[CONTRIBUTION FROM THE DEPARTMENT OF CHEMISTRY OF THE UNIVERSITY OF TEXAS]

The Pressure–Volume–Temperature Relations of 2,2,4-Trimethylpentane

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Introduction.—The determination of the physical properties of selected pure hydrocarbons of a given series will yield data, it is hoped, upon which there may be based some generalizations of value. Thus, in this Laboratory, there has been instituted a systematic program of determining certain physical properties, such as the compressibilities, heat capacities, and heats of evaporation, for a limited number of pure hydrocarbons. The pressure–volume–temperature relations have been reported[2] on three hexanes and one octane; heat capacities of ethane, propane, butane, and isobutane along with heats of vaporization of some hexanes were reported in other papers.[3] The present paper is concerned with a second octane, 2,2,4-trimethylpentane (isooctane); the experimental work on tetramethylbutane will be reported soon.

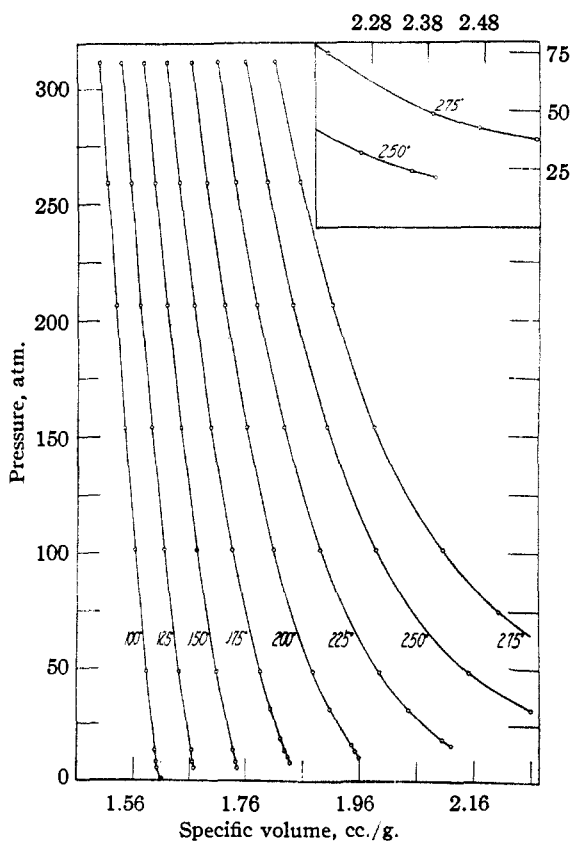

Fig. 1.—Specific volume of 2,2,4-trimethylpentane as a function of the pressure.

This investigation deals with the compressibility of pure 2,2,4-trimethylpentane at eight temperatures: at 25° intervals beginning with 100° and including 275°. No data over any portion of this range were found in the literature. Vapor pressure data have been recorded for isooctane by Smith[4] from approximately 40 to 128°. He also presents a value of 21.507 mm. per degree for the rate of change of the vapor pressure with temperature at the normal boiling point, 99.223°, from which, by use of the approximate Clapeyron equation, there is obtained a value of 7798 cal./mole for the heat of vaporization; this may be compared with the value of 7801 cal./mole (68.3 cal./g.) cited by Doss.[5]

Methods and Apparatus.—All compressibility measurements were made by means of a dead-weight piston gage and accessories; these and the method of operation have been described elsewhere.[6,7]

Material Used.—The sample of 2,2,4-trimethylpentane used in this work was prepared under the direction of Professor Cecil E. Boord of the Department of Chemistry of The Ohio State University as part of the American Petroleum Institute Hydrocarbon Research Project in the Industrial Research Foundation of that University. The material was stated to have a purity better than 99.9 mole per cent. Brooks[8] reports the following physical constants for pure isooctane: d.(g./cc.) at 20° = 0.69189 (0.6918); b. p. (normal) = 99.233°; f. p. = −107.3°; and $n^{20}D$ 1.39155 (1.39156); the values in parentheses were obtained by the authors on the sample used in this investigation.

The Data.—The experimental results are presented graphically in the accompanying figure, specific volumes (cc./g.) being presented as functions of the pressure at different temperatures. From such large scale graphs, the specific volumes at each temperature were read off at rounded pressures; these values, together with the corresponding molar densities, are presented in Table I. No attempt was made to determine the specific

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(2) (a) Kelso with Felsing, THIS JOURNAL, **62**, 3132 (1940); (b) Kelso with Felsing, *J. Ind. Eng. Chem.*, **34**, 161 (1942); and (c) Felsing and Watson, THIS JOURNAL, **64**, 1822 (1942).

