Physical Properties of Hydrocarbons

Part 17—C_4-C_5 Branched Hydrocarbons

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IN PREVIOUS ARTICLES, the physical properties of straight chain hydrocarbons have been presented. This article covers the C_4-C_5 branched chain hydrocarbons. All four of these compounds (isobutane, isobutylene, isoprene, and isopentane) are important commercial products. Isobutane production is over one-half billion pounds a year. Isobutylene and isoprene are part of one of the most dramatic and successful engineering achievements—the development of synthetic rubber during World War II.

Critical Properties and Vapor Pressures. The critical properties recorded in Table 17-1 were taken from the data of the ASTM.[1] Other literature sources agree closely with these values.[2, 3, 4, 5]

The vapor pressures of isobutane,[2, 4, 7] isobutylene,[2, 5] and isopentane[2, 8, 9] have been measured up to the critical point. Data for isoprene are available only up to the boiling point.[2] The data have been extended to the critical point by the equation recommended by Miller.[10] This equation, discussed in the preceding part of this series, gave an average error of 1.4 percent when compared to 8 experimental values for isobutane and isopentane. Above 50° C, the error averaged only 0.5 percent.

Heat of Vaporization. Canjar and co-workers[4] have compiled the thermodynamic properties and P-V-T data for isobutane as part of their extensive series on thermodynamic properties of hydrocarbons. Additional data up to the critical point is available for isobutane[7] and isobutylene.[5] The limited data for isopentane and isoprene[1, 3] have been extended by the Kharbanda nomograph[11] of the Watson equation. When compared to 11 experimental points for isobutane and isobutylene, this method gave an average error of 2.9 percent and a maximum error of 7.1 percent.

Heat Capacity. Kobe[12] presents vapor heat capacity data for isopentane over the entire temperature range. Scott has experimentally determined the heat capacity up to 215° C.[13] His data agree within 1 percent with the data of Kobe. The heat capacity of isobutane has been measured up to 420° C.[14, 15] The method of Doraiswamy and Rihani[16] has been used to calculate the vapor heat capacity of isobutane from 500 to 1,000° C and for isoprene and isobutylene over the entire 0-1,000° C range. This is an extremely accurate estimation method, giving an average error of 0.5 percent when compared to 20 experimental points for isobutane and isopentane. Sage and Lacey have determined the effect of pressure on the heat capacity of isobutane in the 20-110° C range.[7] This information is presented in Fig. 17-5.

With very little experimental data available,[1] the liquid heat capacity was calculated as in the previous article (density times heat capacity equals a constant). This method gave an average error of 1.8 percent when compared to experimental data on isobutane.[7] Hadden[17] has recently proposed a new method of calculating the liquid heat capacities of hydrocarbons. This method requires a knowledge only of the boiling point but is limited to temperatures below the boiling point. The author found this method to give essentially the same results as the other estimation method.

Density. Only the density of isobutylene has been measured up to the critical point.[5] The method of Francis[18] has been used to calculate the liquid densities up to the critical point for the other three compounds. When compared with experimental data on isobutane,[1, 19] isobutylene,[5] and isopentane,[8] the average error for 18 points was 0.9 percent.

Viscosity. Vapor viscosity data are available up to 120° C for isobutane[20, 21] and up to 200° C for isopentane.[20, 22] The estimation method of Bromley and Wilks[23] has been used to provide the data for all four compounds over the temperature range of 0-500° C. This method gave an average error of 1.8 percent when compared with experimental data. Fig. 17-9 shows the effect of pressure on the viscosity of isobutane.[24]

TABLE 17-1—Physical Properties of C_4 - C_5 Branched Hydrocarbons

	Boiling Point °C	Freezing Point °C	Molecular Weight	Critical Properties T_c °C	P_c psia	d_c g/ml
Isobutane (2-methylpropane)	−11.7	−159.6	58.12	135.0	529	0.222
Isobutylene (2-methylpropene)	− 6.9	−140.3	56.10	144.7	580	.234
Isoprene (2-methyl 1, 3-butadiene)	34.1	−146.0	68.11	241*	558*	.247*
Isopentane (2-methylbutane)	27.8	−159.9	72.15	187.2	483	.234

