Physical Properties of Hydrocarbons

Part 39—Benzene Compounds

From charts you can get these properties for benzene compounds:

- Vapor Pressure
- Heat of Vaporization
- Heat Capacity
- Density
- Viscosity
- Surface Tension
- Thermal Conductivity

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BENZENE is one of the most important raw materials in the petrochemical industry. The 1970 demand is expected to be close to 10 billion pounds. Most of this benzene is produced by the petroleum industry by reforming or by dealkylation of toluene. Styrene accounts for almost 40 percent of benzene usage. Phenol and cyclohexane account for 50 percent of the rest. The future growth of benzene depends largely on the growth of these three end-use markets.

Cumene is produced by alkylating benzene with propylene. Most of the cumene is converted to phenol and acetone. In 1970 cumene production will top one billion pounds.

Ethylbenzene is made by the alkylation of benzene and then dehydrogenated to produce styrene monomer. About 4 billion pounds of ethylbenzene will be produced in 1970. Propylbenzene has not achieved the significant commercial importance accorded to benzene, cumene and ethylbenzene.

Critical Properties and Vapor Pressure. The critical temperatures and pressures of all four compounds and the critical densities of benzene and ethylbenzene have been measured.[1] The critical densities of propylbenzene and cumene were estimated by the method of Lydersen, with a probable error of 1-2 percent.[9]

The vapor pressures have been determined up to the critical point for benzene[7,8] and ethylbenzene,[1,3] and to the boiling point for propylbenzene[3] and cumene.[1,3] The vapor pressures above the boiling point were estimated by the method used in previous articles in this series.[10]

Heat of Vaporization. Data are reported in the literature for benzene up to the critical temperature[1,8] and at the boiling point for ethylbenzene.[1] The equation proposed by Giacalone was used to calculate the heat of vaporization at the boiling point for propylbenzene and cumene.[9] For ethylbenzene, this equation gave a value in exact agreement with the experimental data. The nomograph of Kharbanda was used to extend the boiling point value to other temperatures.[11]

Heat Capacity. Vapor heat capacities have been determined for all four compounds.[2,8,12-14]

Liquid heat capacities are available for benzene from 0-80°C;[1,8,15,16] for ethylbenzene from −92°C to +27°C;[17] and from −92°C to +98°C for propylbenzene.[14] The heat capacity of cumene at 20°C was calculated by the technique of Johnson and Huang.[9] The data were extended to 200°C by the equation, density times heat capacity equals a constant. For five experimental values, the error averaged 2.1 percent.

Density. The densities have been measured from 0°C to the critical point for benzene;[1,8,18-20] from −80°C to +130°C for ethylbenzene[1,18,21] and propylbenzene;[1,18,21] and from 0°C to 40°C for cumene.[18,21] The data were extended to the critical point by the Lydersen method.[9] For five experimental values, the error averaged 0.2 percent.

Viscosity. The vapor viscosities have been estimated, with a probable error of 3-5 percent.[22]

Liquid viscosity data are available to the critical point

TABLE 39-1—Physical Properties of Benzene Compounds

	Boiling Point, °C	Freezing Point, °C	Molecular Weight	Critical Properties Tc °C	Pc psia	dc g/ml
Benzene	80.1	5.5	78.11	289	714	0.304
Ethylbenzene	136.2	−95.0	106.16	344	536	0.284
Propylbenzene	159.5	−99.6	120.19	366	473	0.286*
Cumene	152.4	−96.1	120.19	358	467	0.288*

* Estimated.

PHYSICAL PROPERTIES OF HYDROCARBONS . . .

