Physical Properties of Hydrocarbons

Part 18—C_6—C_8 Branched Hydrocarbons

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THIS ARTICLE PRESENTS the physical properties of four C_6-C_8 branched-chain hydrocarbons. These compounds are found as major components of refinery streams. Only 2, 2, 4-trimethylpentane (better known as isooctane) has achieved commercialization as a relatively pure compound. The combination of a relatively high boiling point, high evaporation rate, and low toxicity makes it a popular solvent.

Critical Properties and Vapor Pressures. Kay has determined the critical properties of isohexane.[1] Ambrose reports the critical temperature for isohexane, 2-methylheptane, and isooctane.[2] Several investigators have experimentally determined the other critical properties of isooctane.[3,4] The ASTM reports critical property data for all four compounds.[5]

The vapor pressures of the four compounds up to their boiling points are available in the extensive vapor pressure data compilation by Stull.[6] Data up to the critical point are available only for isooctane.[3,4] The vapor pressures of the other three compounds were calculated by the same method described in previous articles.[7] For isooctane, the method gave an average error of 1.4 percent.

Heat of Vaporization. Experimental data are available up to the boiling point for all four compounds.[5,8,9,10] These data have been extended to the critical point by the previously described nomograph of Kharbanda.[11]

Heat Capacity. The vapor heat capacity for all four compounds was calculated by the method of Rihani and Doraiswamy.[12] When compared with data in the 0-700° C range reported by the American Petroleum Institute[13] for isohexane, the average error was 0.3 percent and the maximum error for five points was 0.6 percent. As can be seen from Fig. 18-3, the vapor heat capacities are almost identical for the four compounds over the entire 0-1,000° C range.

The liquid heat capacities have been determined from −40° C to +25° C.[5,14,15,16] The data have been extended up to 160° C by the calculation method described in the previous article.

For seven experimental points, the average and maximum error was 2.9 percent and 5.6 percent, respectively.

Density. The density of isohexane has been experimentally determined from 0-80° C;[9,17] 2-methylhexane from 0-60° C;[5,13] and 2-methylheptane from 0-60° C.[17,18] Kay[3] has measured the density of isooctane over the temperature range of 50° C to its critical point at 271° C. These data have been supplemented by the data of Beattie[4] and Geist.[17] The densities up to the critical point were calculated for the four compounds by the method of Francis.[19] Compared with the experimental data for isooctane from 0° C to within five degrees of the critical temperature, this amazingly accurate estimation method yielded average and maximum errors of 0.2 percent and 0.6 percent, respectively. For five experimental points on the other three compounds, the error averaged 0.5 percent.

Viscosity. The vapor viscosity for all four compounds has been estimated by the method proposed by Flynn and

TABLE 18-1

	Boiling Point °C	Melting Point °C	Molecular Weight	Critical Properties °C T_c	psia P_c	g/ml d_c
Isohexane (2-methylpentane)	60.3	−135.7	86.17	224.3	440	0.235
2-methylhexane	90.1	−118.3	100.20	257.2	400	.234
2-methylheptane	117.6	−109.0	114.22	286.4	364	.235
Isooctane (2,2,4-trimethylpentane)	99.2	−107.4	114.22	271.1	375	.237

