Physical Properties of Hydrocarbons

Part 16—C_5-C_8 Alkenes

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As with the C_5-C_8 alkanes covered in the previous article, the C_5-C_8 alkenes (1-pentene, 1-hexane, 1-heptene, 1-octene) are largely encountered as components in petroleum refinery streams. As pure compounds, they have found use as monomers for copolymers.

None of the 1-alkenes has been extensively studied. Consequently, it has been necessary to estimate many of the physical properties. Fortunately, estimation methods for hydrocarbons are generally very accurate.

Critical Properties and Vapor Pressure. The critical properties recorded in Table 16-1 were taken from the data of the ASTM.[1] The critical temperatures of all four compounds have been experimentally determined. The critical pressures and densities, except for 1-pentene, were estimated by the ASTM.

The vapor pressure of 1-pentene has been determined up to the critical point.[2,3,4,5] Data for the other three compounds are available only up to the boiling point.[4,6,7,8] The vapor pressure from the boiling point to the critical point for these three compounds has been estimated from the equation:

$$\log P_r = A(1 - 1/T_r)$$

where
P_r = reduced pressure
T_r = reduced temperature
A = a constant which is determined from experimental data (i.e., the boiling point)

Miller[9] has evaluated the available vapor pressure equations and has found this equation to be very reliable for hydrocarbons from the boiling point to the critical point. The error is less than 2 percent. The author found an average error of 0.7 percent for 1-pentene.

Heat of Vaporization. Heat of vaporization data are available only up to the boiling point.[1,2,3,6,8] The data have been extended by Kharbanda's nomograph of the Watson equation.[10]

Heat Capacity. The vapor heat capacities have been estimated by the method of Rihani and Doraiswamy.[11] When compared to experimental data on 1-pentane,[3] the estimated values gave an average error of 0.3 percent.

The liquid heat capacity has been experimentally determined at 25° C for all four compounds[1], but only 1-pentene has been studied over a wide temperature range.[12,13] The liquid heat capacities for the other three compounds were estimated from the equation:

$$d\ C_p = k$$

where
d = density, g/ml
C_p = heat capacity, cal/g — °C
k = a constant

For hydrocarbons, k is generally assumed to be 0.35. However, this assumption gives average errors of about 5 percent. The author has found much better results by calculating k from a known liquid heat capacity (in this case, 25° C). By this method k was 0.336 for 1-pentene; 0.345 for 1-hexene; 0.36 for 1-heptene; and 0.368 for 1-octene. For 1-pentene, this method gave an average error of 1.2 percent when compared to 7 experimental points over the temperature range of −23° C to +105° C.

Density. Liquid density data for the four compounds are available only in the 0-100° C temperature range.[1,2,5,6,14] The data have been extended to cover the −40° C to the critical temperature range by the equation proposed by Francis[15]:

$$D_s = A - Bt - C/(E - t)$$

where
A = density at 20° C plus .05
B, C = constants
t = temperature, ° C
E = the critical temperature plus 34, in °C

Francis has evaluated B and C for a wide range of hydrocarbons for which experimental densities are available. Using this compilation, it is possible to estimate the constants for the C_5-C_8 alkenes. Although Francis generally recommends that A be calculated as the density at 20° C plus .06, the author found a better fit for the C_5-C_8 alkenes using .05 instead of .06. For 12 points, the author found a maximum error of 1.6 percent and an average error or only 0.9 percent. This is amazingly good accuracy for a method that is simple and requires only a knowledge of the room temperature density and the critical temperature.

Viscosity. The vapor viscosity has been estimated by the method of Bromley and Wilke.[10]

The liquid viscosities of 1-hexene and 1-octene have

PHYSICAL PROPERTIES OF HYDROCARBONS . . .