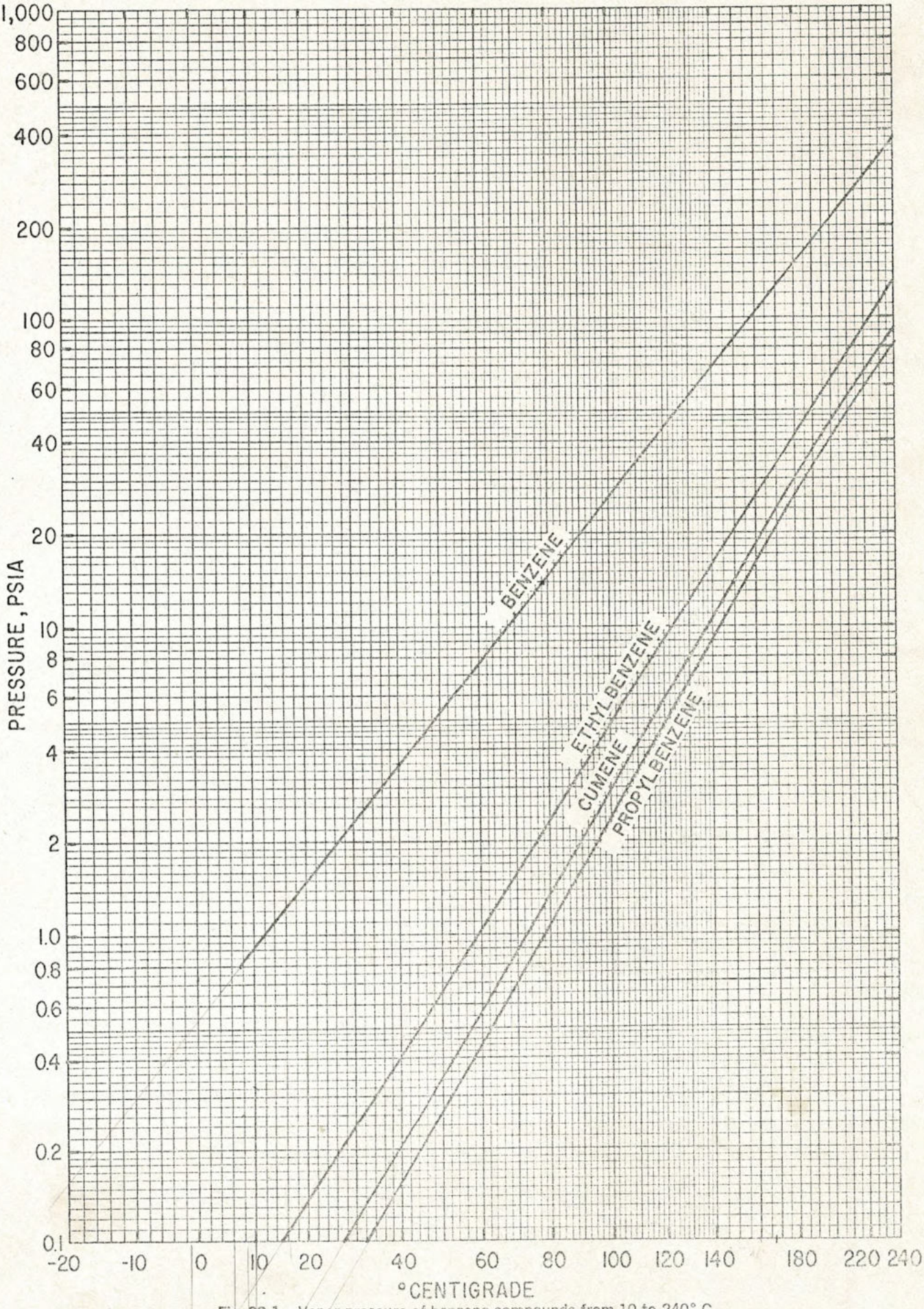

Fig. 39-1---Vapor pressure of benzene compounds from 10 to 240° C.

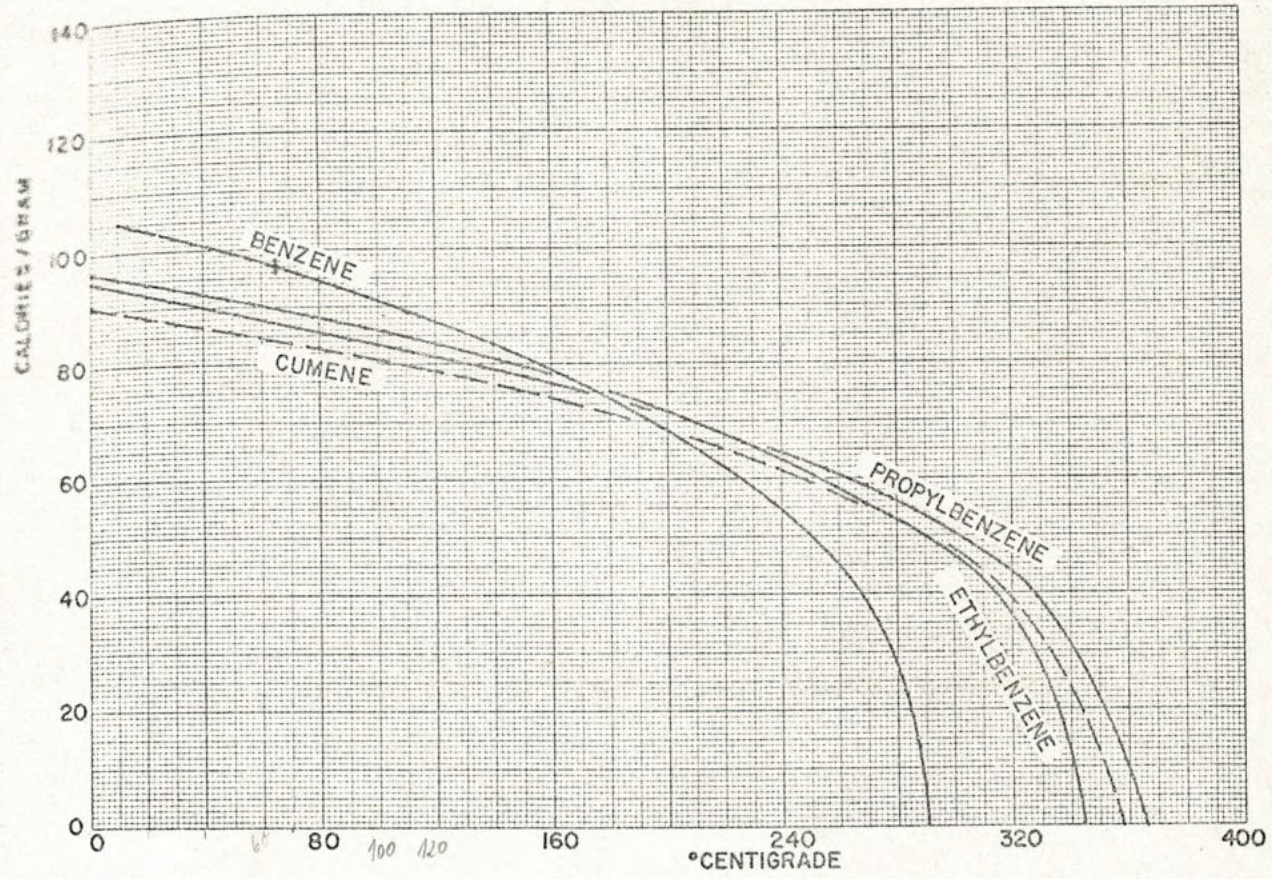

Fig. 39-2—Heat of vaporization of benzene compounds from 0 to 360° C.