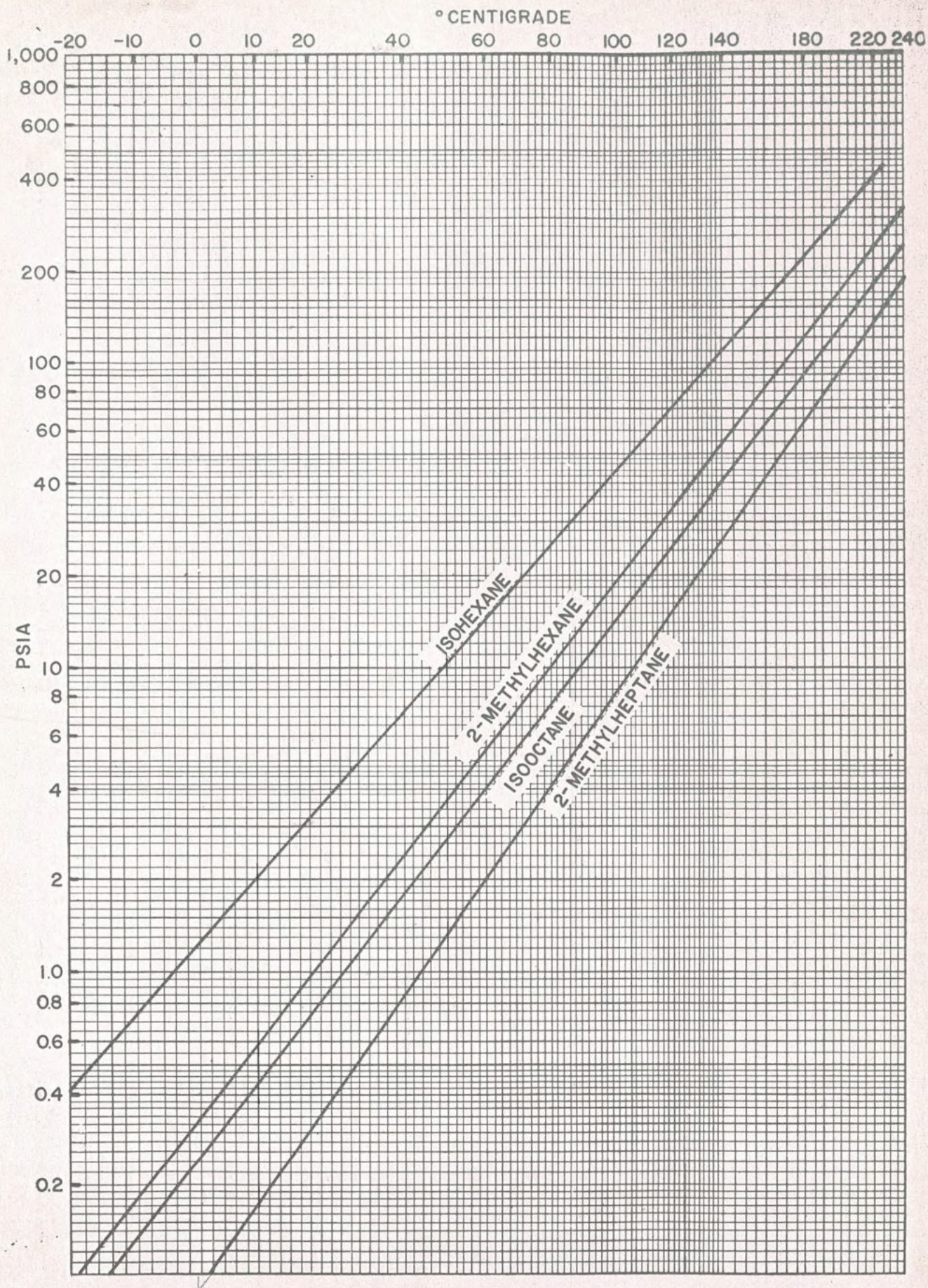

Fig. 18-1—Gives the vapor pressure for C_6—C_8 branched hydrocarbons from —20° C to +240° C.