* Estimated by ASTM

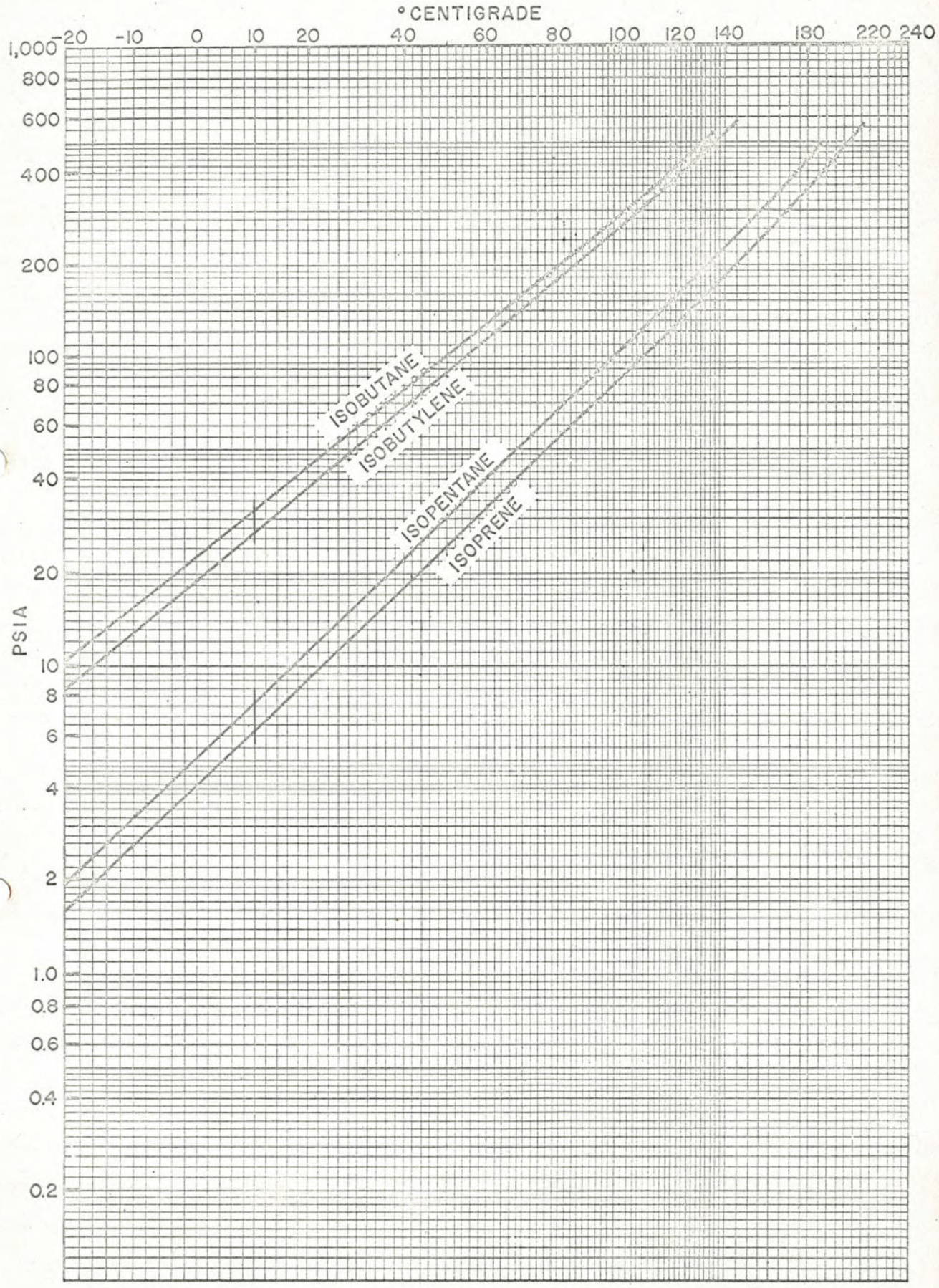

Fig. 17-1—Gives vapor pressure for C_4-C_5 branched hydrocarbons from —20° C to +220° C.

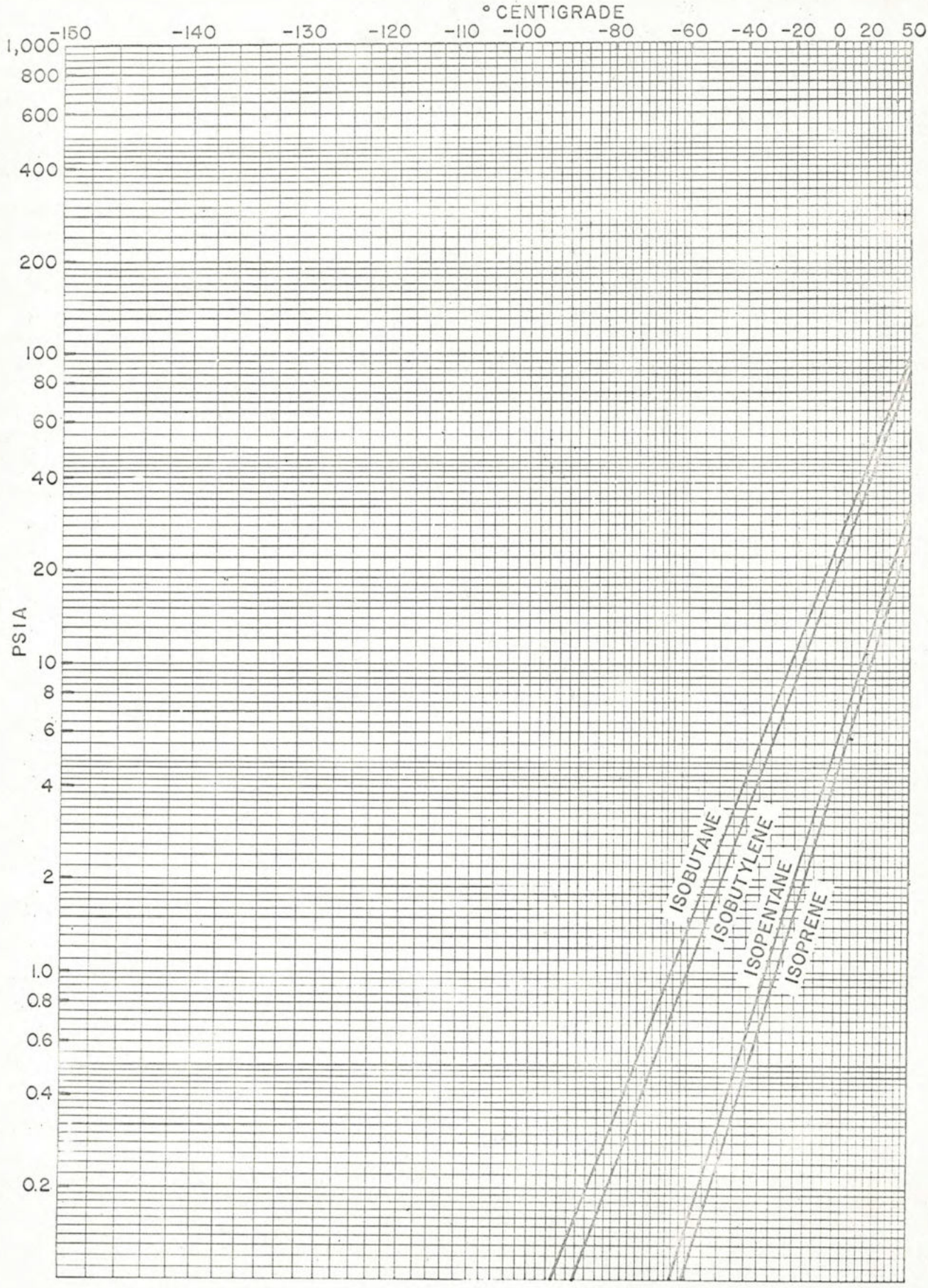

Fig. 17-2—Gives vapor pressure for C_4-C_5 branched hydrocarbons from —90° C to +50° C.