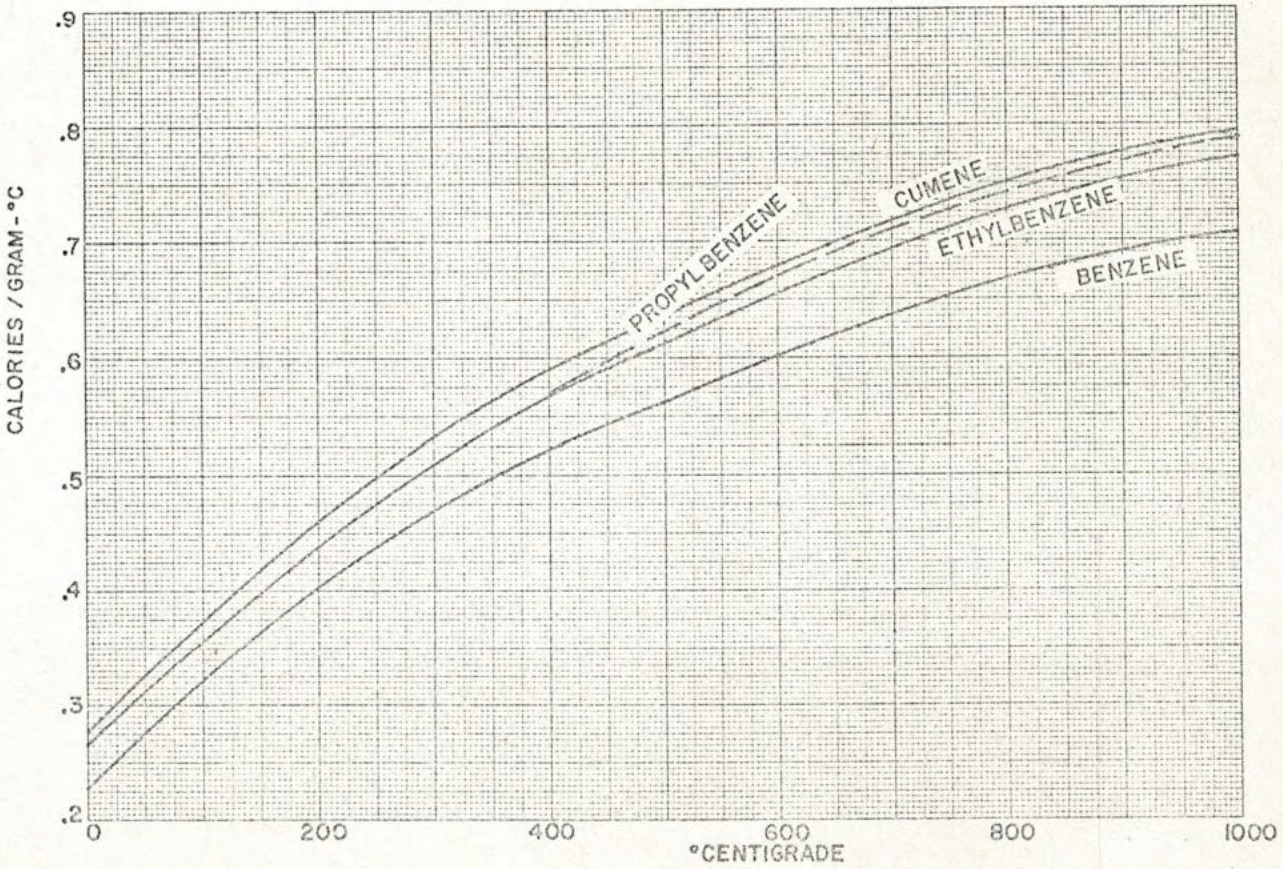

Fig. 39-3—Vapor heat capacity of benzene compounds from 0 to 1000° C.