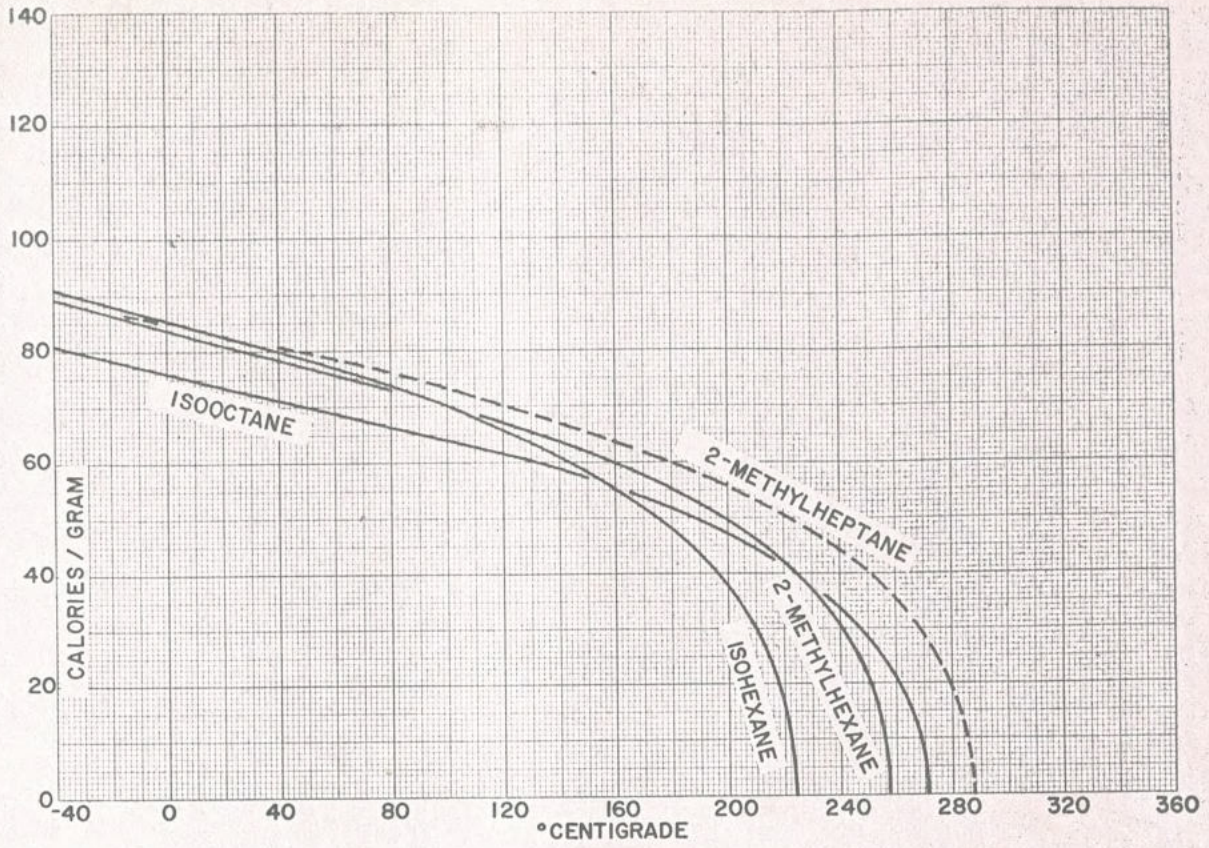

Fig. 18-2—Gives heat of vaporization for C_6—C_8 branched hydrocarbons from —40° C to +280° C.

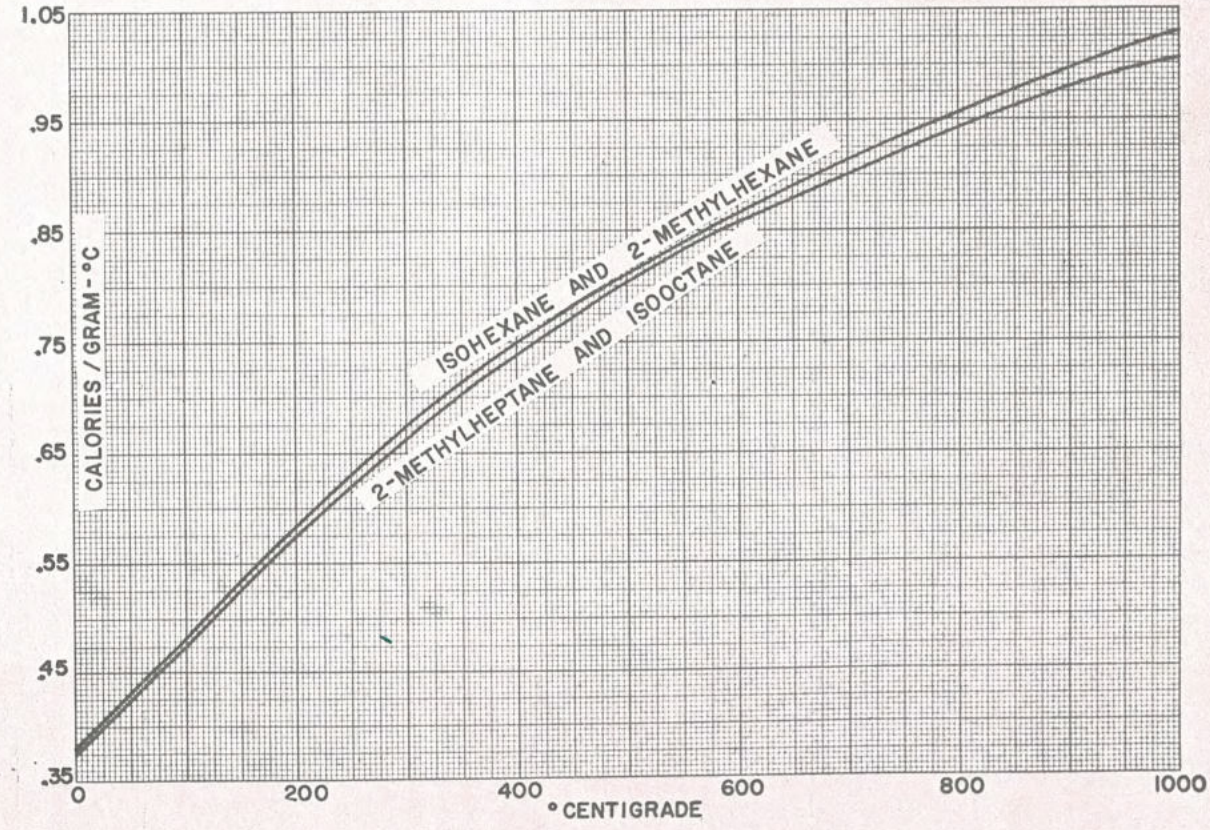

Fig. 18-3—Gives vapor heat capacity for C_6—C_8 branched hydrocarbons from 0° C to +1000° C.