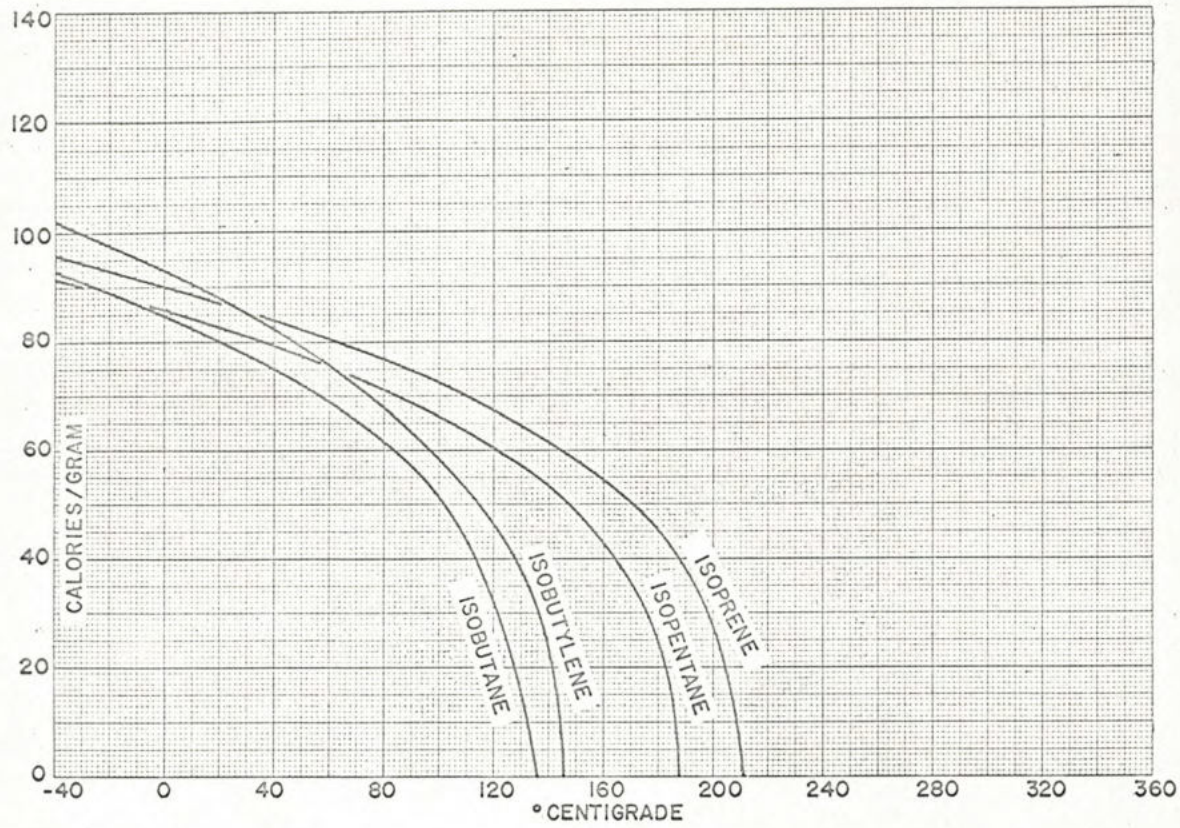

Fig. 17-3—Gives heat of vaporization for C_4-C_5 branched hydrocarbons from —40° C to +210° C.

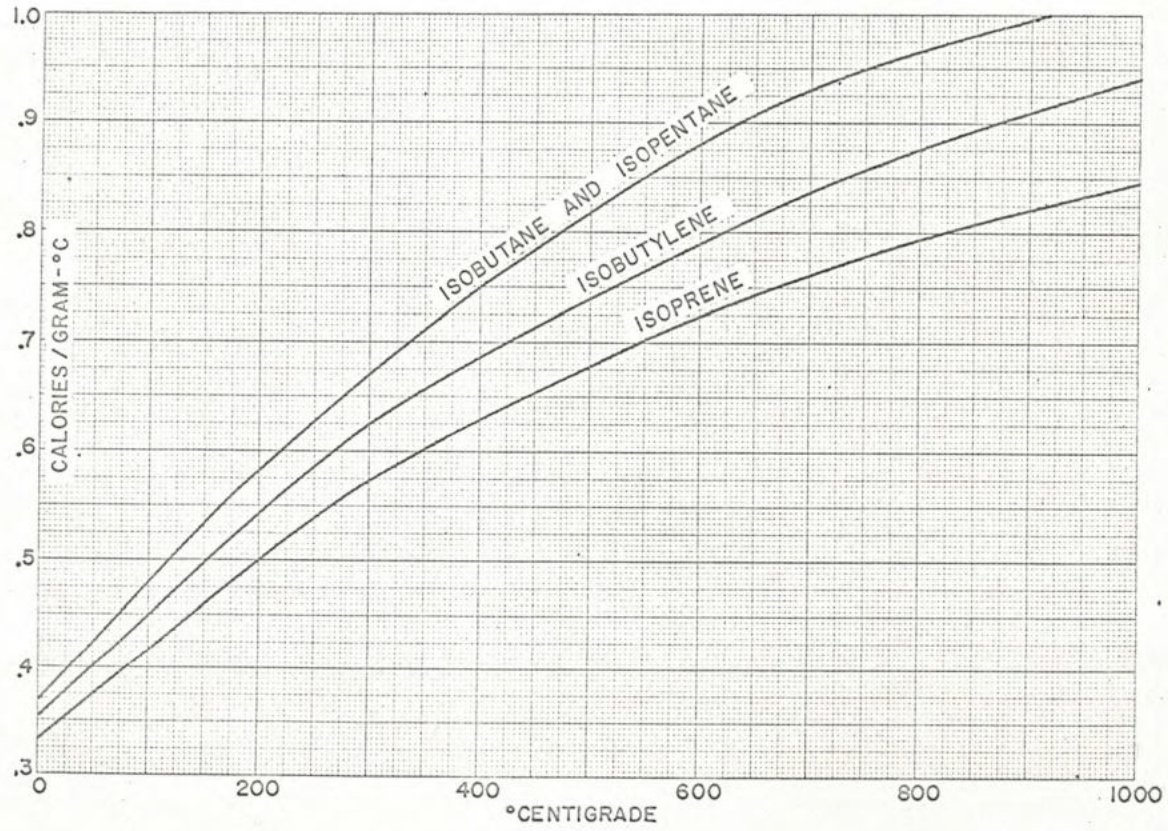

Fig. 17-4—Gives vapor heat capacity for C_4-C_5 branched hydrocarbons from 0° C to +1000° C.