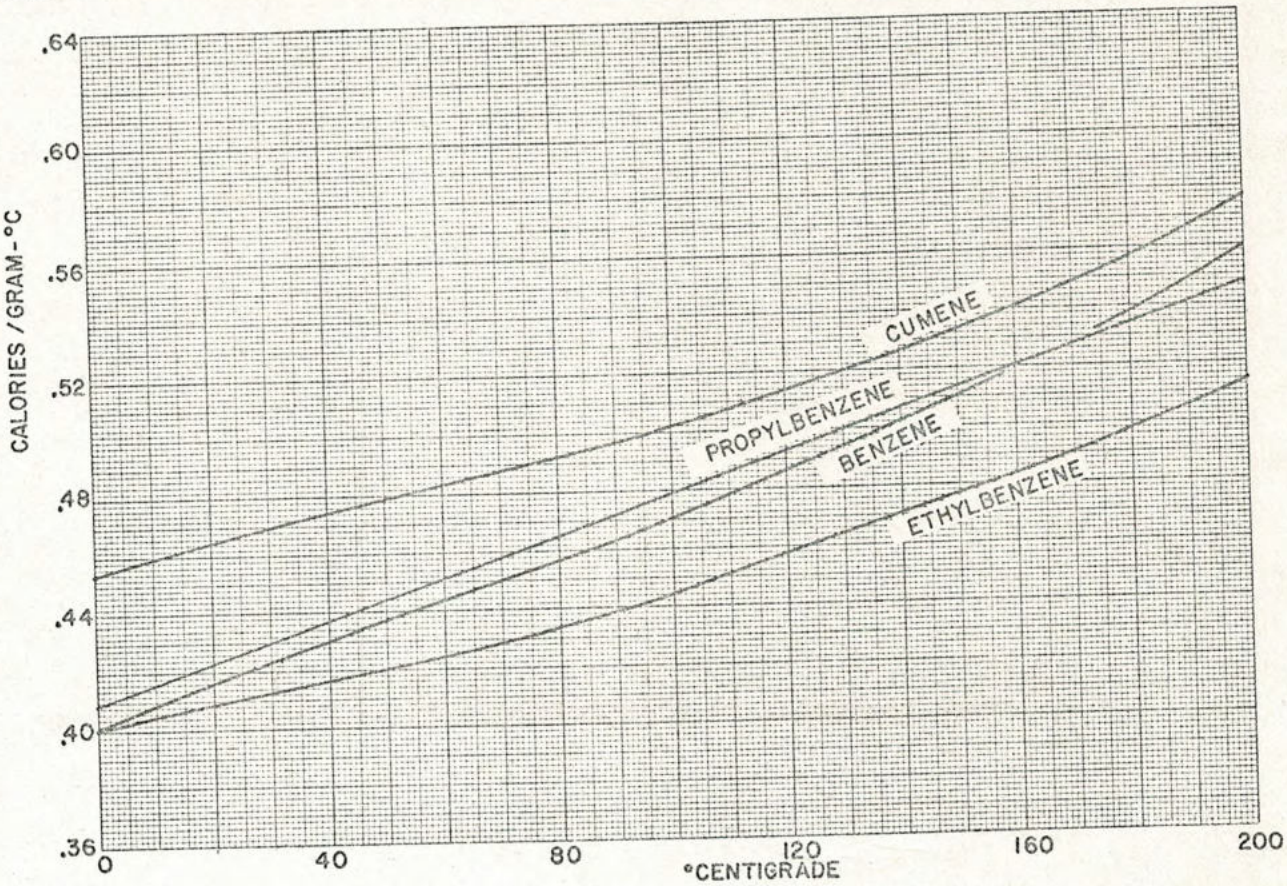

Fig. 39-4—Liquid heat capacity of benzene compounds from 0 to 200° C.

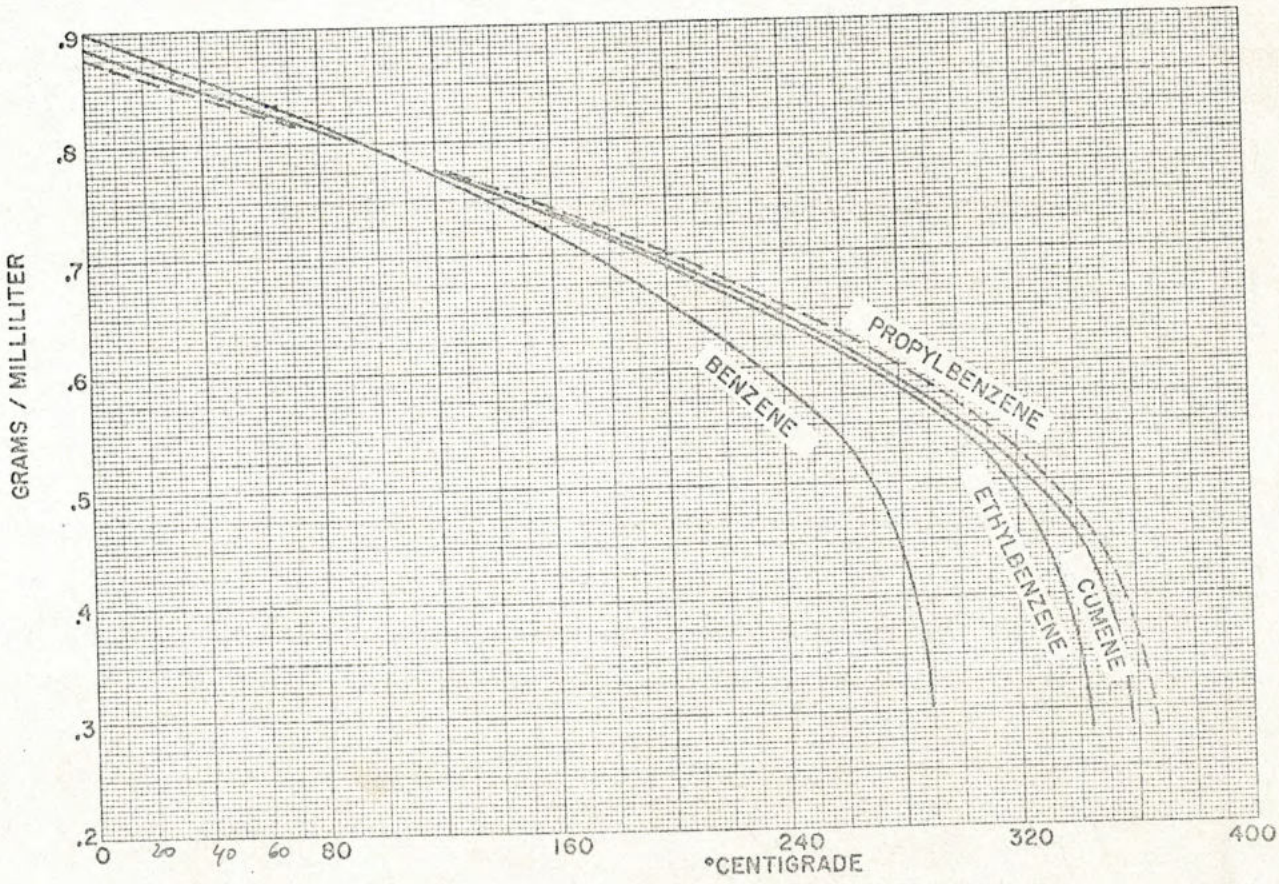

Fig. 39-5—Liquid density of benzene compounds from 0 to 360° C.