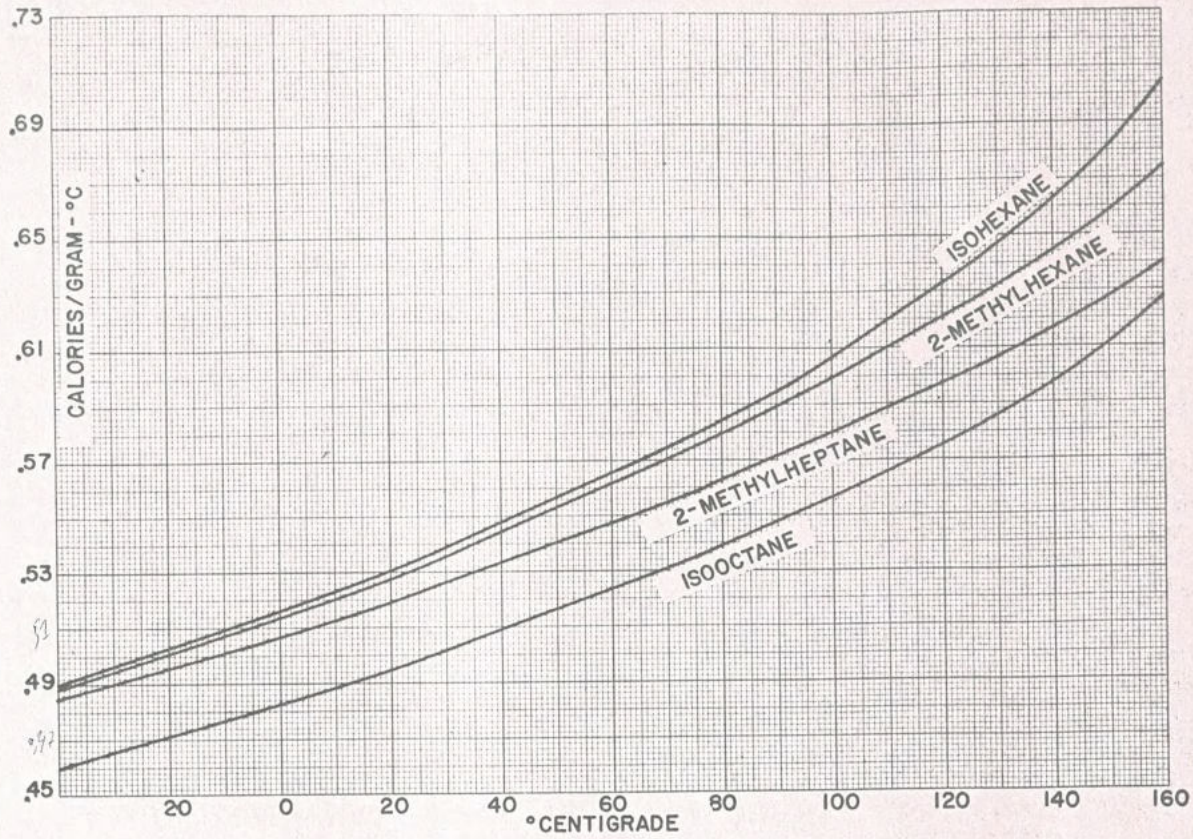

Fig. 18-4—Gives liquid heat capacity for C_6—C_8 branched hydrocarbons from —40° C to +160° C.