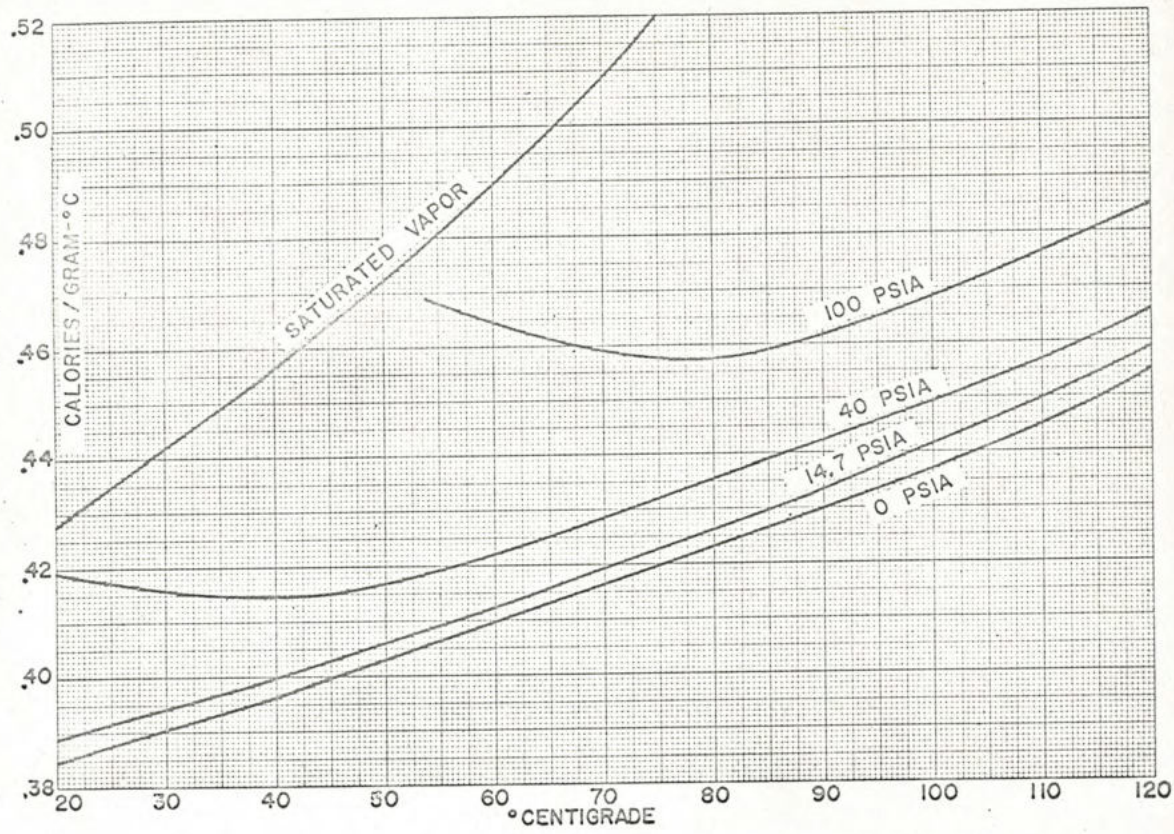

Fig. 17-5—Gives isobutane heat capacity pressure effect from 20° C to 120° C.

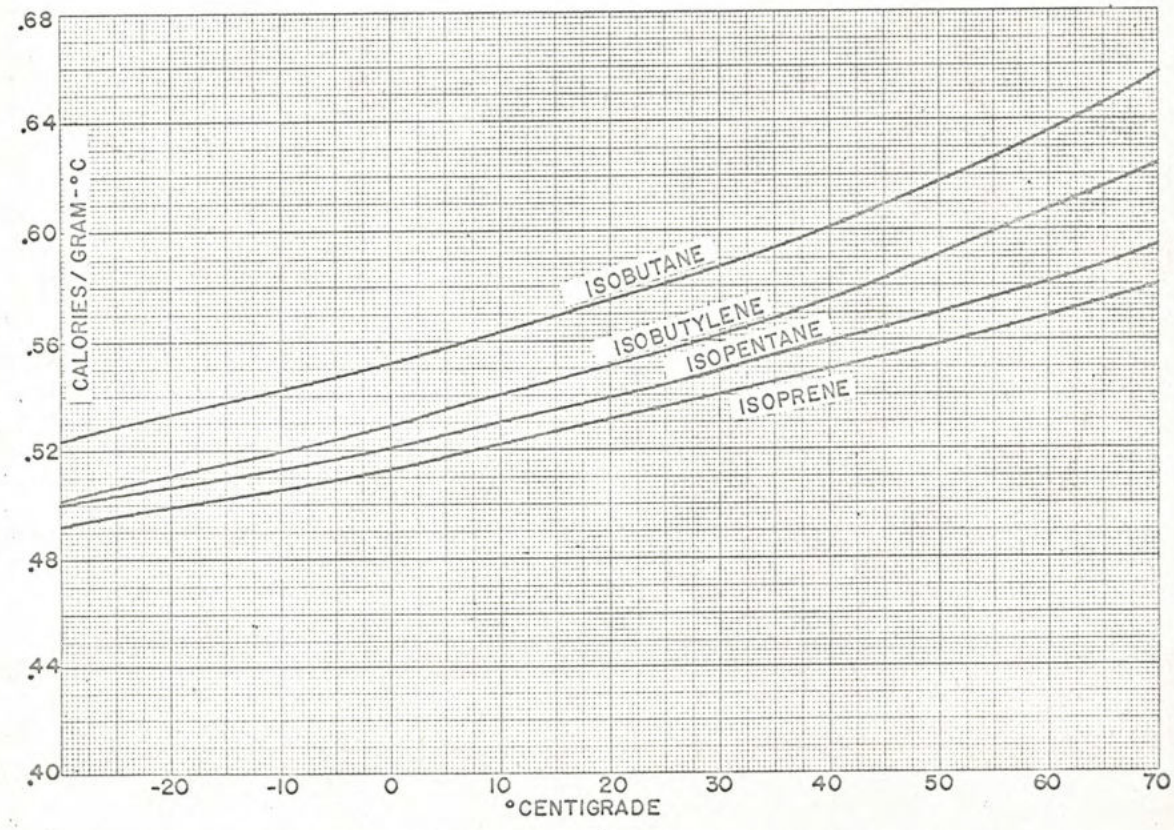

Fig. 17-6—Gives liquid heat capacity for C_4-C_5 branched hydrocarbons from —30° C to +70° C.