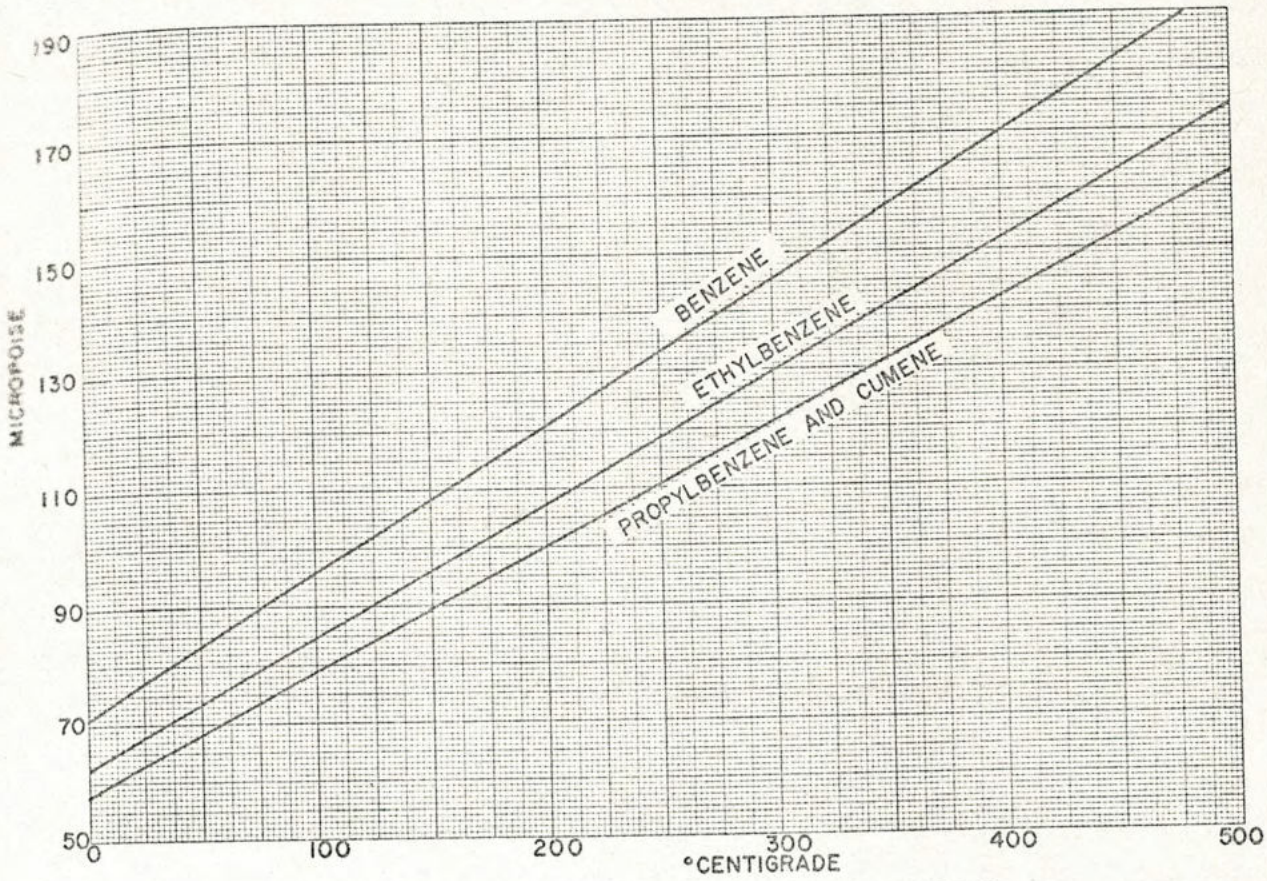

Fig. 39-6—Vapor viscosity of benzene compounds from 0 to 500° C.

