1012 *J. Chem. Eng. Data* **2002,** *47,* 1012−1016

Vapor−Liquid Critical Properties of *n*-Alkylbenzenes from Toluene to 1-Phenyltridecane

Eugene D. Nikitin,* Alexander P. Popov, and Nataliya S. Bogatishcheva

Institute of Thermal Physics, Ural Branch of the Russian Academy of Sciences, Amundsena Street, 106,
620016 Ekaterinburg, Russia

Yuri G. Yatluk

Institute of Organic Synthesis, Ural Branch of the Russian Academy of Sciences, GSP-147,
Sof 'i Kovalevskoi Street, 20, 620219 Ekaterinburg, Russia

This paper gives experimental critical temperatures and pressures of 10 *n*-alkylbenzenes $C_6H_5C_nH_{2n+1}$ with the number of carbons in the side chain $n = 1$, 2, 4, 5, 6, 7, 8, 10, 11, and 13. *n*-Alkylbenzenes that are heavier than butylbenzene are thermally unstable at their critical points. The method of pulse heating of a wire probe placed into the liquid under study has been used. Residence times are from (0.01 to 1) ms. Equations for the correlation of the critical temperatures and pressures of *n*-alkylbenzenes with the number of carbon atoms in the side chain, molar mass, and normal boiling point have been obtained. The experimental critical constants of alkylbenzenes have been compared with the values calculated by the methods of Lydersen, Joback and Reid, and Constantinou and Gani.

Introduction

Akylbenzenes $C_6H_5C_nH_{2n+1}$ are one the most important groups of aromatic hydrocarbons. However, experimental critical constants are known for only five normal alkylbenzenes: benzene, toluene (methylbenzene), ethylbenzene, propylbenzene, and butylbenzene.[1] This is probably explained by the fact that butylbenzene and heavier *n*-alkylbenzenes are unstable at their critical temperatures.[2] In this paper we report our measurements of the critical temperatures and pressures of 10 alkylbenzenes with $n =$ 1, 2, 4, 5, 6, 7, 8, 10, 11, and 13 using the pulse-heating method applicable to thermally unstable substances.[3−5]

Experimental Section

Method. A brief outline of the pulse-heating method is given below. Additional details can be found in several publications.[3−5] The method is based on measuring the pressure dependence of the temperature of the attainable superheat (spontaneous boiling-up) of a liquid with the help of a thin wire probe heated by pulses of electric current. When the pressure in the liquid approaches the critical pressure, the temperature of the attainable superheat approaches the critical temperature.[6−8]

The liquid under study fills the chamber, the pressure in which is measured with a dial gauge. A platinum wire probe, 2×10^{-3} cm in diameter and (1 to 3) cm in length, is placed in the liquid. It is heated by rectangular pulses of electric current of duration from (0.015 to 1.2) ms. By the end of a pulse, the probe and the thin liquid layer that surrounds it are heated to the temperature of spontaneous boiling-up. The amplitude of pulses is chosen in such a way that the time from the start of a pulse to the moment of boiling-up t^* is from (0.01 to 1.0) ms. At the moment of boiling-up, the conditions of heat transfer from the probe to the liquid change abruptly against the background of a smooth temperature increase, and a temperature perturbation caused by boiling-up takes place. The probe temperature at this moment is determined from its resistance. The pressure in the chamber increases step by step until the negative temperature perturbation decreases to the level of the apparatus sensitivity for this parameter (1×10^{-3} K). This pressure is taken to be equal to the measured value of the critical pressure p_c^m, and the temperature of the attainable superheat at this pressure is taken to be equal to the measured value of the critical temperature T_c^m.