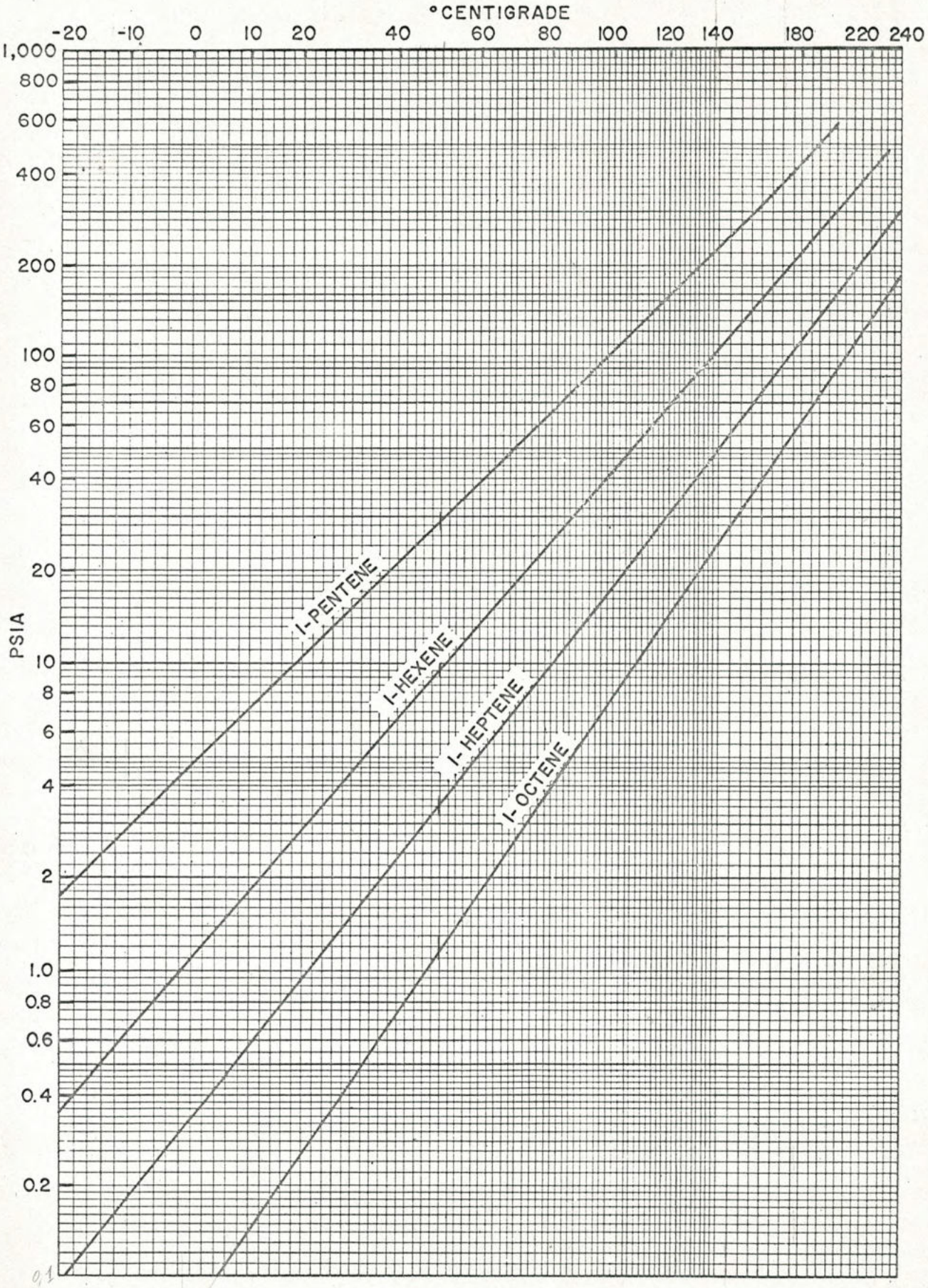

Fig. 16-1—Gives vapor pressure for C_5-C_8 alkenes from −20° C to +240° C.