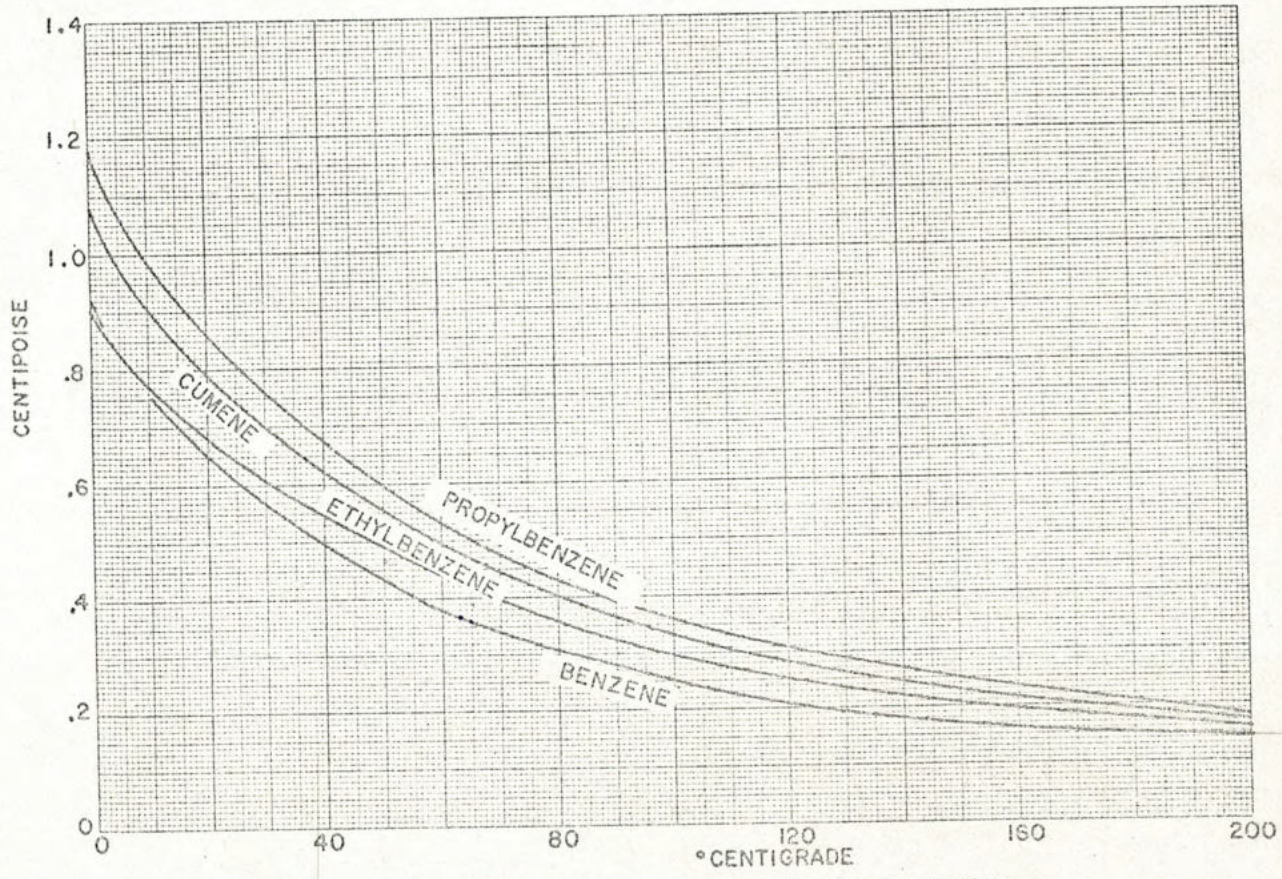

Fig. 39-7—Liquid viscosity of benzene compounds from 0 to 200° C.

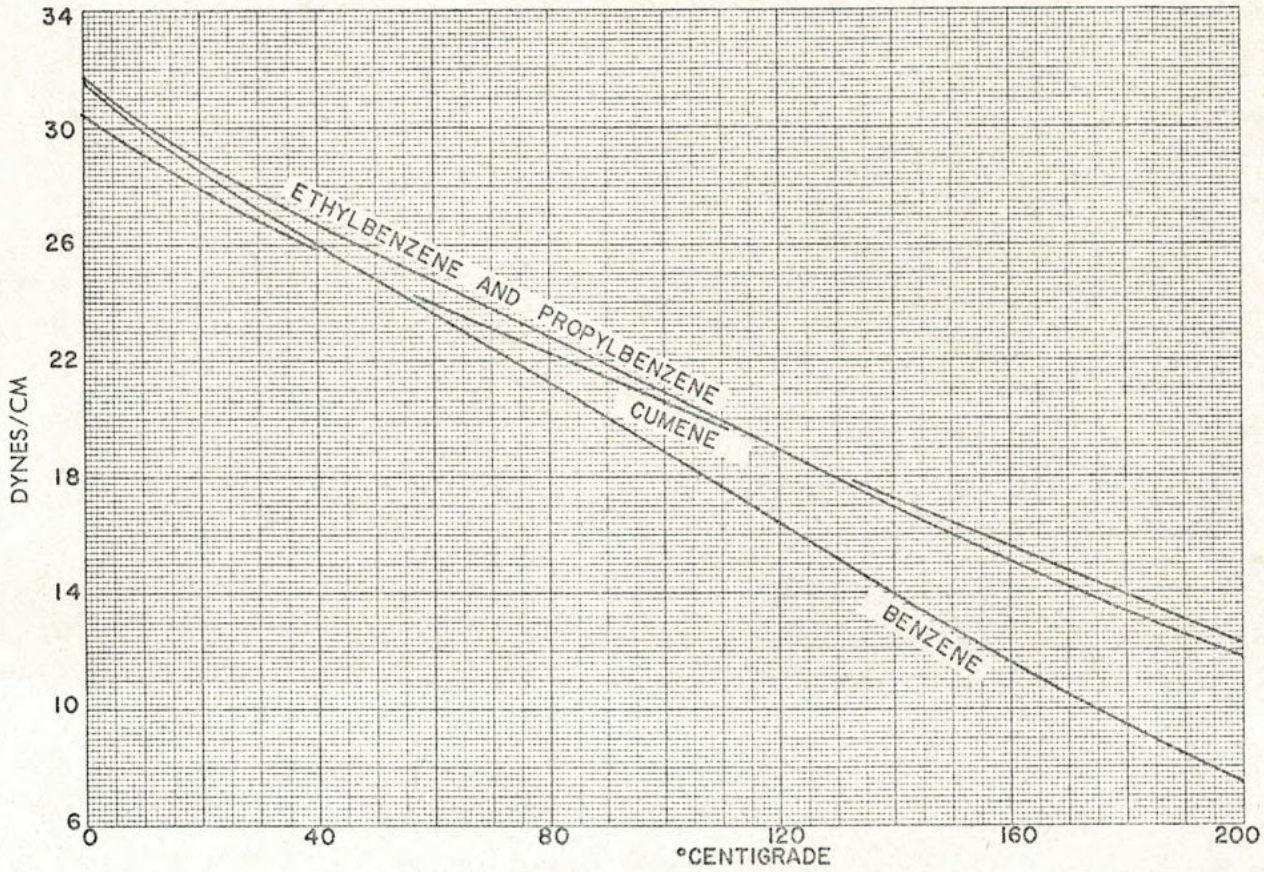

Fig. 39-8—Surface tension of benzene compounds from 0 to 200° C.