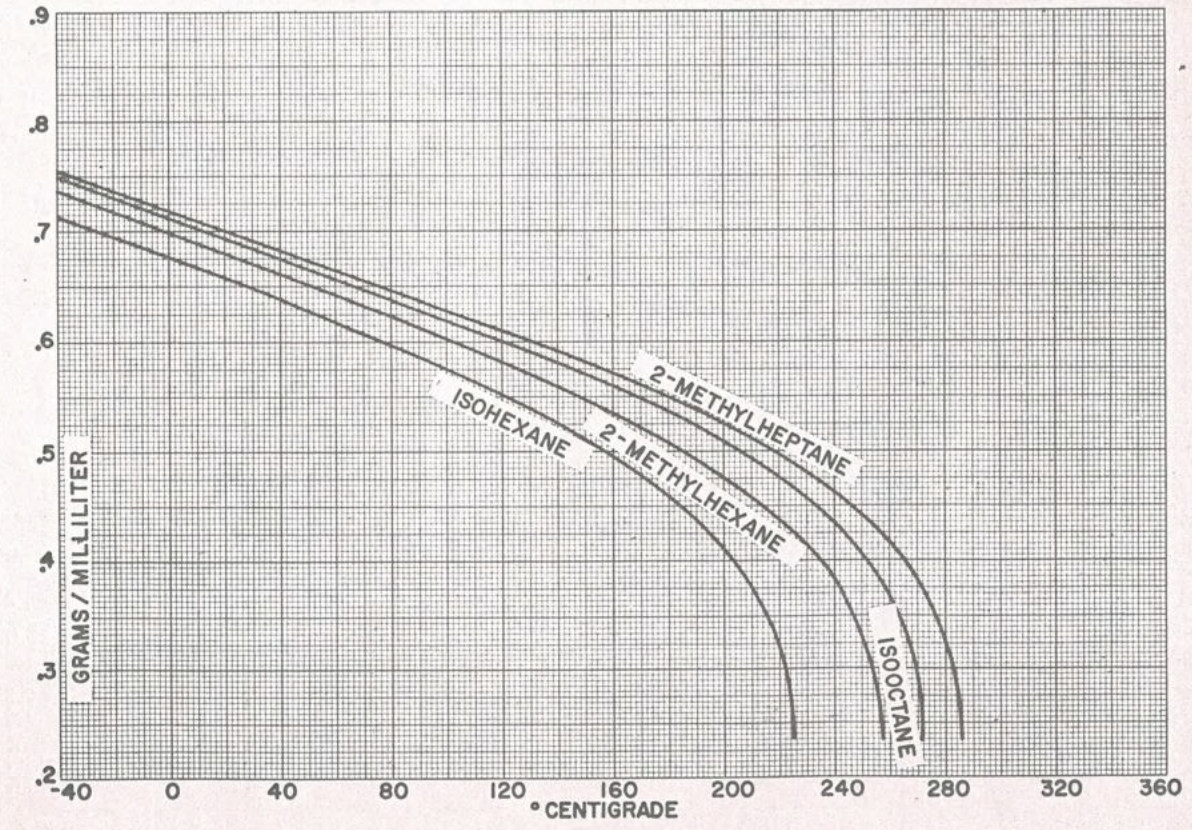

Fig. 18-5—Gives liquid density for C_6—C_8 branched hydrocarbons from —40° C to +280° C.

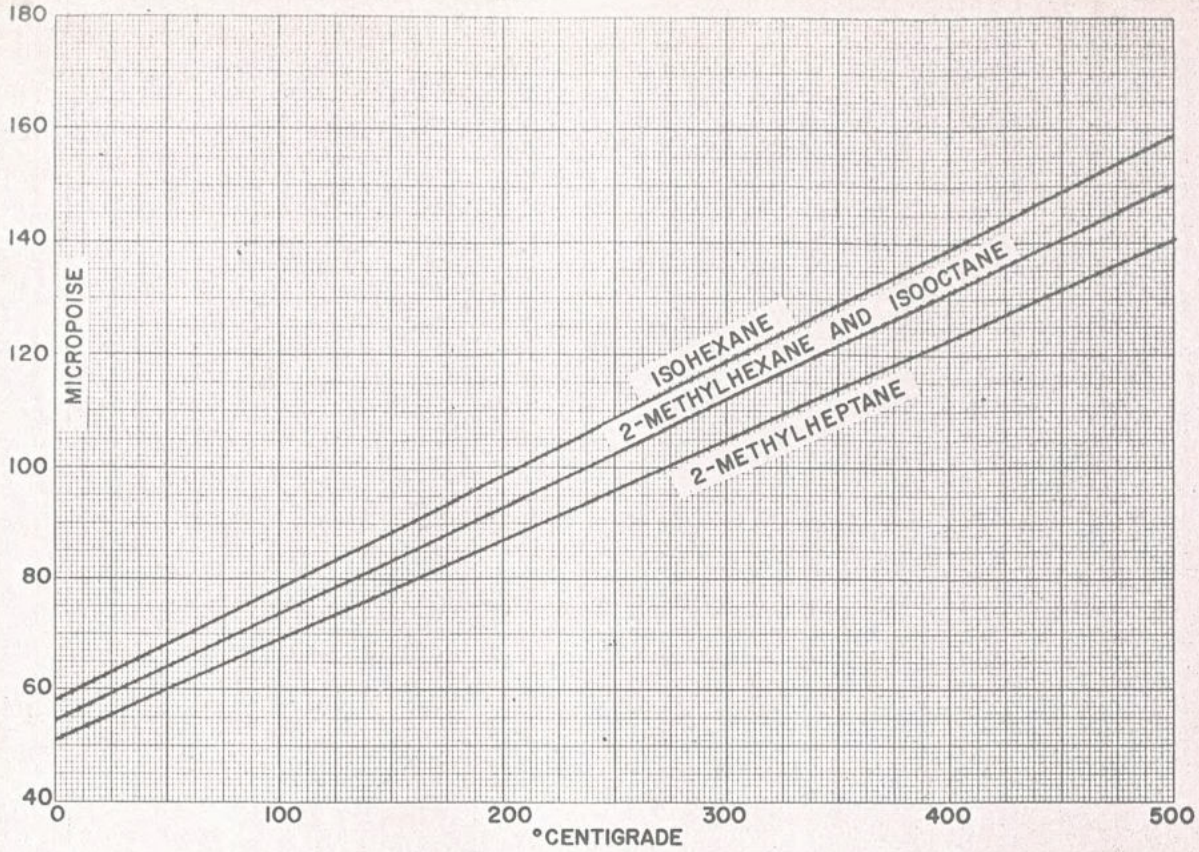

Fig. 18-6—Gives vapor viscosity for C_5—C_8 branched hydrocarbons from 40° C to 500° C.