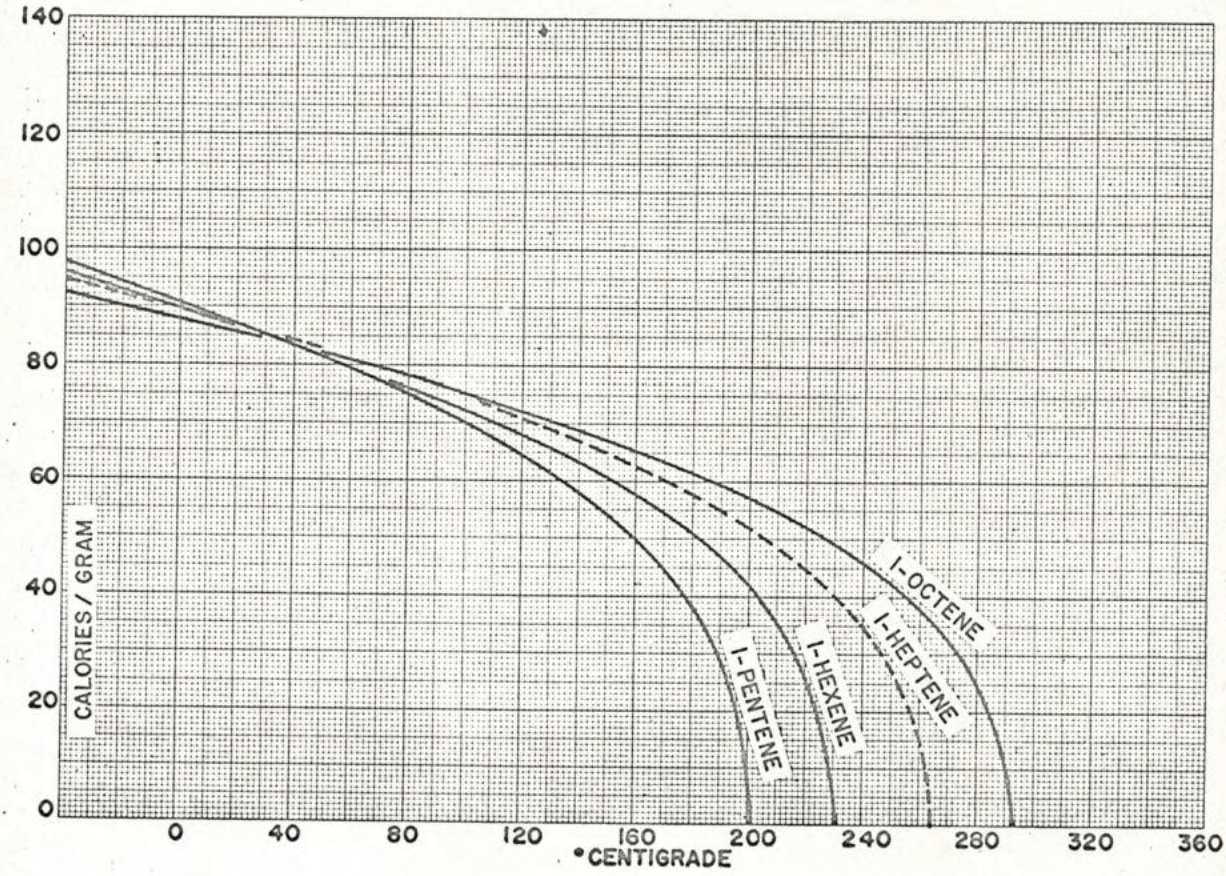

Fig. 16-2—Gives heat of vaporization for C_5-C_8 alkenes from −40° C to 294° C.

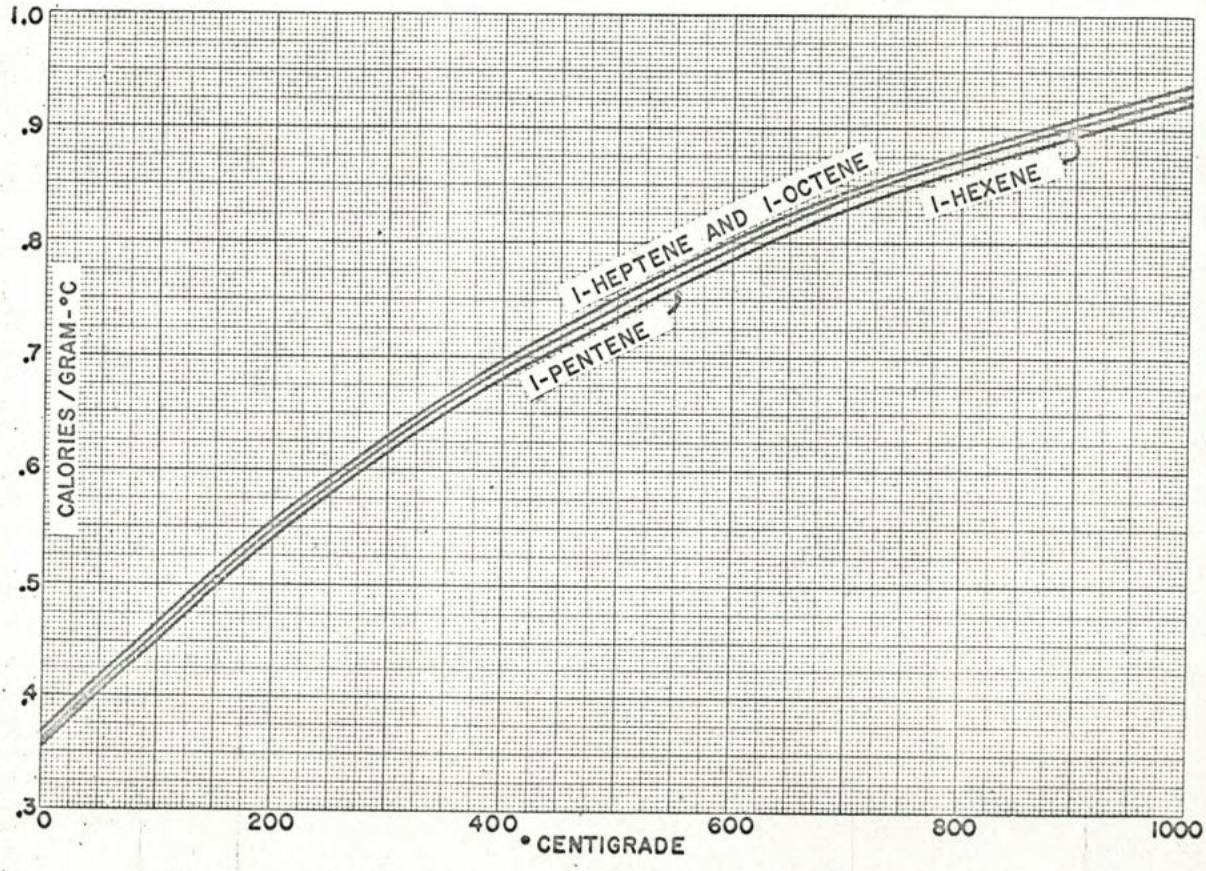

Fig. 16-3—Gives vapor heat capacity for C_5-C_8 alkenes from 0° C to +1,000° C.