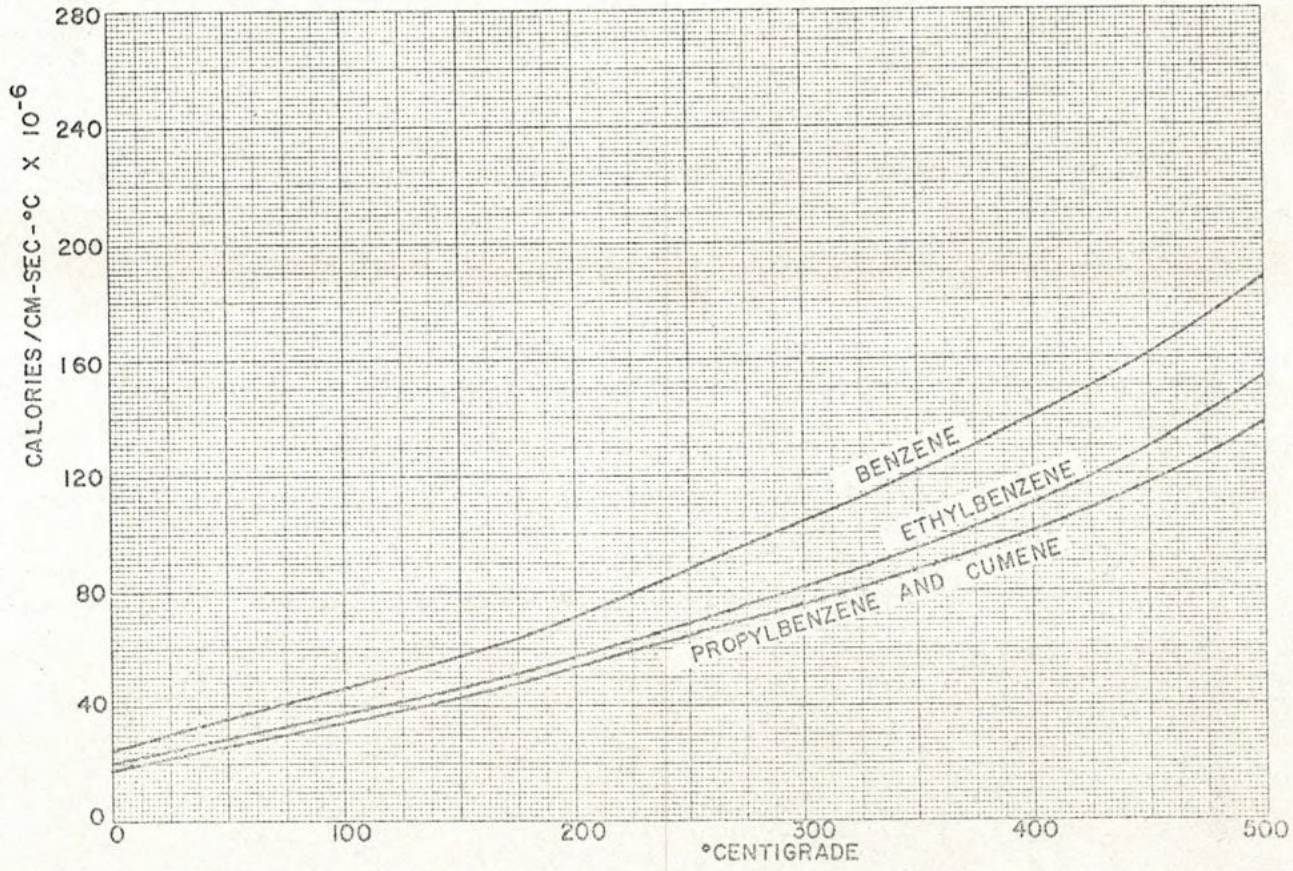

Fig. 39-9—Vapor thermal conductivity of benzene compounds from 0 to 500°C.