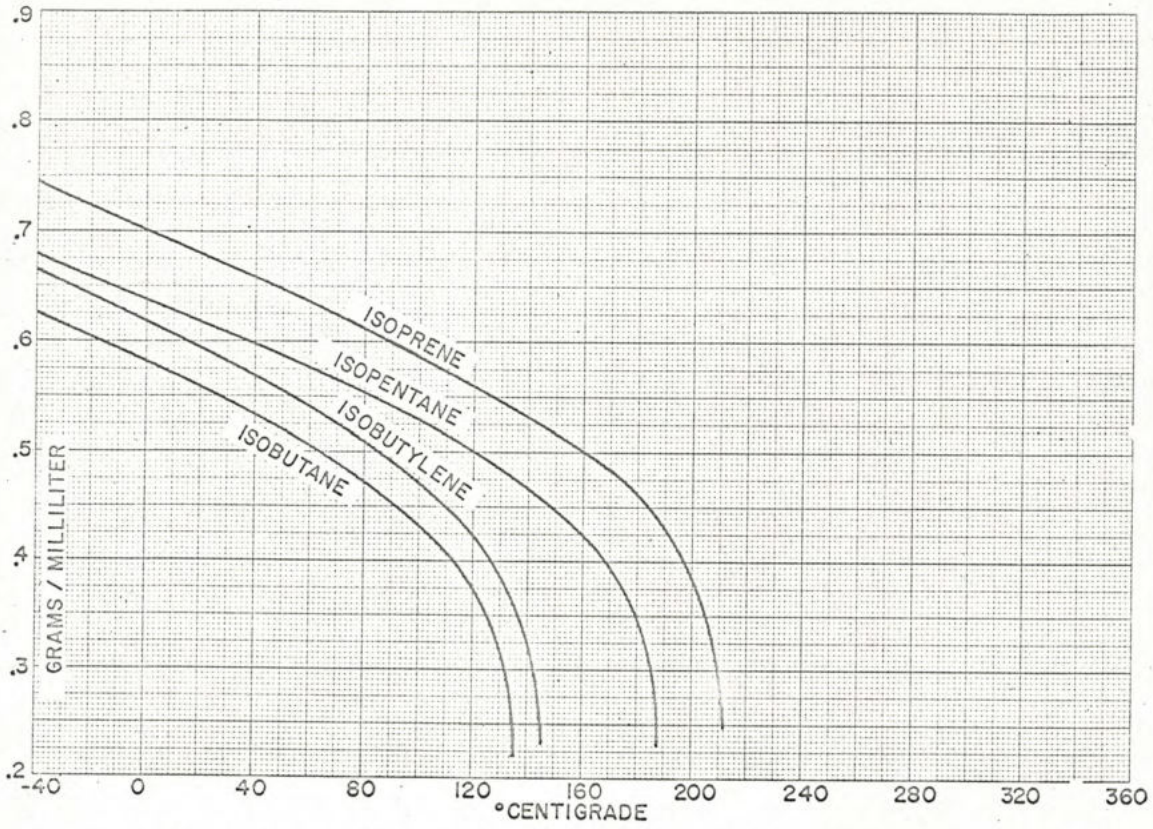

Fig. 17-7—Gives liquid density for C_4-C_5 branched hydrocarbons from —40° C to +210° C.