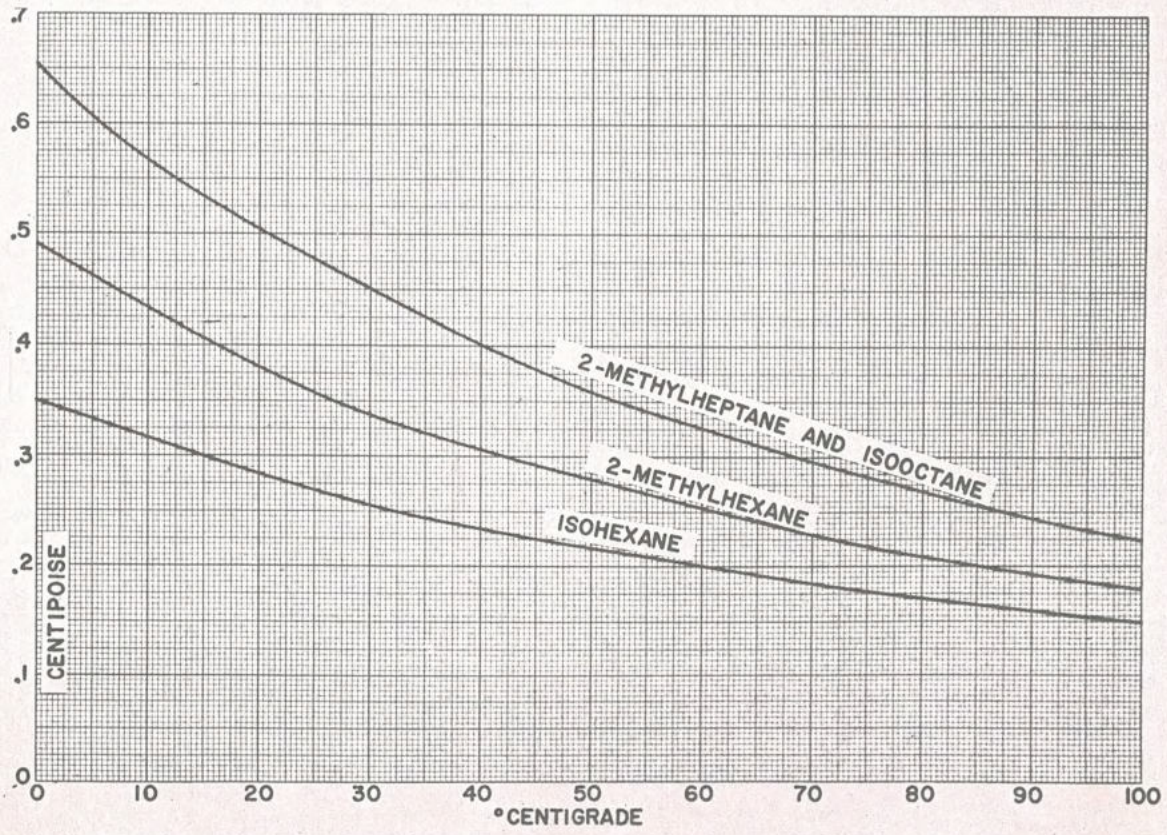

Fig. 18-7—Gives liquid viscosity for C_6—C_8 branched hydrocarbons from 0° C to 100° C.