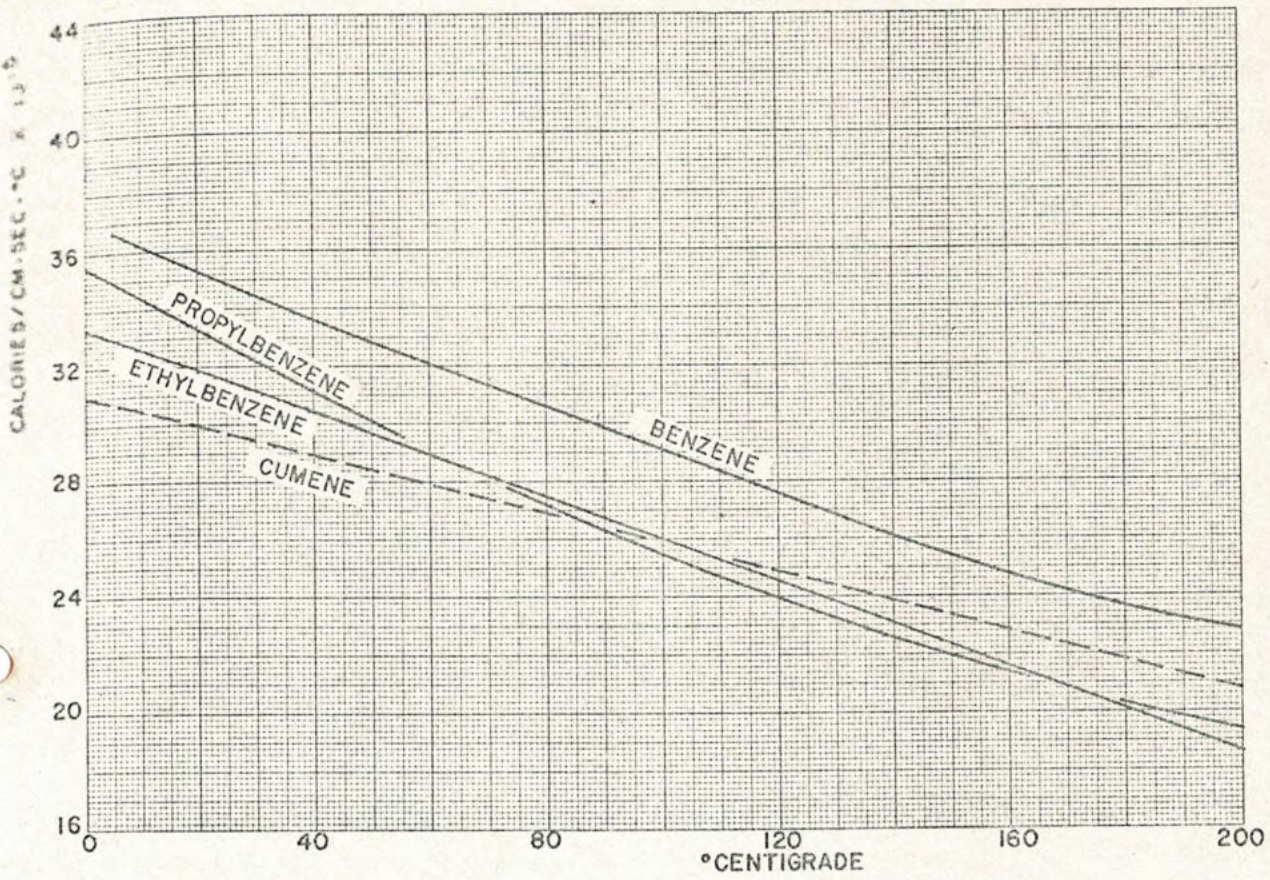

Fig. 39-10—Liquid thermal conductivity of benzene compounds from 0 to 200° C.

benzene[1,7] and from the melting point to +40°C for the other three compounds.[21,23] The experimental data were used to calculate the constant in the Thomas equation.[9] From this, the viscosities were calculated at higher temperatures, with an average error of 2.0 percent.

Surface Tension. The International Critical Tables[19] report the surface tension of benzene from 0°C to the critical point. Donaldson and Quayle[18] have measured the surface tension of all four compounds over the 20-40°C range. These data were used to calculate the constant in the Sugden equation and the data were extended to 200°C, with a probable error of 2-4 percent.

Thermal Conductivity. The vapor thermal conductivities were calculated by the method used in previous articles.[24]

Liquid thermal conductivity data are reported in the literature for benzene from 0-170°C;[25-29] at 20 and 80°C for ethylbenzene;[29] and from 0-100°C for cumene.[28,30] The various investigators agree within about 10 percent. The method of Robbins and Kingrea[29] was used to calculate the thermal conductivity over the 0-200°C. The error averaged 7.3 percent when compared to nine experimental values.

LITERATURE CITED

[1] Timmermans, J., Physico-Chemical Constants of Pure Organic Compounds, Elsevier Publishing Co., Inc., New York (1950).
[2] Stull, D. R., *Industrial and Engineering Chemistry* 35, pp. 1303-4 (1943).
[3] Stull, D. R., *Ibid.*, 39, pp. 517-550 (April 1947).
[4] Ambrose, D., et al *Transactions of the Faraday Society* 56, pp. 1452-9 (1960).
[5] Ambrose, D. and Grant, D. G., *Ibid.* 53, pp. 771-8 (1957).
[6] Bond, D. L. and Thodos, L. *Journal of Chemical and Engineering Data* 5, pp. 289-92 (1960).
[7] Hecks, J. R. and Orban, E., *Journal of Physical Chemistry* 60, pp. 1025-7 (1956).
[8] Organick, E. I. and Studhalter, W. R., *Chemical Engineering Progress* 44, pp. 847-54 (1948).
[9] Reid, R. C. and Sherwood, T. K., The Properties of Gases and Liquids, McGraw-Hill Book Co., New York (1958).
[10] Miller, D. G., *Industrial and Engineering Chemistry* 56 (3), pp. 46-57 (March 1964).
[11] Kharbanda, O. P., *The Industrial Chemist*, pp. 124-7 (March 1955).
[12] Kobe, K. A. and Long, E. G., *Petroleum Refiner* 28 (7), pp. 145-8 (1949).
[13] Brickwedde, F. G., et al, *Journal of Chemical Physics* 13, pp. 547-53 (1945).
[14] Messerly, J. F., et al, *Journal of Physical Chemistry* 69 (12), 4304-11 (1965).
[15] Burlew, J. S., *Journal of the American Society* 62, pp. 696-700 (1940).
[16] Oliver, G. D., et al, *Ibid.* 70, pp. 1502-5 (1948).
[17] Guthrie, G. B. et al, *Ibid.* 66, pp. 2120-1 (1944).
[18] Donaldson, R. D. and Quayle, O. R., *Ibid.* 72, pp. 35-6 (1950).
[19] International Critical Tables, McGraw-Hill Book Co., New York (1926).
[20] Gornowski, E. J., *Industrial and Engineering Chemistry* 39, pp. 1348-52 (1947).
[21] Geist, J. M. and Cannon, M. R., *Ibid. Analytical Edition* 18, pp. 611-13 (1946).
[22] Bromley, L. A. and Wilke, C. R. *Ibid.* 43 (7), pp. 1641-48 (1951).
[23] Barlow, A. J., et al, *Proceedings of the Royal Society (London)* A 292 (1430), pp. 322-42 (1967).
[24] Owens, E. J. and Thodos, G., *AIChE Journal* 6 (4), pp. 676-81 (December 1960).
[25] Horrocks, J. K. and McLaughlin, E., *Ibid.* A273, pp. 259-74 (1963).
[26] Scheffy, W. J. and Johnson, E. F., *Journal of Chemical and Engineering Data* 6, pp. 245-9 (1961).
[27] Venart, J. E., *Ibid.* 10 (3), pp. 239-41 (1965).
[28] Briggs, D. K., *Industrial and Engineering Chemistry* 49, pp. 418-21 (1957).
[29] Robbins, L. A. and Kingrea, C. K., *American Petroleum Institute, Division of Refining* 42 (III), pp. 52-61 (1962).
[30] Mason, H. L., *Transactions of the ASME* 76, pp. 817-21 (1954).

Indexing Terms: Benzene-9, Computations-4, Cumene-9, Ethyl Benzene-9, Heat-7, Hydrocarbons-9, Isopropyl Benzene-9, Liquid Phase-5, Physical Properties-7, Pressure-6, Properties/Characteristics/-7, Propyl Benzene-9, Temperature-6, Vapor Phase-5.