(3) (a) Dailey with Felsing, *ibid.*, **65**, 42 (1943); *ibid.*, **65**, 44 (1943); (b) Lemons with Felsing, *ibid.*, **65**, 46 (1943).

(4) Smith, *Bur. Standards J. Research*, **24**, 229 (1940).

(5) Doss, "Physical Constants of the Principal Hydrocarbons," The Texas Company, New York, N. Y., 1942, p. 3.

(6) Kelso with Felsing, THIS JOURNAL, **62**, 3132 (1940).

(7) Beattie, *Proc. Am. Acad. Arts Sci.*, **69**, 389 (1934).

(8) Brooks, *Bur. Standards J. Research*, **24**, 44 (1940).

TABLE I

COMPRESSIBILITY OF LIQUID 2,2,4-TRIMETHYLPENTANE

Molecular weight, 114.224; pressures are in normal atmospheres and temperatures are on the International Temperature Scale.

Press., atm.	Specific volumes, cubic centimeters per gram at 100.00°	125.00°	150.00°	175.00°	200.00°	225.00°	250.00°
5.0	1.604						
10.0	1.600	1.666	1.741	1.835			
15.0	1.597	1.661	1.736	1.827	1.949		
20.0	1.595	1.658	1.731	1.818	1.936	2.098	
25.0	1.592	1.655	1.726	1.812	1.924	2.074	2.337
30.0	1.590	1.652	1.722	1.805	1.912	2.053	2.280
50.0	1.582	1.639	1.707	1.783	1.874	1.990	2.144
100.0	1.563	1.614	1.672	1.735	1.808	1.892	1.990
150.0	1.545	1.593	1.646	1.698	1.762	1.830	1.906
200.0	1.530	1.573	1.621	1.670	1.724	1.782	1.847
250.0	1.515	1.556	1.600	1.645	1.694	1.746	1.803
300.0	1.502	1.541	1.581	1.623	1.668	1.715	1.765

volumes of the liquid isooctane under its own vapor pressure at each of the temperatures under investigation. However, Smyth and Stoops[9] have given a value of the density at 100° of 0.6206 g./cc. (or 1.6113 cc./g.). This experimental value has been included in the authors' graph and is shown to be in excellent accord with their values at higher pressures at 100°.

Since the last temperature of this investigation (275°) is above the critical point (t_c = 271.1°; p_c = 25.46 atm.), as given by Gilliland and Parekh,[10] the values for the specific volumes at this temperature are presented separately in Table II.

TABLE II

DENSITIES AND MOLAR VOLUMES OF ISOOCTANE AT 275°

Press., atm.	Specific volume, cc./g.	Density, moles/liter
35.0	2.637	3.320
40.0	2.514	3.483
50.0	2.378	3.681
100.0	2.110	4.149
150.0	1.991	4.397
200.0	1.918	4.564
250.0	1.862	4.702
300.0	1.818	4.816

Discussion of Results.—These compressibility data are believed to be accurate to 0.10% at the lower pressures and temperatures and to 0.1–0.2% at the higher pressures and temperatures. Temperature measurements are correct at least to 0.01°. The uncertainty in the measurement of volume is 0.05–0.10%, in the determination of mass less than 0.01%, and in the measurement of pressures less than 0.03%. At 275° there is evidence of a slight amount of decomposition: three separate loadings were made; the first two indicated a very slow decomposition, while the third loading did not show any signs of decomposition. Hence, in view of this evidence, the claim for accuracy at this temperature is lowered to 0.2%.

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Summary

1. The compressibility of pure liquid isooctane, 2,2,4-trimethylpentane, has been determined at 25° intervals from 100° to 250° at pressures ranging approximately from the vapor pressures to 300 atmospheres.

2. The compressibility of isooctane was determined at one temperature, 275°, above the critical point.

3. The data are presented tabularly and graphically, the specific volume being related to the pressure at different temperatures.

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(9) Smyth and Stoops, THIS JOURNAL, **50**, 1883 (1928).

(10) Gilliland and Parekh, *Ind. Eng. Chem.*, **34**, 360 (1942).