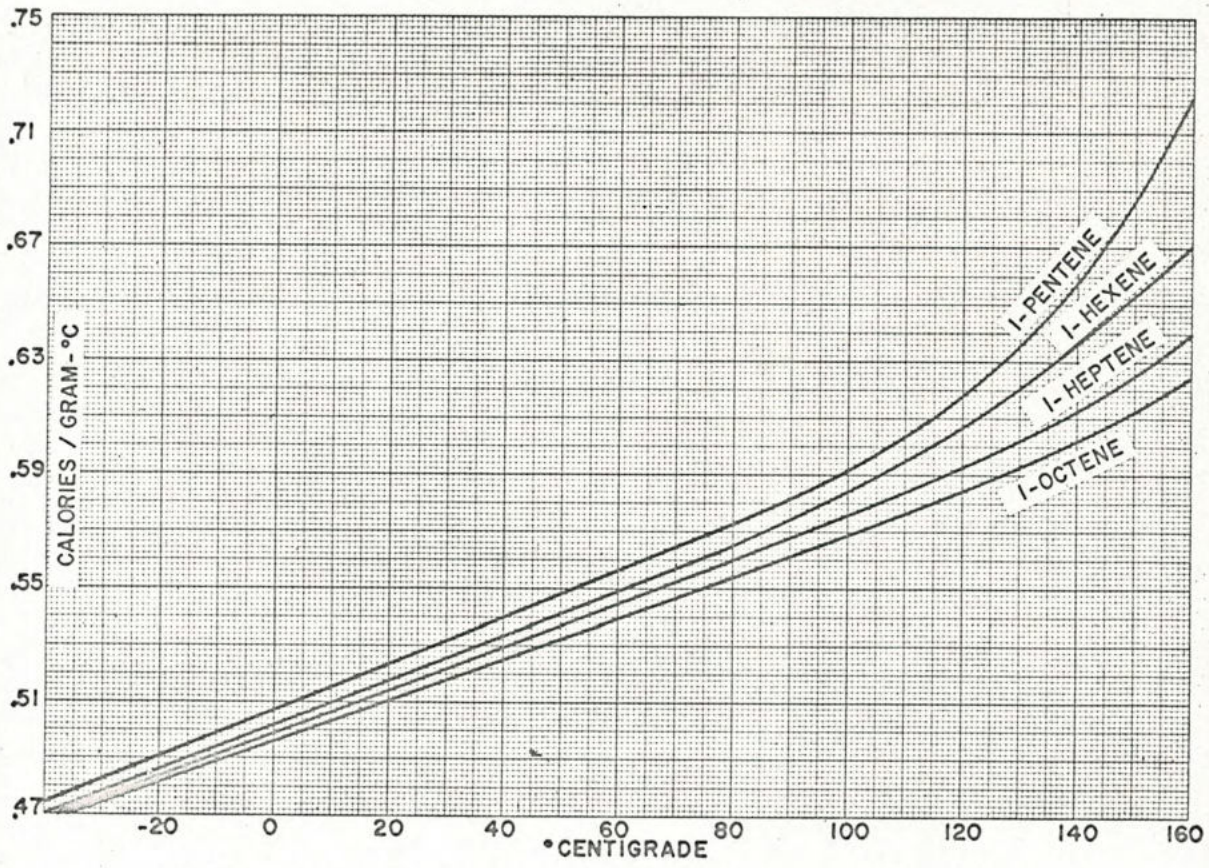

Fig. 16-4—Gives liquid heat capacity for C_5-C_8 alkenes from −40° C to +160° C.