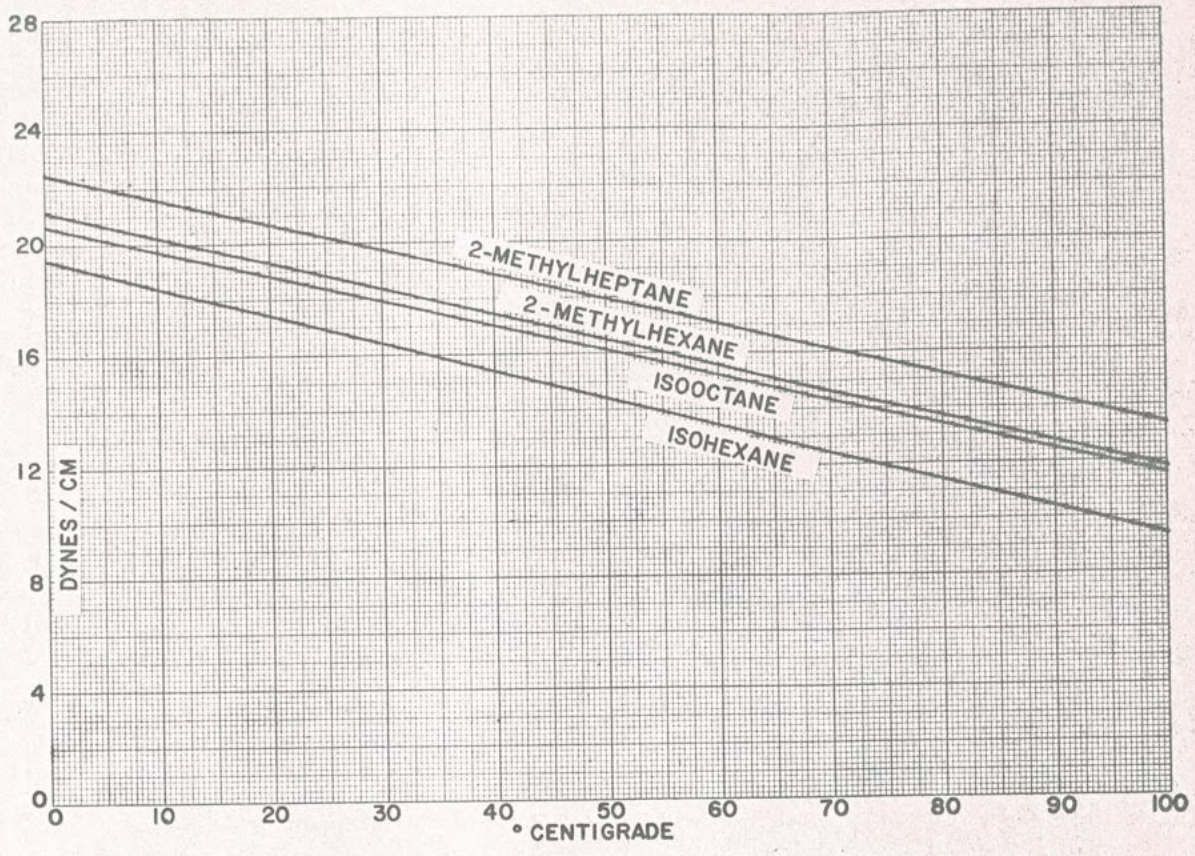

Fig. 18-8—Gives surface tension for C_6—C_8 branched hydrocarbons from 0° C to 100° C.

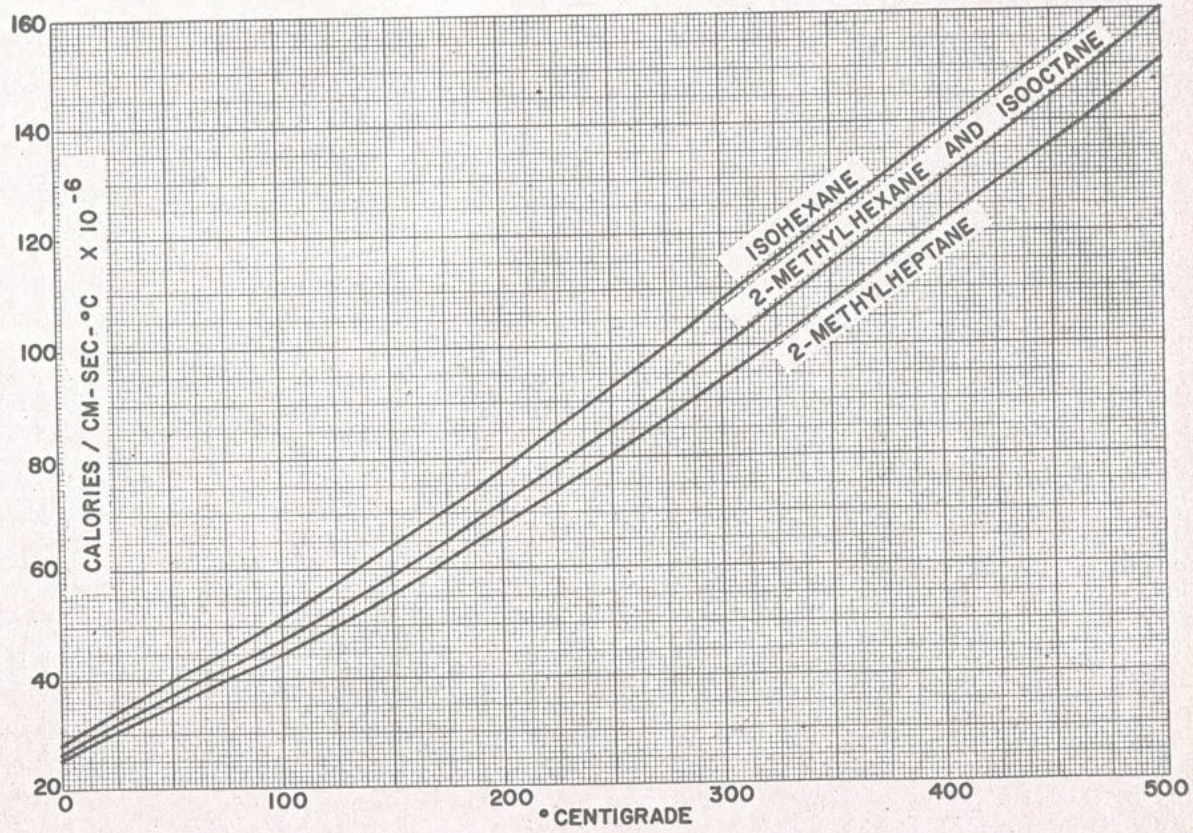

Fig. 18-9—Gives vapor thermal conductivity for C_6—C_8 branched hydrocarbons from 0° C to 500° C.