The true critical pressure p_c and critical temperature T_c values of stable compounds are calculated by the following equation:

$$p_c = p_c^m/\pi_0, \quad T_c = T_c^m/\tau_0 \tag{1}$$

where π_0 and τ_0 are the reduced pressure and temperature of the liquid under study at which, according to the boiling-up theory, the amplitude of a negative temperature perturbation is equal to the apparatus sensitivity (1×10^{-3} K). The equation for calculating this amplitude is given in our previous paper.[3] This equation contains the thermophysical properties of the substance under investigation near the critical point, which are estimated using the principle of corresponding states. The appropriate formulas are given in our previous paper.[9] To use them, it is necessary to know the acentric factor of the liquid under study or the analogous parameter suggested by Filippov:[10]

$$A = 100\frac{p_s(T/T_c = 0.625)}{p_c}$$

---

* To whom correspondence should be addressed. E-mail: e-nikitin@mail.ru. Fax: +7-3432-678800.

10.1021/je025514n CCC: $22.00

where p_s is the vapor pressure. In this paper, we use the Filippov parameter because for its determination it is enough to know the vapor pressure at a lower temperature in comparison with the acentric factor where $T/T_c = 0.7$, and in the literature, there are more data on the vapor pressures of alkylbenzenes at low temperatures. The acentric factor ω and the Filippov parameter A are related by the following empiric equation:[10]

$$\omega = 0.401 - 0.664 \log_{10} A$$

Filippov's parameters of *n*-alkylbenzenes were estimated in the following way. Filippov's parameters of alkylbenzenes from benzene to butylbenzene were calculated using the critical properties recommended by Tsonopoulos and Ambrose.[1] The vapor pressures of benzene to ethylbenzene were taken from ref 11, and those for propylbenzene and butylbenzene were in accordance with ref 12. Filippov's parameters and the critical constants of the other alkylbenzenes were calculated by an iteration method. At first, as the critical constants we used p_c^m and T_c^m; the vapor pressures of pentyl-, hexyl-, heptyl, octyl-, decyl-, and tridecylbenzenes were taken in accordance with refs 12 and 13 and the TRC recommendations.[14] In the literature, we did not find the vapor pressures of undecylbenzene, only the normal boiling point. The value reported by Morton et al.[15] ($T_b = 569$) K and recommended by TRC[14] seems too low; we consider the T_b value given in the *Aldrich Handbook*[16] ($T_b = 589.2$ K) more realistic. Then we calculated the vapor pressures of undecylbenzene using the Clapeyron equation. It is, of course, a rough estimation, but the values of π_0 and τ_0 are not very sensitive to variations in A. For example, for methylbenzene a change of 10% in A causes a change of about 0.1% in p_c and 0.01% in T_c. Then we calculated π_0 and τ_0 and by eq 1 p_c and T_c. As the second iteration, Filippov's parameters and the critical properties were calculated using corresponding values after the first iteration. Two iterations were enough because, as discussed above, the values of π_0 and τ_0 are little affected by variations of Filippov's parameter.

The ideal gas capacity was also used in calculating the heat capacity of the liquid under study. It was calculated by the method of Rihani and Doraiswamy as presented by Reid et al.[17] As a result of a special experiment, the factor G_T (for the definition of this factor, see our previous paper[3]) was estimated at 1.5 K^{-1}.

For thermally unstable substances, p_c and T_c determined in such a way depend on the time from the pulse beginning to the moment of boiling-up t^* (the heating rate) because of the change in the chemical composition in the process of heating. The true values of the critical constants of thermally unstable compounds are determined by extrapolation of p_c and T_c as functions of t^* to $t^* = 0$. The procedure of extrapolation is described in refs 3 and 18. Alkylbenzenes, beginning from butylbenzene, are unstable at their critical points, but for all the studied alkylbenzenes, the change in the chemical composition by time t^* was apparently so small that the dependences $p_c(t^*)$ and $T_c(t^*)$ were not observed, and extrapolation was not used.

We used measuring probes of (1, 2, and 3) cm in length. Usually at the beginning of an experiment, the 1 cm probe was placed into the chamber with alkylbenzene and measurements of the critical constants were carried out at heating times $t^* = (0.03, 0.07, 0.12, 0.24, 0.48,$ and $0.95)$ ms. Then the measurements were repeated with (2 and 3) cm probes at the same set of heating times. Thereafter, the chamber was filled with a new portion of alkylbenzene and measurements were performed again with new measuring probes. The number of the alkylbenzene portions was from 3 to 5; the number of the probes of each length was from 3 to 5. Then the values of p_c^m and T_c^m were averaged.