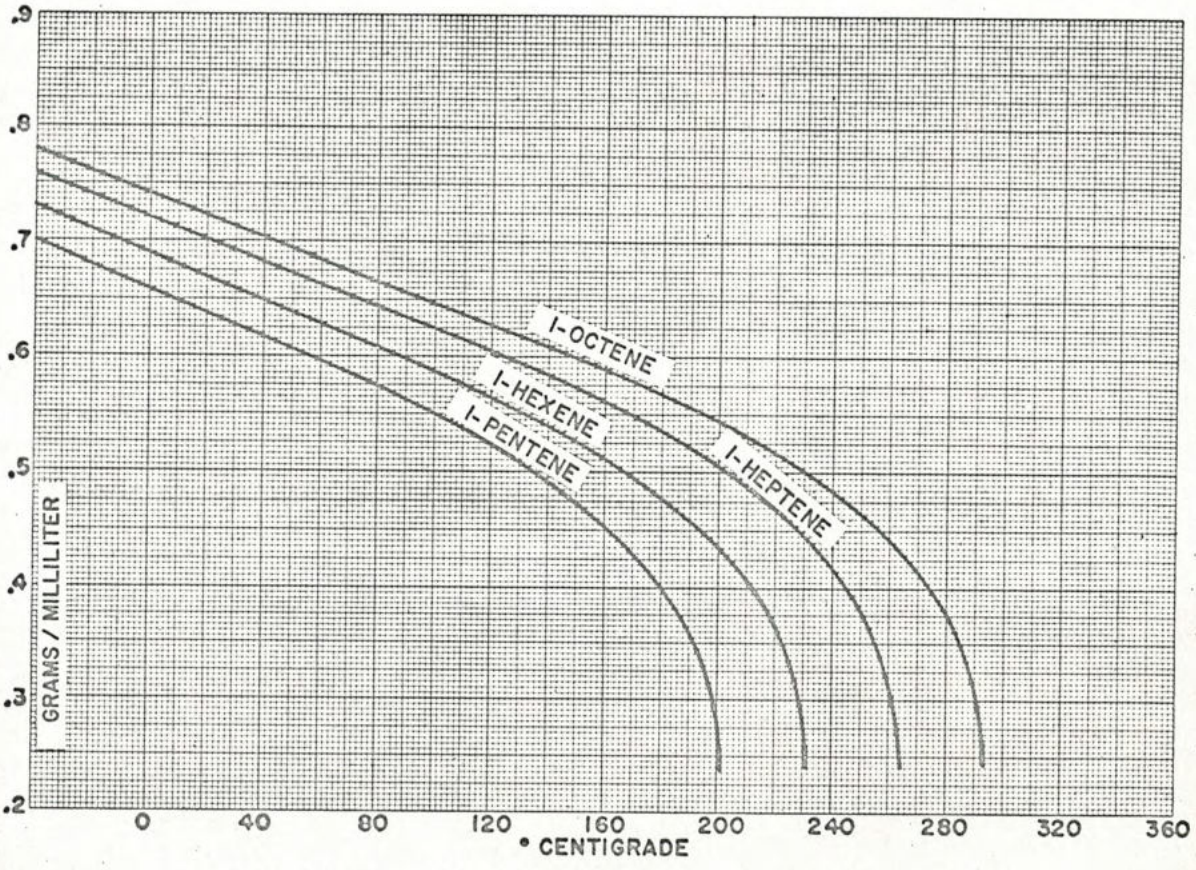

Fig. 16-5—Gives liquid density for C_5-C_8 alkenes from −40° C to +293° C.

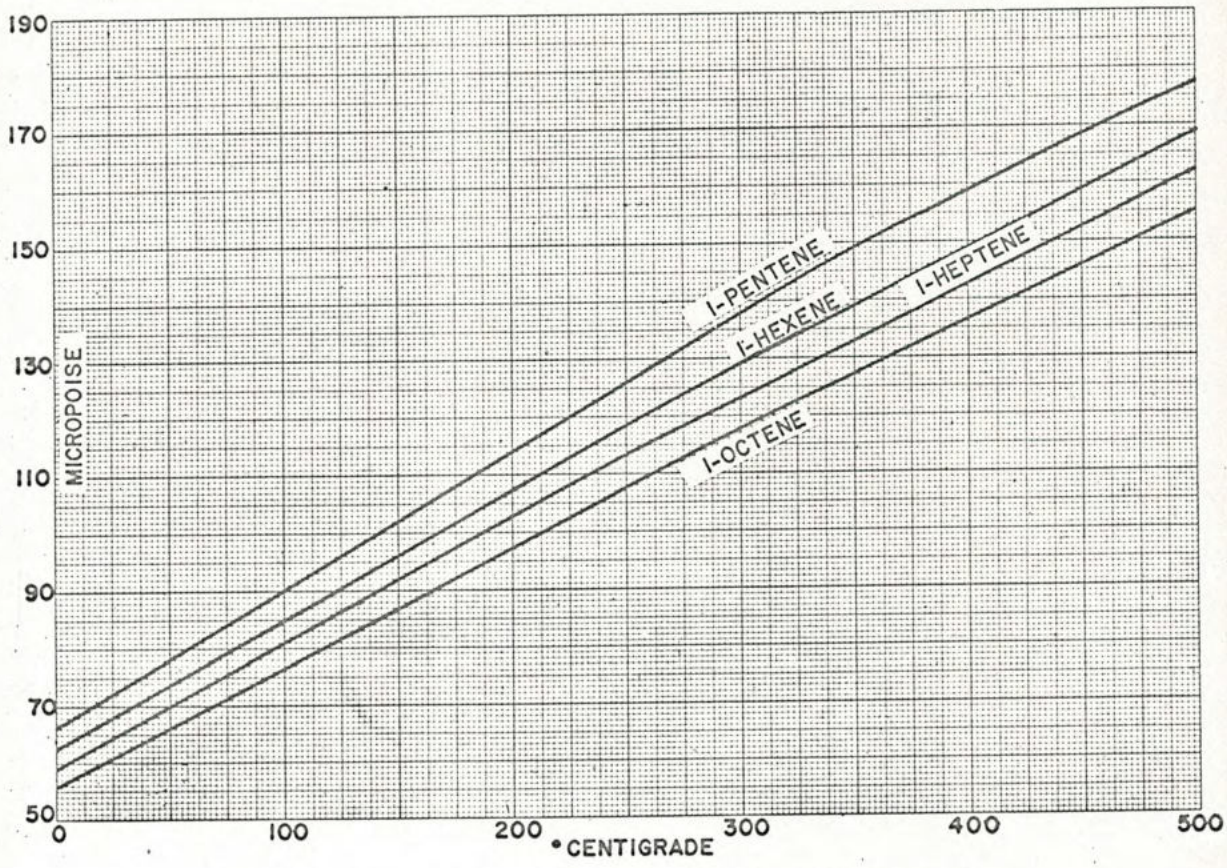

Fig. 16-6—Gives vapor viscosity for C_5-C_8 alkenes from 0° C to + 500° C.