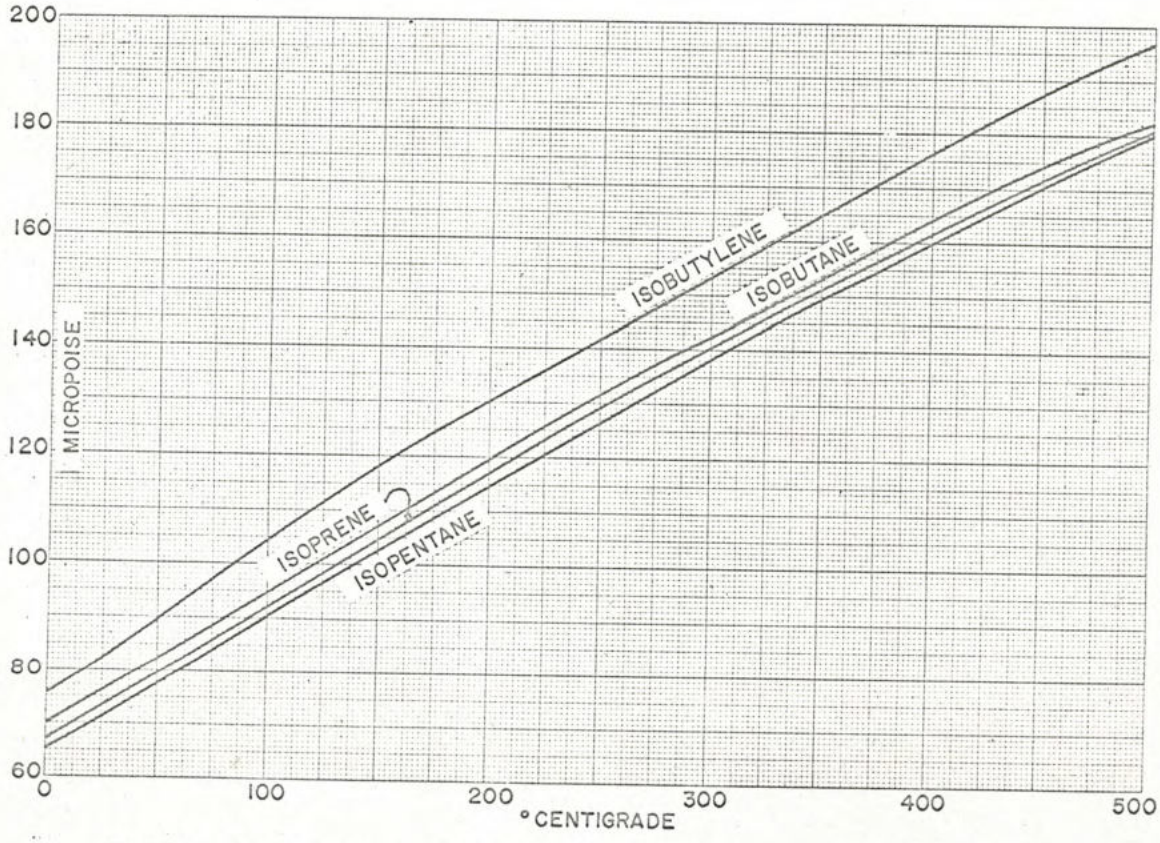

Fig. 17-8—Gives vapor viscosity for C_4-C_5 branched hydrocarbons from 0° C to +500° C.

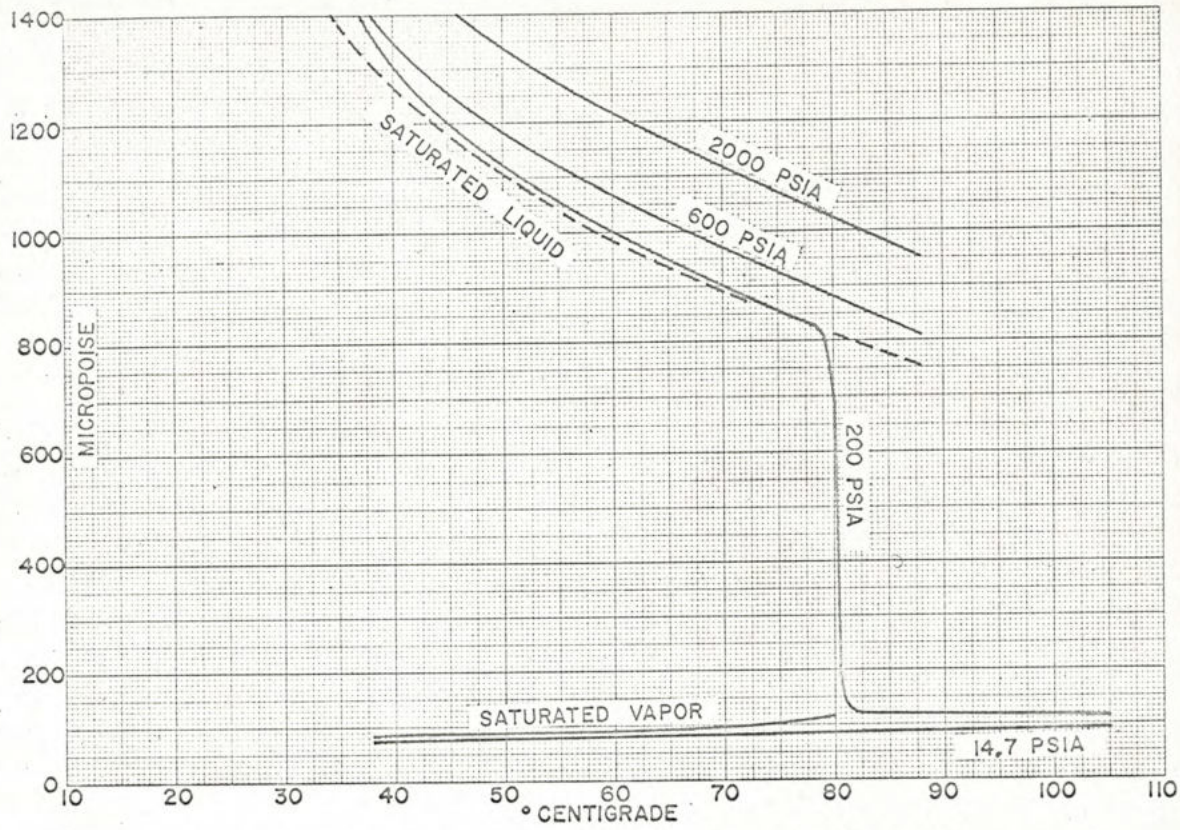

Fig. 17-9—Gives viscosity pressure effect for isobutane 35° C to 85° C.

