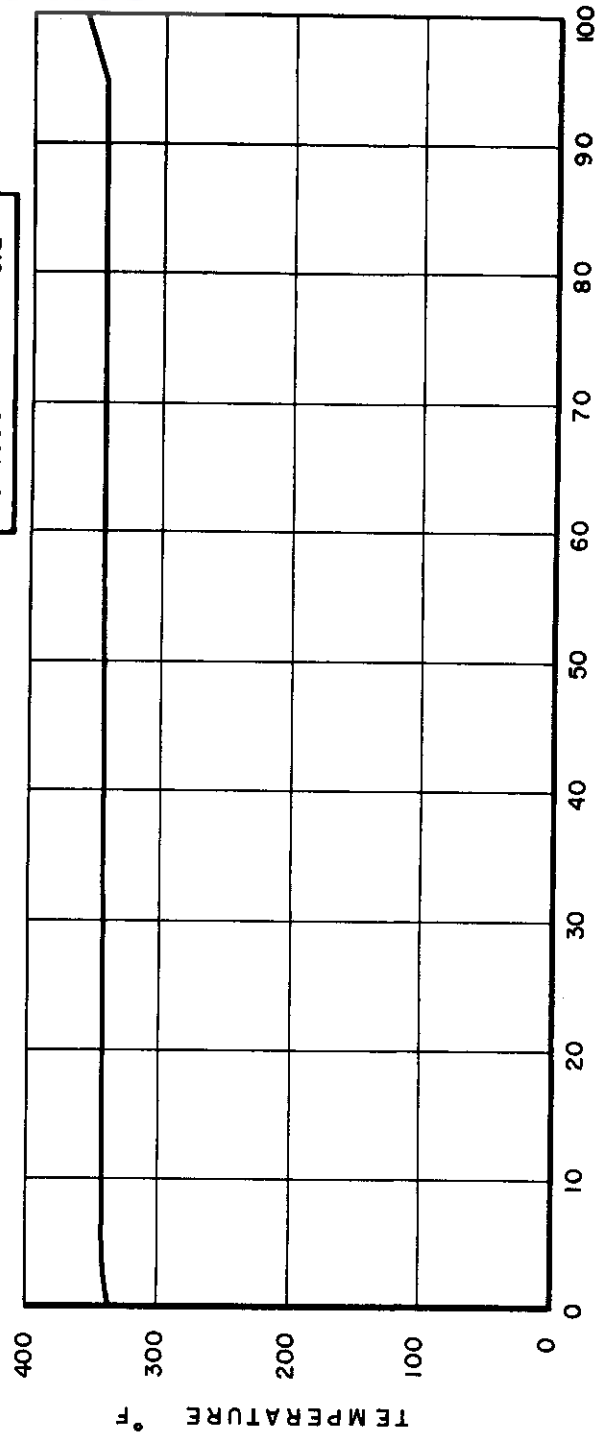


FIGURE 14. DISTILLATION PLOT

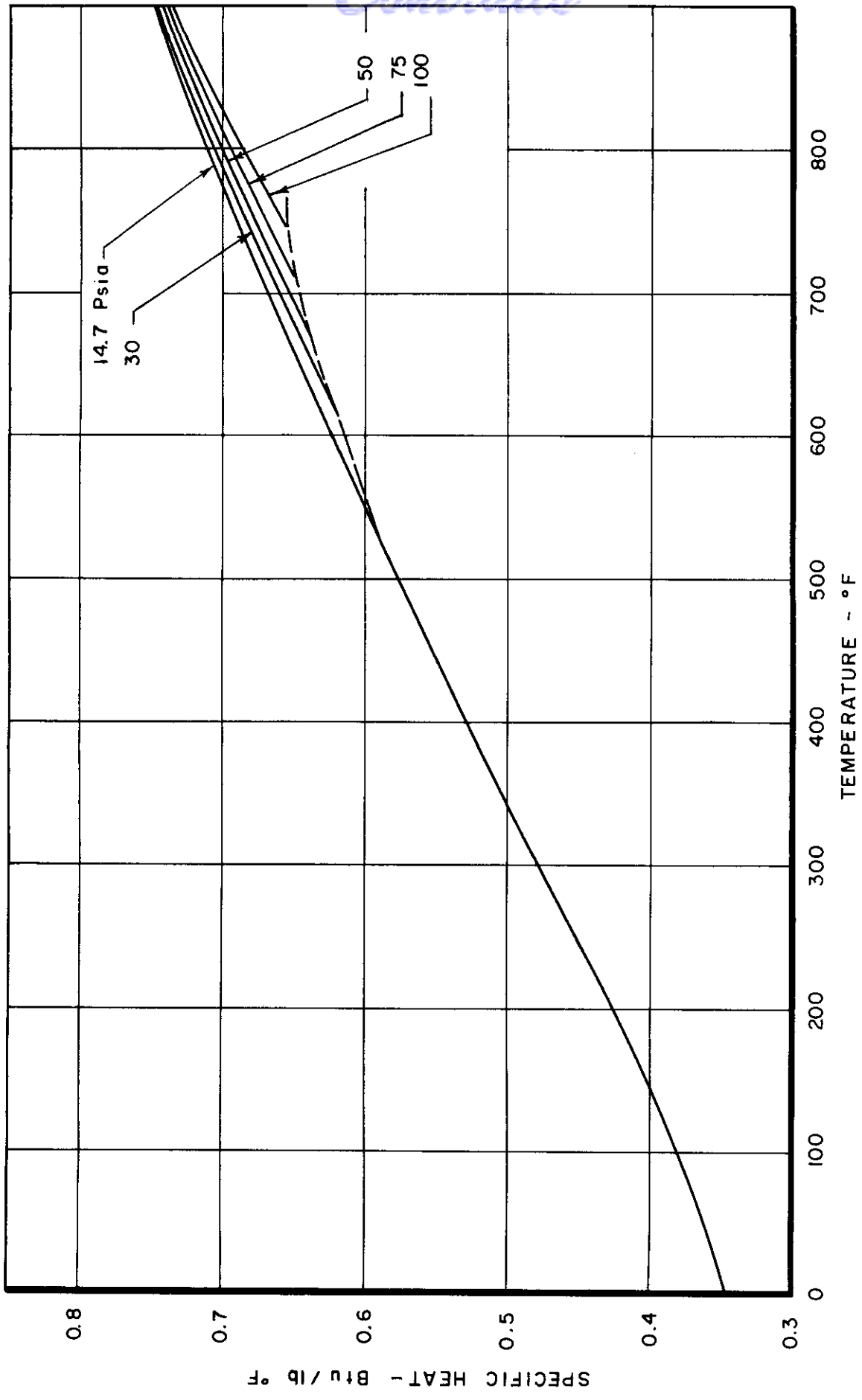


FIGURE 15. VAPOR SPECIFIC HEAT OF ISOPROPYLDICYLCHEXYL

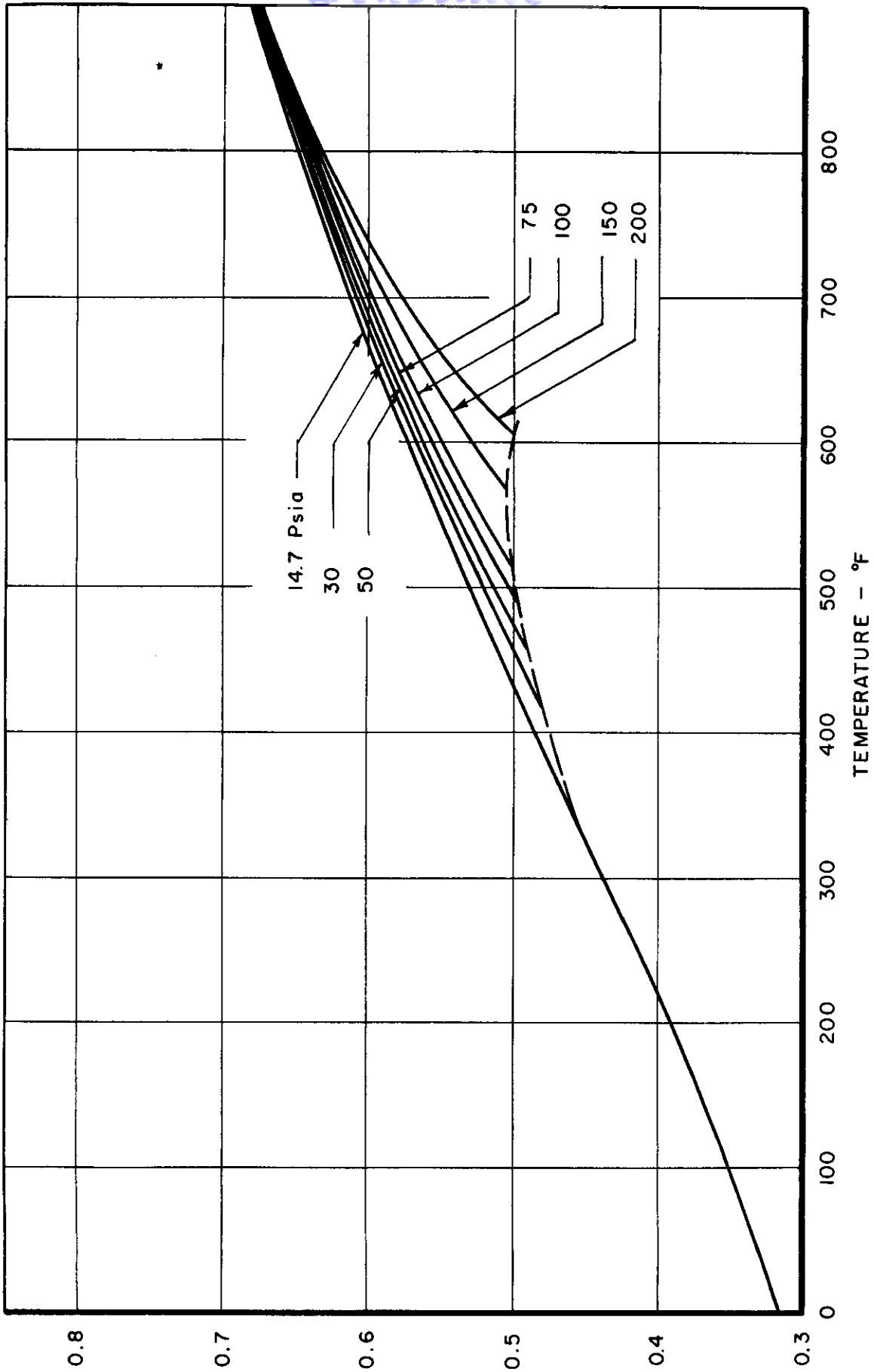


FIGURE 16. VAPOR SPECIFIC HEAT OF DIETHYLCYCLOHEXANE

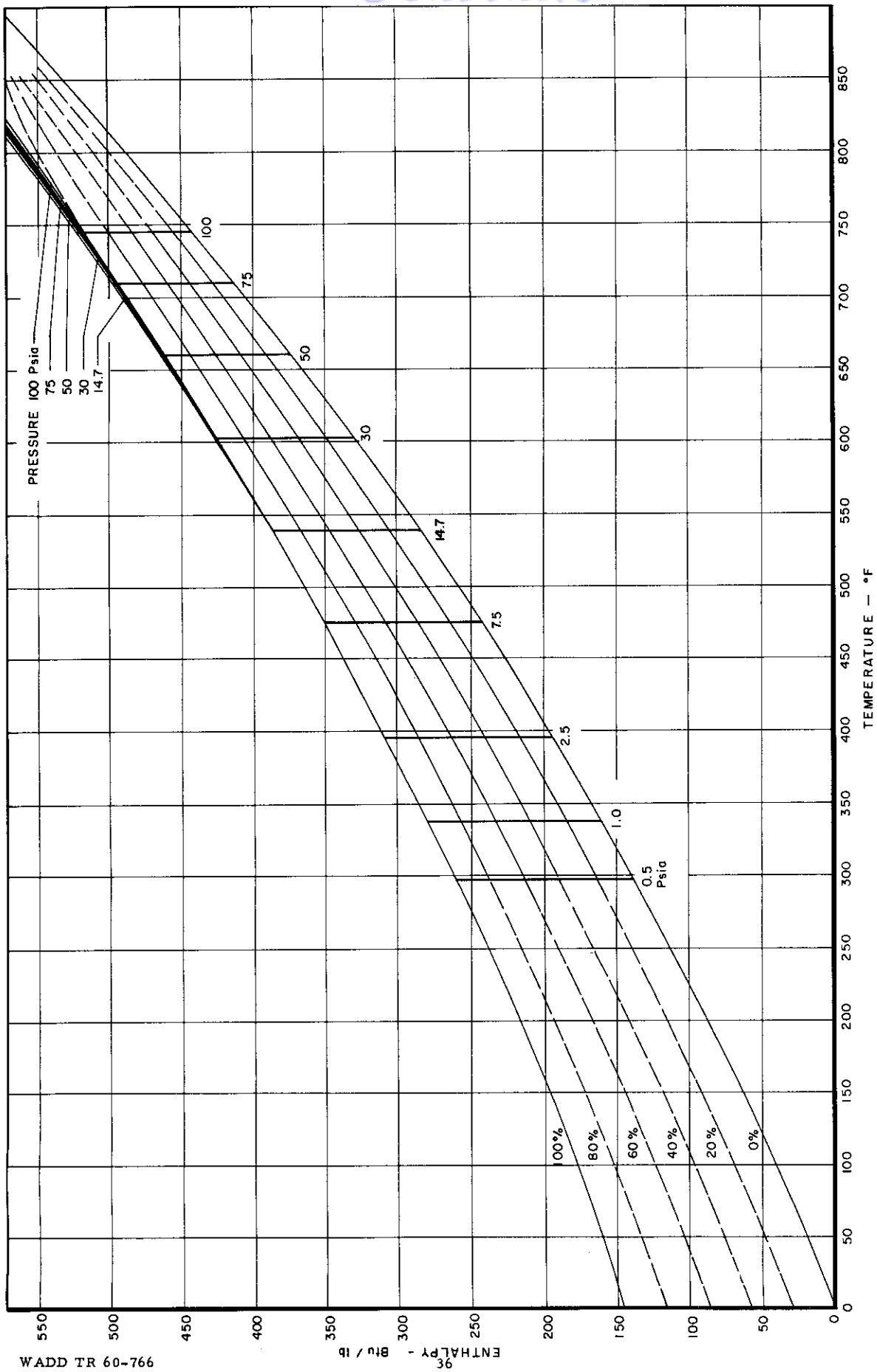