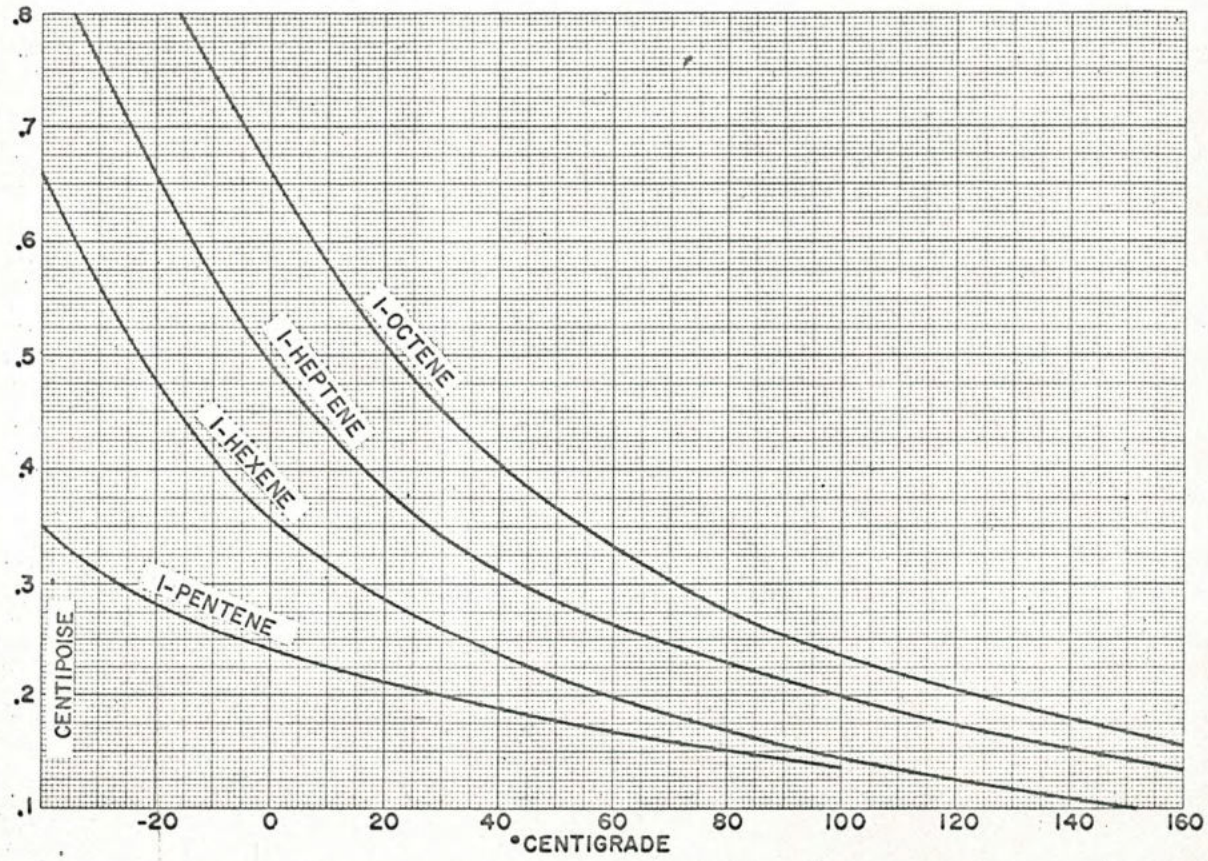

Fig. 16-7—Gives liquid viscosity for C_5-C_8 alkenes from −40° C to +160° C.