Table 1. Purities of Materials Used in Critical Point Measurements

compound	supplier	purity/% supplier	purity/% real
methylbenzene	Merck	99	99.9
ethylbenzene	Merck	99	>99.9
butylbenzene	Aldrich	99+	99.6
pentylbenzene	Aldrich	99	99.2
hexylbenzene	Fluka	>99.8	99.9
phenylheptane	Fluka	>99	99.3
phenyloctane	Aldrich	99	99.0
phenyldecane	Fluka	>98	98.2
phenylundecane	Aldrich	99	99.5
phenyltridecane	Aldrich	99	99.0

Sources and Purities of the Substances Studied. The sources and purities are given in Table 1. Only for 1-phenyldecane was the purity less than 99%. Before the critical constants were measured, the purities were verified by gas chromatography (Shimadzu GS-Ha). Some samples (ethyl-, butyl-, heptyl-, undecyl-, and tridecylbenzenes) were also analyzed after the measurements of the critical properties. Gas chromatography could not detect a change in the composition of the samples.

It is interesting that samples exposed to air and sunlight for several months had appreciably lower purities. We discovered this by repeating the analysis after several months of storage. For the original samples, the concentration of the main substance fell by from (0.5 to 1)%, and for the samples that were used in the critical constants measurements, it fell by from (0.5 to 1.5)%. Alkylbenzenes are known to oxidize in accordance with the following scheme:[19]

$$\begin{aligned} &\qquad\qquad\qquad\qquad\qquad C_6H_5OH + RCHO \quad (2)\\ &C_6H_5CH_2R + O_2 \rightarrow C_6H_5CHROOH \rightarrow\\ &\qquad\qquad\qquad\qquad\qquad C_6H_5CRO + H_2O \quad (3)\\ &\qquad\qquad\qquad\qquad\qquad C_6H_5CHROH + C_6H_5CH_2R \quad (4) \end{aligned}$$

We compared the dependencies of the logarithm of the retention time of an impurity on the carbon number in the side chain of an alkylbenzene in the GC experiments and came to the conclusion that the impurities formed one homologous series derivative from the initial one. The proton magnetic spectroscopy of the sample that contained the greatest quantity of impurities showed the presence of small signals with chemical shifts of 2.95 ppm and 4.90 ppm (the greatest) which corresponded to products **3** and **4**. A signal from product **2**, aldehyde, in the field from (9.6 to 9.8) ppm was absent. Thus, the reaction goes in the direction of the formation of alcohol with some ketone.

Uncertainties. The uncertainty of the results of the measurement of the critical pressure of a stable substance consists of three factors: (i) the uncertainty with which an experimenter determines the pressure in the measuring chamber at which the temperature perturbation decreases to the level of the apparatus sensitivity $u_1(p_c^m)$, (ii) the uncertainty of measuring this pressure with a dial gauge $u_2(p_c^m)$, and (iii) the uncertainty of calculation of π_0 in eq 1. The first factor is associated with the fact that as the pressure approaches the critical value, the amplitude of the negative temperature perturbation decreases smoothly, with a small derivative of the amplitude with respect to

Table 2. Critical Temperatures of *n*-Alkylbenzenes $C_6H_5C_nH_{2n+1}$: Experimental Values and Comparison with Predictive Methods (T_b Is the Normal Boiling Point)

				T_c/K		
n	T_b/K	T_c/K	$\pm\delta T_c$/K	ref 17	ref 23	ref 24
0	353.3[c]	562.05[a]	0.07	562.00	561.63	563.16
1	383.8[c]	591.75[a]	0.15	594.48	593.98	596.17
		588[b]	6			
2	409.3[c]	617.15[a]	0.1	618.50	618.83	620.06
		614[b]	6			
3	432[c]	638.35[a]	0.1	638.00	639.09	639.59
4	456[c]	660.5[a]	0.5	659.26	661.08	657.21
		660[b]	7			
5	478.6[d]	675[b]	7	678.44	680.89	673.28
6	499.3[d]	695[b]	7	695.01	698.03	688.03
7	512.5[e]	708[b]	7	701.51	704.97	701.68
8	536.5[e]	725[b]	7	723.12	727.01	714.36
10	566.2[f]	752[b]	8	742.81	747.20	737.35
11	589.2[g]	763[b]	8	764.00	768.60	747.83
13		790[b]	8			767.13
AAPE[h]/%				0.36	0.39	1.05