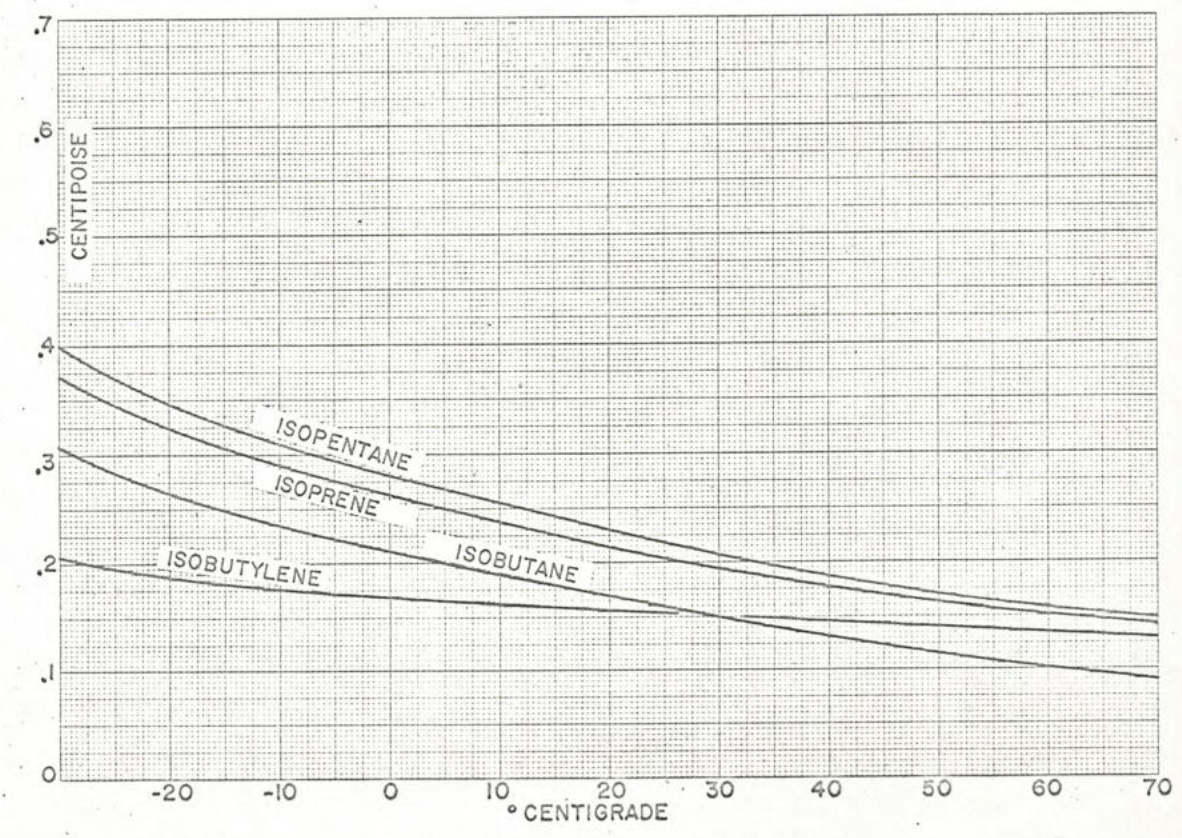

Fig. 17-10—Gives liquid viscosity for C_4-C_5 branched hydrocarbons from —30° C to +70° C.

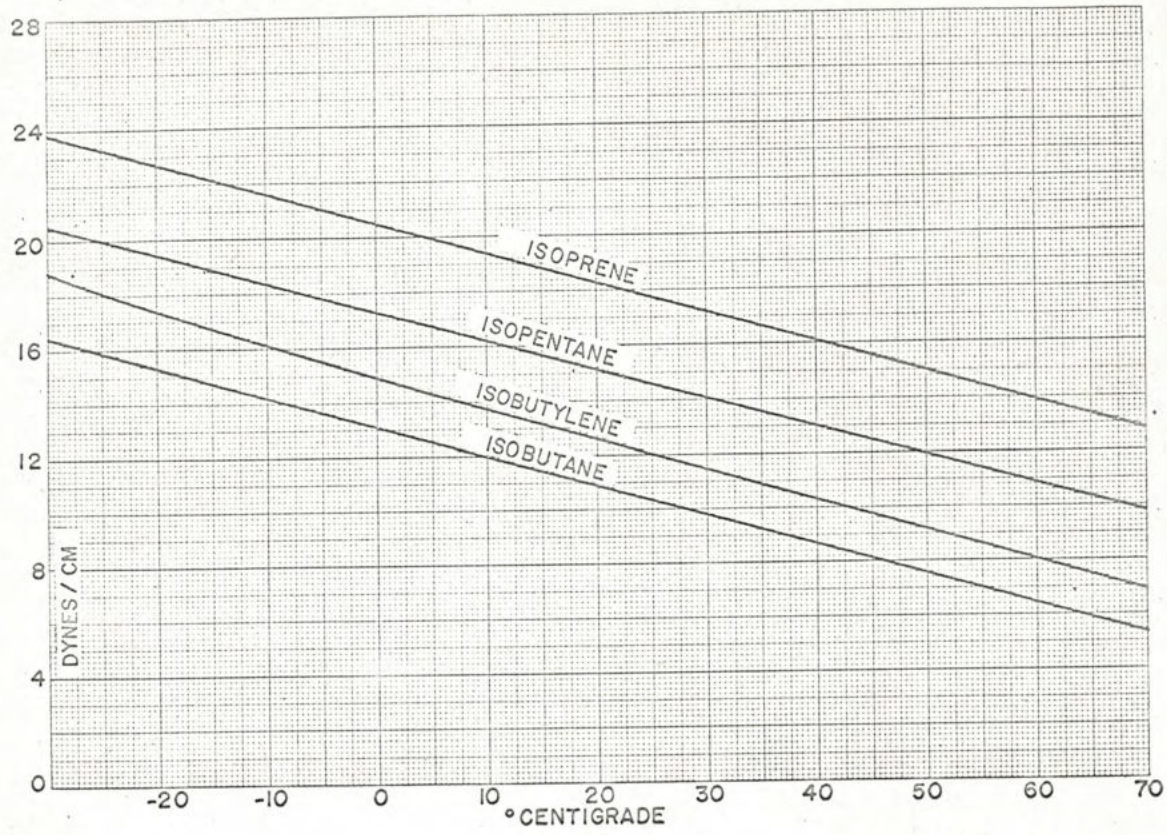

Fig. 17-11—Gives surface tension for C_4-C_5 branched hydrocarbons from −30° C to +70° C.