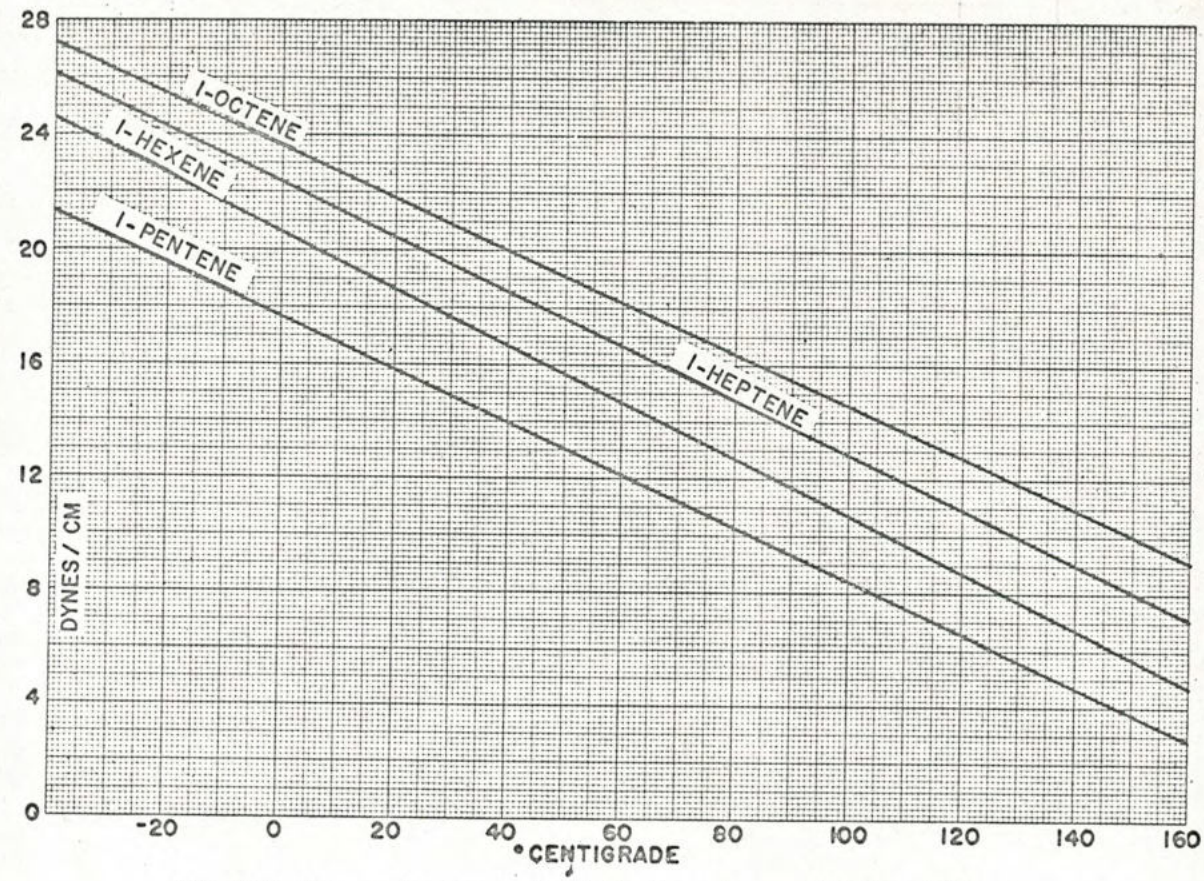

Fig. 16-8—Gives surface tension for C_5-C_8 alkenes from −40° C to +160° C.

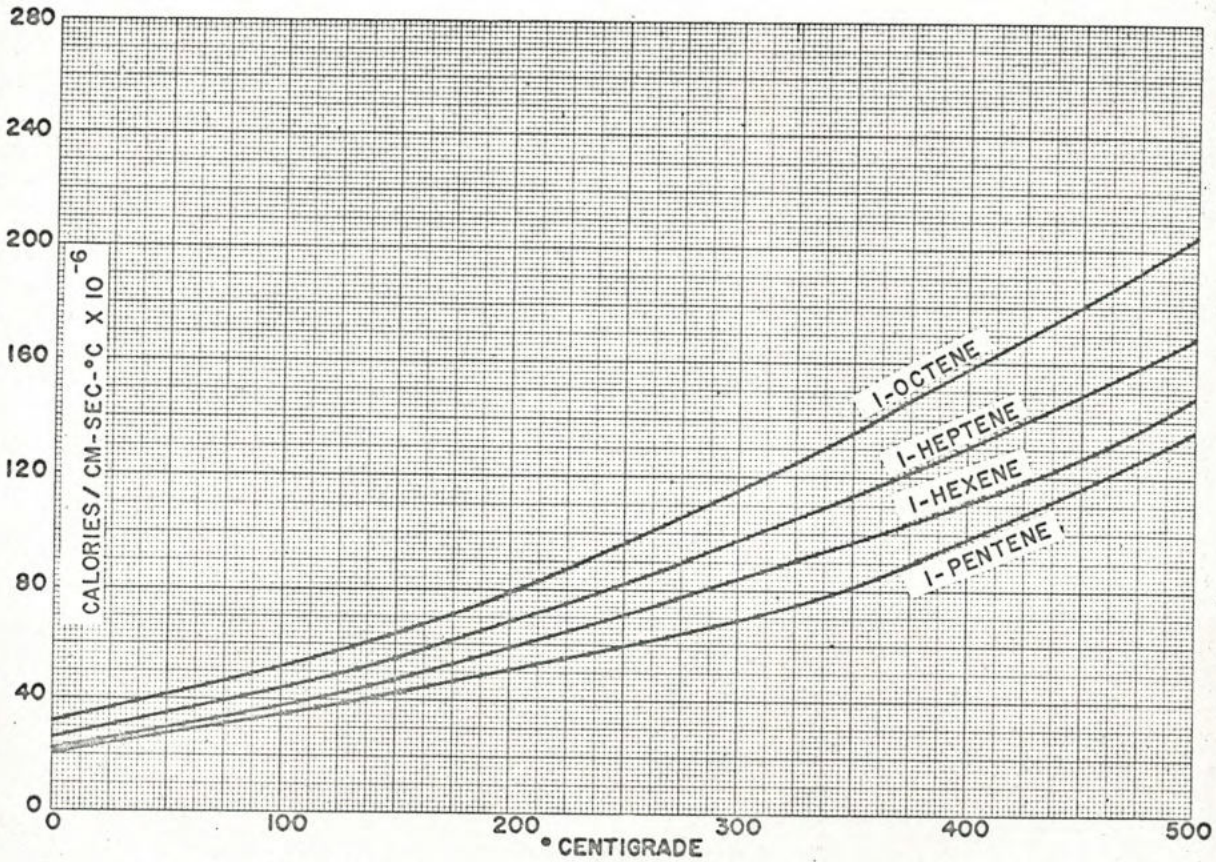

Fig. 16-9—Gives vapor thermal conductivity for C_5-C_8 alkenes from 0° C to +500° C.