FIGURE 17. ENTHALPY DIAGRAM FOR ISOPROPYLDICYCLOHEXYL

WADD TR 60-766

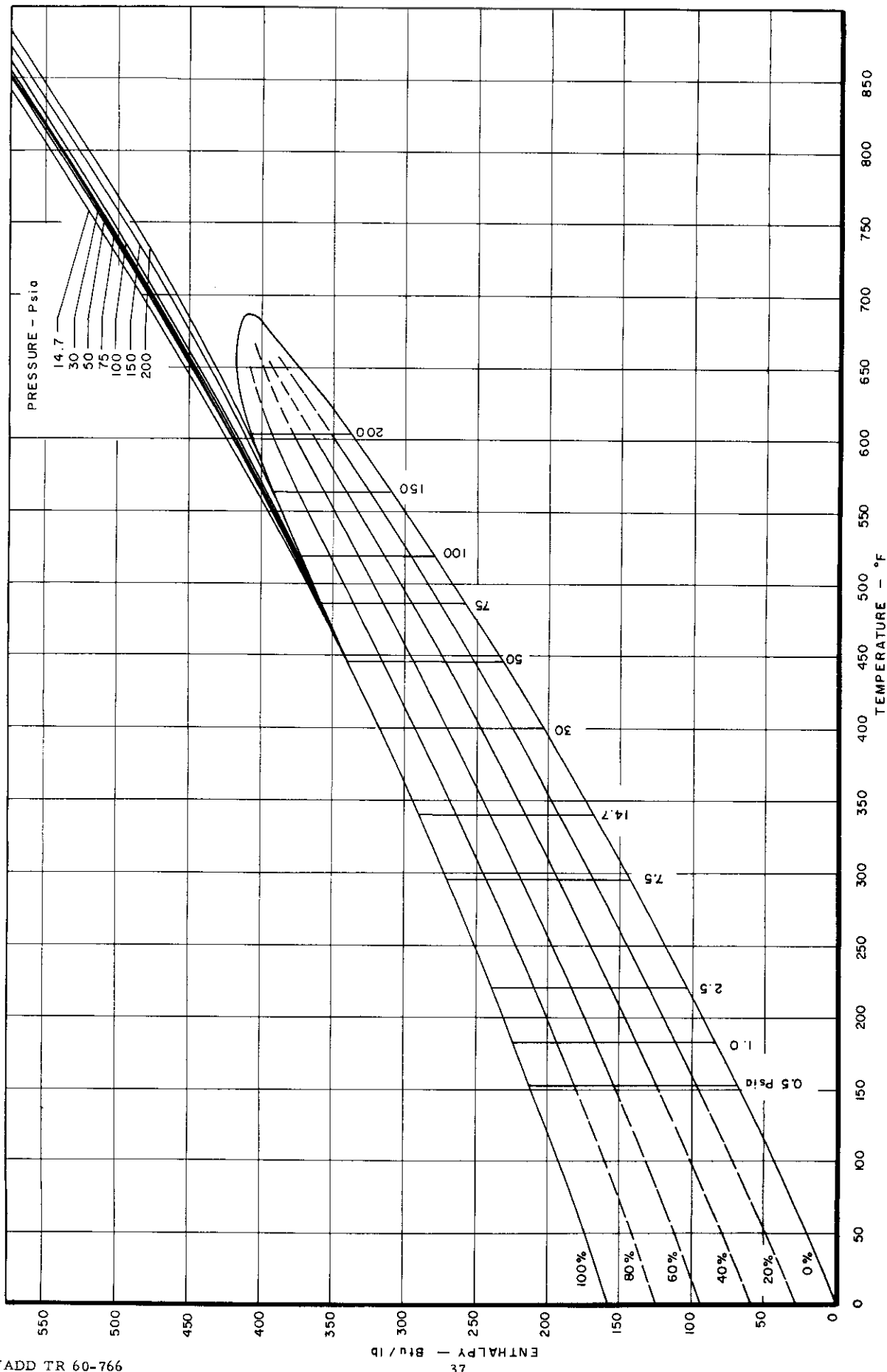


FIGURE 18. ENTHALPY DIAGRAM FOR DIETHYLCYCLOHEXANE

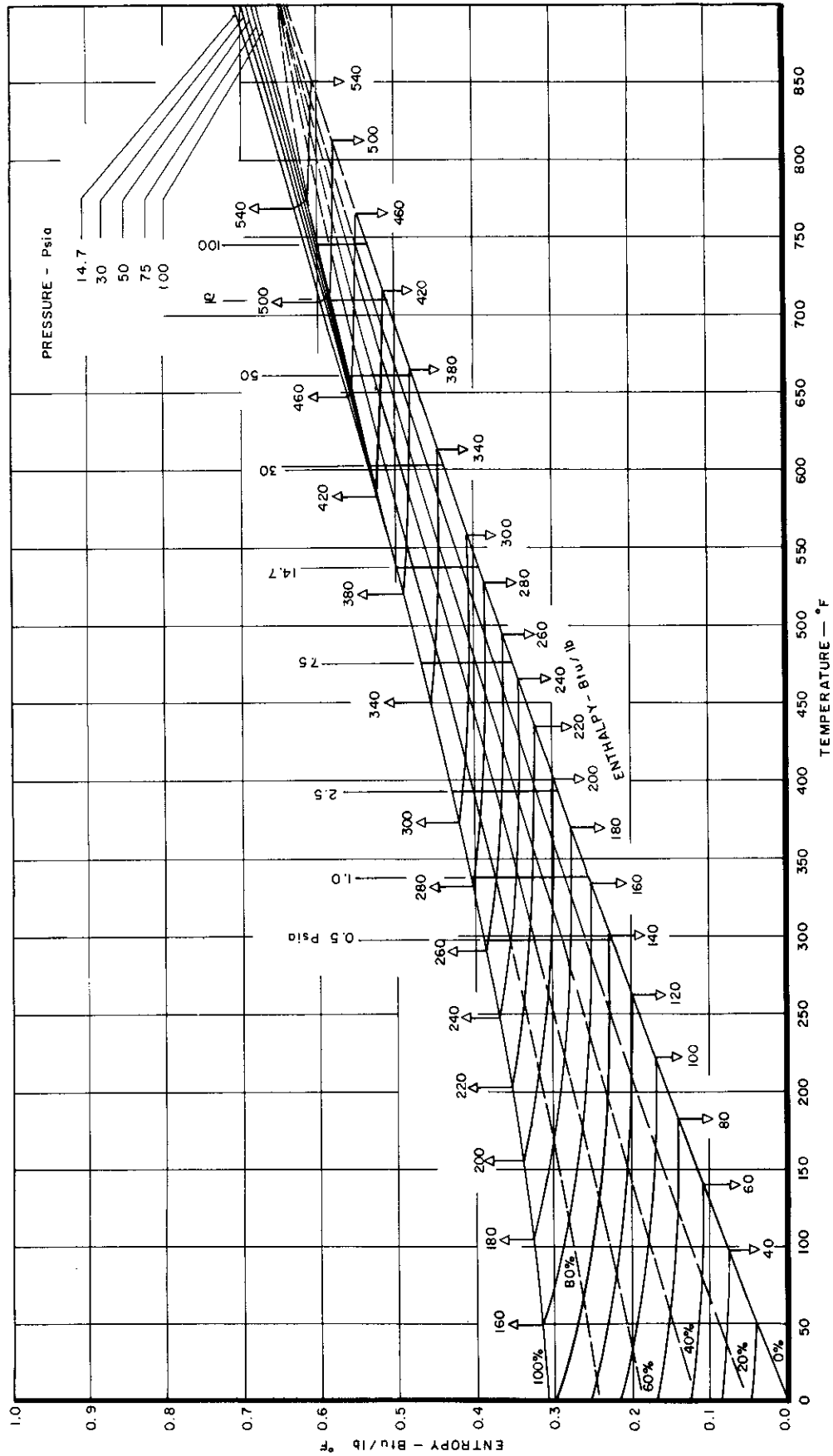


FIGURE 19. TEMPERATURE - ENTROPY DIAGRAM FOR ISOPROPYLCYCLOHEXYL

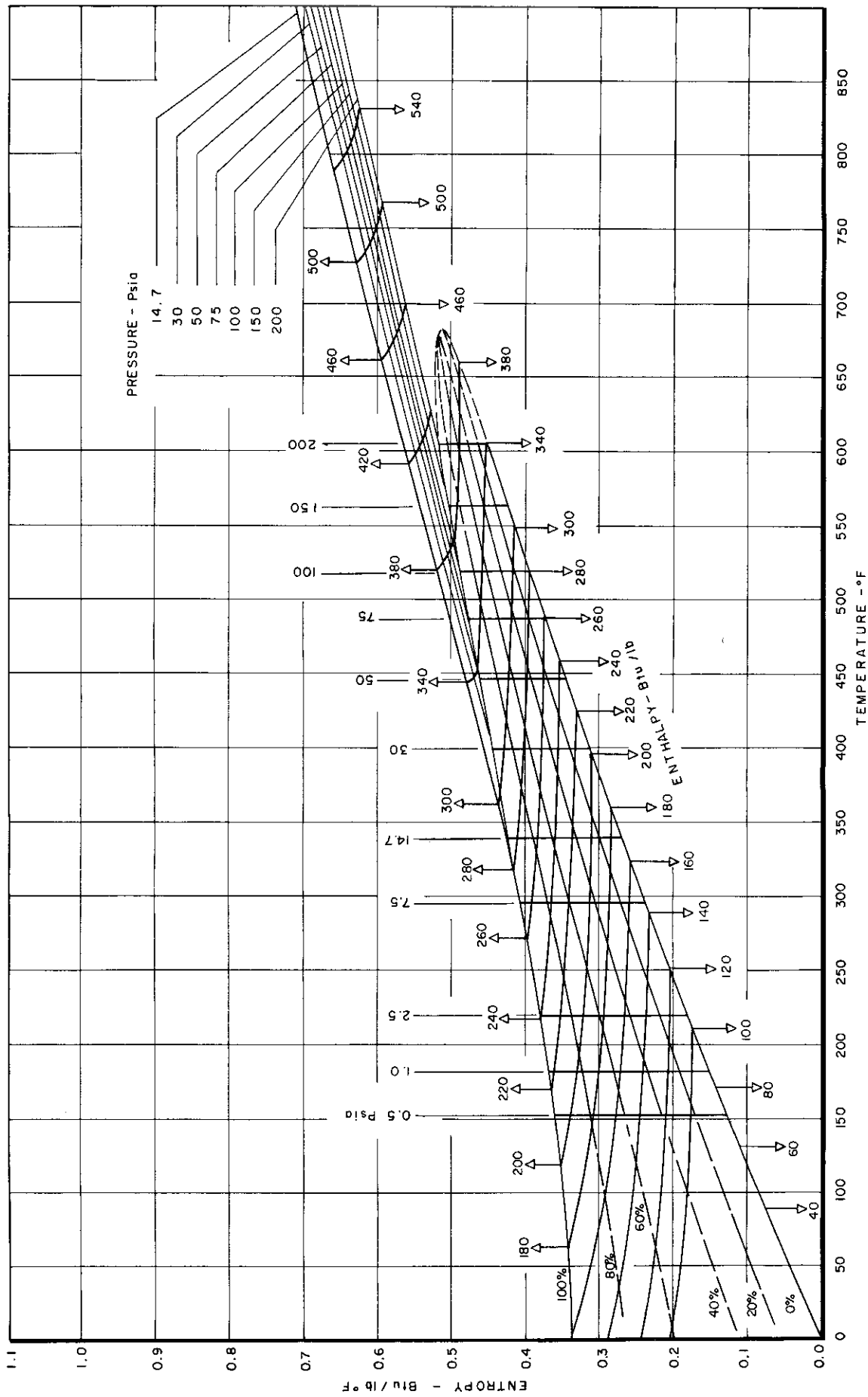