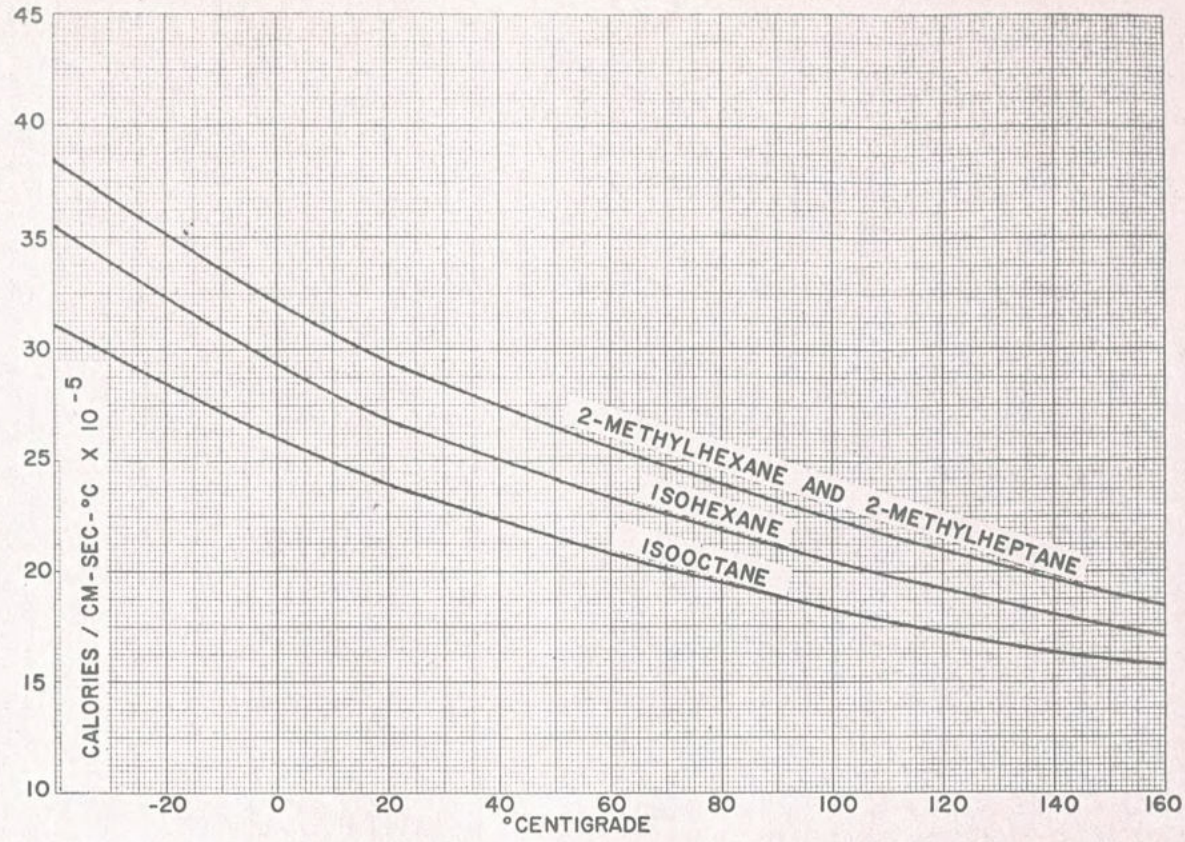

Fig. 18-10—Gives liquid thermal conductivity for C_6—C_8 branched hydrocarbons from —40° C to +160° C.

Thodos,[20] with an expected error of 2-4 percent.

The liquid viscosity is available from 0-40° C for isohexane[14,17] and 2-methylheptane.[17] For 2-methylhexane the viscosity has been measured only at 20° C.[14] Geist and Cannon[17] have determined the viscosity of isooctane from 0-90° C. The viscosities of 2-methylhexane from 0-100° C has been estimated by the method of Souders.[21] For isohexane and 2-methylheptane, the data have been extended over the 0-100° C range by a plot of the log of the viscosity versus the reciprocal of the absolute temperature.

Surface Tension. Surface tension data are available for all four compounds over the 0-100° C range.[5,8,13,14,18,22]

Thermal Conductivity. There are only a few data points on the vapor[23] and liquid[24] thermal conductivities. Consequently, estimation methods have been used to calculate the vapor[25] and liquid[26] thermal conductivities.

About the author

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Indexing Terms: Computations-4, Heat-7, Isohexane-9, Isooctane-9, Liquid Phase-5, 2-Methylheptane-9, 2-Methylhexane-9, Physical Properties-7, Pressure-6, Properties/Characteristics/-7, Temperature-6, Vapor Phase-5.

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Part 19 "Chlorinated C_2's" will appear in an early issue.