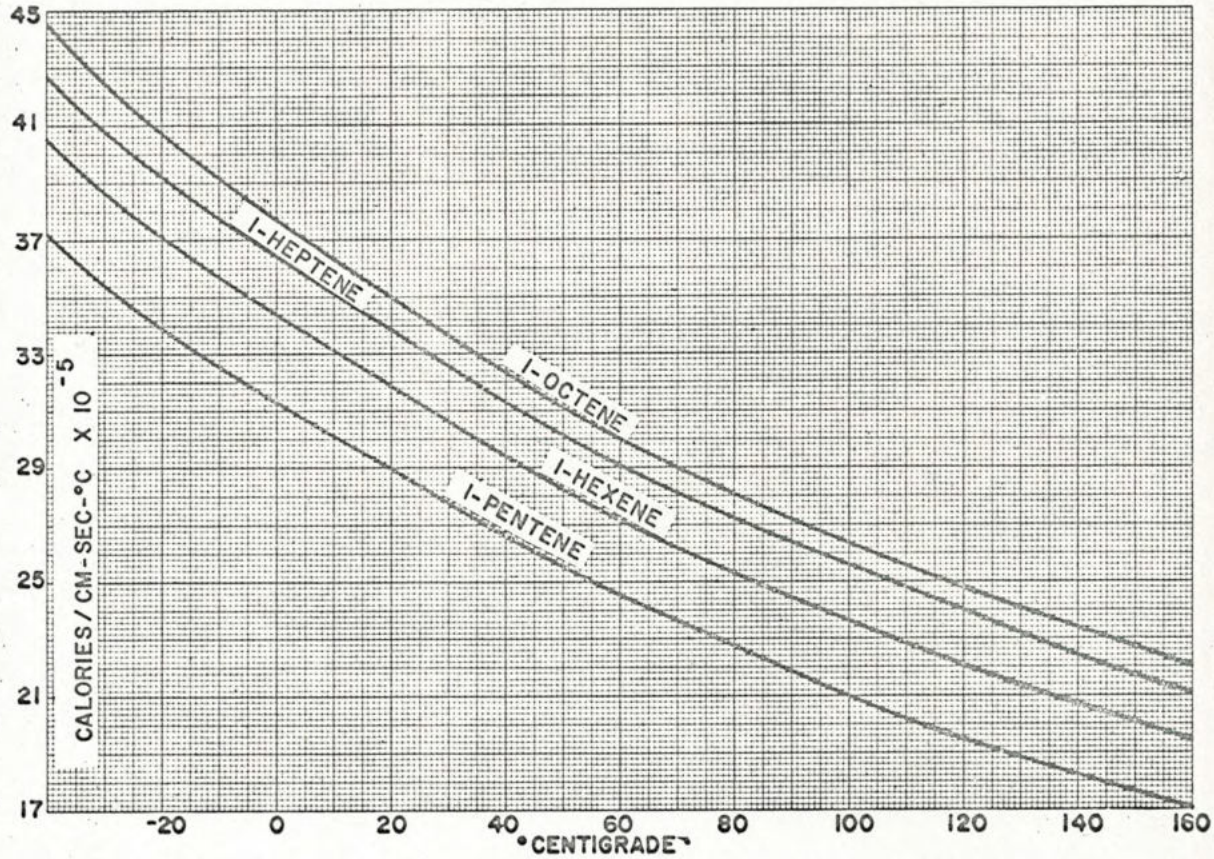

Fig. 16-10—Gives liquid thermal conductivity for C_5-C_8 alkenes from −40° C to +160° C.

been measured by Wright[14] up to the boiling point. Souder's equation[10] has been used to estimate the viscosity of 1-pentene and 1-heptene from 0 to 100° C.

$$\log (\log 10\mu) = md - 2.9$$

where μ = viscosity, in centipoises
m = a constant evaluated from the molecular structure
d = liquid density at the desired temperature

The equation gave an average error of 2.8 percent when compared to experimental data for 1-hexene and 1-octene. The data for all four compounds were extended over the −40 to +160° C range by a plot of the log of the viscosity against the reciprocal of the absolute temperature. This gives a straight line, which can be extrapolated to the other temperatures.

Surface Tension. Jasper and Kerr[16] have measured the surface tension from 0° to the boiling point for 1-hexene, 1-heptene, and 1-octene. The surface tension of 1-pentene is available only at 25° C.[1] The data have been extended by the nomograph of Kharbanda[17], with an average error of 2.6 percent for 9 points which were compared with experimental data.

TABLE 16-1—Physical Properties of C_5-C_8 Alkenes

	Boiling Point (°C)	Melting Point (°C)	Molecular Weight	Critical Properties		
				T_c °C	P_c PSIA	d_c g/ml
1-pentene	30.0	−165.2	70.13	201	586	0.238
1-hexene	63.5	−139.8	84.16	231	471	.240
1-heptene	93.6	−118.9	98.18	264	426	.240
1-octene	121.3	−101.7	112.21	293	395	.242

Thermal Conductivity. Because there are no experimental data for the thermal conductivity, the data were estimated for the vapor[18] and liquid[19] by methods used in previous articles.

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Indexing Terms: Computations-4, Heat-7, Heptene-9, Hexene-9, Liquid Phase-5, Octene-9, Pentene-9, Physical Properties-7, Pressure-6, Properties/Characteristics/-7, Temperature-6, Vapor Phase-5.

Part 17 will appear in an early issue.