FIGURE 20. TEMPERATURE-ENTROPY DIAGRAM FOR DIETHYLCYCLOHEXANE

TABLE I
DENSITY TEMPERATURE DATA

Fuel	Temperature °F	Density gms/cc	Fuel	Temperature °F	Density gms/cc		
Decalin	71	0.889	DCH	-15	0.832		
	161	0.856		60	0.808		
	201	0.840		75	0.803		
	254	0.813		121	0.778		
	313	0.789		163	0.763		
	368	0.772		227	0.735		
	379	0.768		256	0.728		
	398	0.761		300	0.704		
	448	0.731		330	0.697		
	500	0.710		355	0.685		
	IDH	-17		0.915	DCH(16)	404	0.659
1		0.910	407	0.660			
30		0.896	448	0.638			
62		0.886	456	0.632			
73		0.883	488	0.617			
150		0.855	504	0.604			
250		0.818	68	0.804			
350		0.781	60	0.808			
450		0.744	71.6	0.7957			
500		0.725	68	0.800			
IDH(15)		59	0.8854	1:3- DCH(11)		51.8	0.8118
				1:3 - DCH(12)			
				1:3 - DCH(13)			
IDH(15)		59	0.8854	1:4 - DCH(7)		68	0.802

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TABLE II
LIQUID SPECIFIC HEAT DATA

Fuel	Temperature °F	Specific Heat		Fuel	Temperature °F	Specific Heat BTU/lb °F
		Run A	Run B			
Decalin	100	0.402	0.411	IDH	100	0.435
	120	0.415	0.423		120	0.446
	140	0.428	0.435		140	0.458
	160	0.439	0.446		160	0.469
	180	0.451	0.458		180	0.480
	200	0.463	0.469		200	0.490
	220	0.475	0.482		220	0.502
	240	0.488	0.494		240	0.514
	260	0.500	0.505		260	0.524
	280	0.512	0.517		280	0.536
	300	0.526	0.530		300	0.548
	320	0.538	0.542		320	0.561
	340	0.552	0.554		340	0.572
	360	0.565	0.566		360	0.583
	380	0.574	0.580		380	0.595
	400	0.591	0.592		400	0.607
	420	0.604	0.605		420	0.619
	440	0.618	0.618		440	0.631
	460	0.633	0.632		460	0.644
	480	0.646	0.645		480	0.656
500	0.660	0.658	500	0.672		