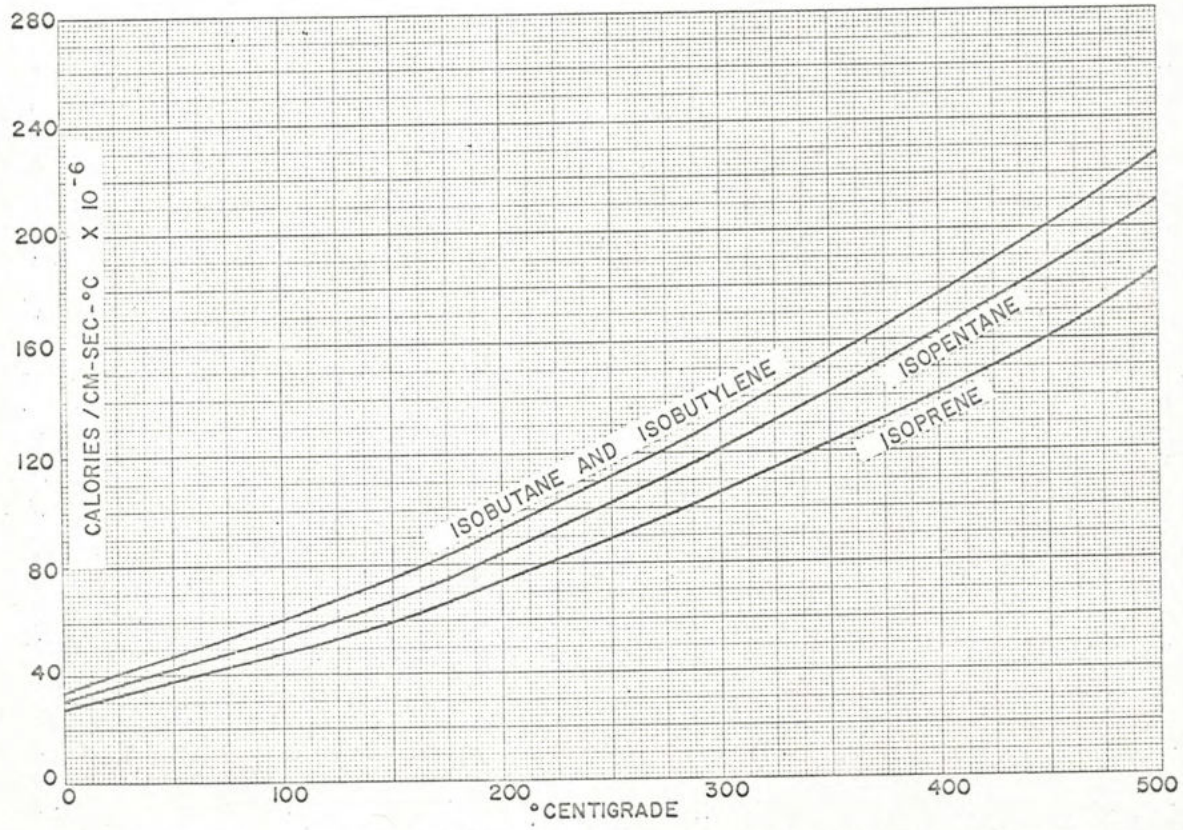

Fig. 17-12—Gives vapor thermal conductivity for C_4-C_5 branched hydrocarbons from 0° C to +500° C.

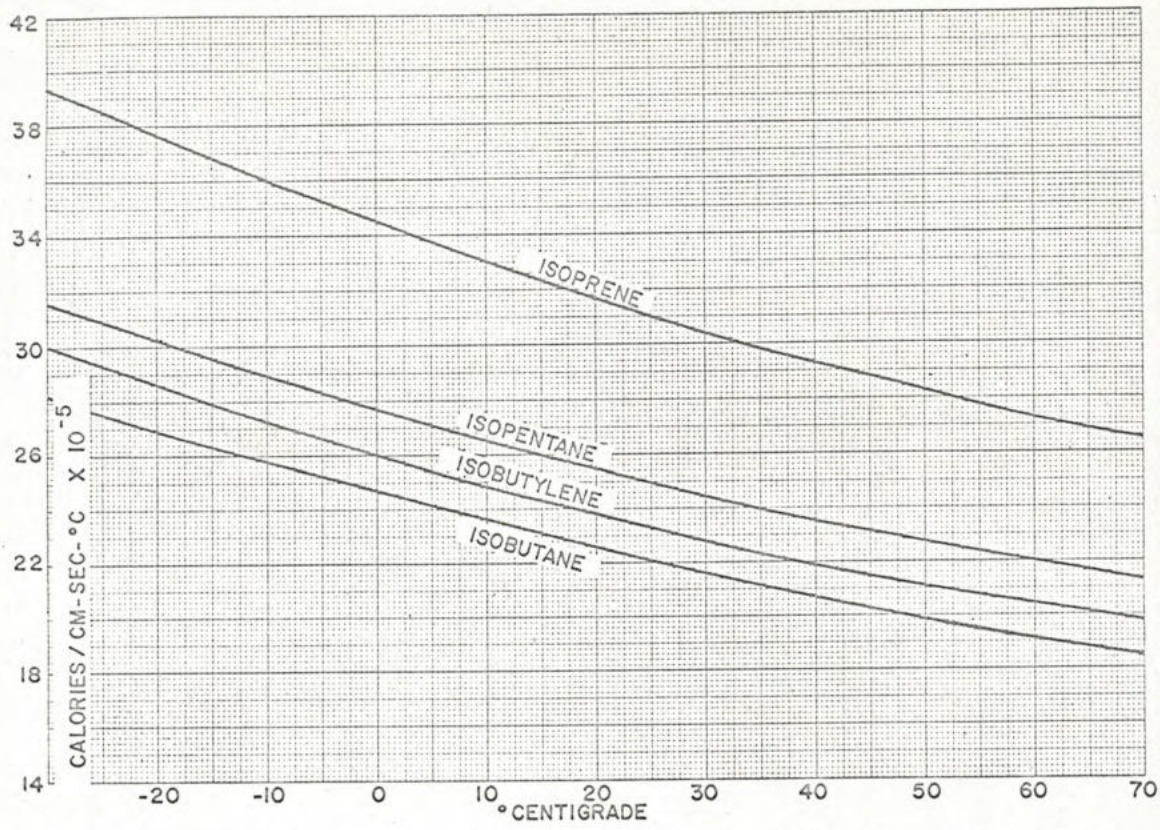

Fig. 17-13—Gives liquid thermal conductivity for C_4-C_5 branched hydrocarbons from —30° C to +70° C.

The liquid viscosity is available from −80° to + 90° C for isobutane;[3,19,24] 0-32° C for isoprene;[25] and −50 to + 30° C for isopentane.[3] The data for isobutylene were estimated by the method of Souders,[21] with a probable error of 3-5 percent. This method was also used to extend the data for isoprene and isopentane up to 70° C.

Surface Tension. The surface tensions are available only around room temperature.[3] These data have been extended over the −30 to +70° C range by Kharbanda's nomograph.[26]

Thermal Conductivity. The thermal conductivities for the vapor[27] and liquid[28] have been estimated by methods described in previous articles.

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Indexing Terms: Computations-4, Heat-7, Isobutane-9, Isobutylene-9, Isopentane-9, Isoprene-9, Liquid Phase-5, Physical Properties-7, Pressure-6, Properties/Characteristics/-7, Temperature-6, Vapor Phase-5.

Part 18—"C_6-C_8 Branched Hydrocarbons" will appear in an early issue.