TABLE II
LIQUID SPECIFIC HEAT DATA (Cont'd)

Fuel	Temperature °F	Specific Heat BTU/lb °F	
		Run A	Run B
DCH	100	0.466	0.464
	120	0.475	0.474
	140	0.485	0.484
	160	0.494	0.493
	180	0.503	0.503
	200	0.512	0.512
	220	0.522	0.524
	240	0.531	0.533
	260	0.540	0.542
	280	0.549	0.552
	300	0.559	0.562
	320	0.568	0.572
	340	0.577	0.581
	360	0.586	0.591
	380	0.597	0.601
	400	0.606	0.611
	420	0.615	0.620
440	0.625	0.631	
460	0.635	0.641	
480	0.644	0.651	
500	0.653	0.661	

TABLE III
VAPOR PRESSURE DATA

Fuel	Temperature °F	Pressure Psia	Fuel	Temperature °F	Pressure Psia
Decalin	225	1.1	DCH	75	<1 mm Hg
	225	1.08		120	0.25
	376	14.7		171	0.29
	400	16.8		199	1.39
	488	50.0		216	2.03
	507	64.5		250	3.50
				298	7.08
				340	14.7
				400	29.8
				500	81.3
IDH	76	<1 mm Hg		575	151.8
	213	0.15		595	181.2
	297	0.51		624	224.5
	348	1.19		647	265.5
	394	2.50		676	332.2
	404	2.84		700	381.0
	457	5.89		710	403.4
	538	14.7		338-340	14.7
	562	20.0		DCH(9,10)	14.7
	600	28.5		DCH(14)	14.7
	607	32.40		DCH(8)	14.4
	654	45.4			
	655	47.5	1:1		
	700	68.7	1:1		
	727	92.5	1:2		
	740	99.0			
	752	171.8	1:3	DCH(11)	344-346
	755	134.3	1:3	DCH(12)	336-343
800	250	1:3	DCH(13)	336-340	
		1:4	DCH(7)	345-349	

TABLE IV

PROPERTIES OF ISOPROPYLDICYCLOHEXL

(MONSANTO CHEMICAL CO.)

(Ref. 15)

Pour point	-66°F
	-55°C
Density (15°C)	0.88536
n_D^{25}	1.4784
Heat of combustion, BTU/lb.	18,447 ± 21
Viscosities (cs)	
60°F	14.10
100°F	6.95
140°F	3.98
177°F	2.60
Flash point °F	270-275
Boiling	276°C(528.8°F)

TABLE V

SHELL DIETHYLCYCLOHEXANE MIXED ISOMERS

(Ref. 16)

Specific Gravity, 20/4°C	0.8040
Specific Gravity, 60/60°F	0.8079
Gravity, API	43.7
Freezing Point, °F	Below-110
Flash Point, PMCC, °F	116
Kinematic Viscosity at -30°F, CS	4.38
Aniline Point, °C	55.2
Carbon, % w	85.63
Hydrogen, % w	14.36
Sulfur, % w	0.0001
Aromatics, % w. UV	0.6
Existent Gum	less than 1 mg/dl
Accelerated Gum(16 hrs. at 100°C, 100 psi O ₂)	less than 1 mg/dl
CFR Coker Test (475°F preheater, 500°F filter, 6 lbs./hour flow rate)	
Filter pressure drop	almost nil
Filter merit rating	85
Preheater-slight coking;better performance than any jet fuel tested at this temperature.	
Heat of combustion at 25°C	
K Cal/gram	10.31
M BTU/lb.	18.61
M BTU/gal.	125.1

TABLE V
SHELL DIETHYLCYCLOHEXANE MIXED ISOMERS (Cont'd)

ASTM Distillation,	<u>D-86, °F</u>	<u>D-1078, °C</u>
Recovery, %w		
IBP	335	173.4
10	338	175.6
50	340	176.1
90	340	176.5
95	340	176.6
End point	351	---
Dry point	---	176.8

Gas - Liquid Chromatography Analysis

C ₉ and lighter naphthenes, %w	0.62
C ₁₀ naphthenes	98.50
C ₁₀ aromatics)	
C ₁₁ and heavier naphthenes)	<u>0.88</u>
	100.00