[a] According to Tsonopoulos and Ambrose.[1] [b] This work. [c] According to the TRC recommendation.[14] [d] According to Weast and Grasselli.[25] [e] The average between the data by Weast and Grasselli[25] and Aldrich Chemical Co.[26] [f] According to Aldrich Chemical Co.[26] [g] According to Aldrich Chemical Co.[16] [h] AAPE = average absolute percent error; AAPE/% = $^1/_N\Sigma(|T_c^{\mathrm{exp}} - T_c^{\mathrm{calc}}|/T_c^{\mathrm{calc}}) \times 100\%$, where N is the number of experimental data points, T_c^{exp} is the experimental value of the critical temperature, and T_c^{calc} is the calculated value of the critical temperature.

Table 3. Critical Pressures of *n*-Alkylbenzenes $C_6H_5C_nH_{2n+1}$: Experimental Values and Comparison with Predictive Methods

			p_c/MPa		
n	p_c/MPa	$\pm\delta p_c$/MPa	ref 17	ref 23	ref 24
0	4.895[a]	0.006	4.888	4.769	4.862
1	4.108[a]	0.010	4.144	4.114	4.179
	4.09[b]	0.12			
2	3.609[a]	0.010	3.597	3.651	3.596
	3.60[b]	0.11			
3	3.200[a]	0.010	3.177	3.262	3.203
4	2.89[a]	0.04	2.845	2.931	2.874
	2.90[b]	0.09			
5	2.58[b]	0.08	2.576	2.649	2.595
6	2.35[b]	0.07	2.353	2.405	2.357
7	2.14[b]	0.06	2.166	2.194	2.151
8	1.98[b]	0.06	2.006	2.009	1.973
10	1.72[b]	0.05	1.762	1.703	1.681
11	1.64[b]	0.05	1.643	1.576	1.560
13	1.54[b]	0.05	1.466	1.361	1.358
AAPE[c]/%			1.16	2.73	2.01

[a] According to Tsonopoulos and Ambrose.[1] [b] This work. [c] AAPE = average absolute percent error; AAPE/% = $^1/_N\Sigma(|p_c^{\mathrm{exp}} - p_c^{\mathrm{calc}}|/p_c^{\mathrm{calc}}) \times 100$, where N is the number of experimental data points, p_c^{exp} is the experimental value of the critical pressure, and p_c^{calc} is the calculated value of the critical pressure.

the pressure.[3] The uncertainty of the results of measuring the critical temperature consists of the uncertainty $u_1(T_c^m)$ that has a nature analogous to $u_1(p_c^m)$, the uncertainty of the measurement of the probe temperature from its resistance $u_2(T_c^m)$, and the uncertainty of calculation of τ_0. The uncertainties $u_1(p_c^m)$ and $u_1(T_c^m)$ can be reduced by repeated measurements and statistical analysis of the data to the values $0.01p_c^m$ and $0.001T_c^m$. The uncertainty $u_2(p_c^m)$ depends on the type of the dial gauge and in our experiments does not exceed the value $0.004p_c^m$. The uncertainty $u_2(T_c^m)$ is also determined by the equipment used (resistance box and oscilloscope) and is evaluated by us to about $0.007T_c^m$. The uncertainties of calculating π_0 and τ_0 are difficult to estimate in an independent way, since the formulas for their calculation[3,9] were obtained by solving a complex thermophysical problem in the course of which some assumptions were made.[20] In this situation, it is easier to estimate directly the uncertainties of $u(T_c)$ and $u(p_c)$. For this purpose, we measured the critical constants of several "standard" substances: pentane, hexane, heptane, water,[3] and naphthalene.[21] The critical properties of these compounds are known with comparatively small uncertainties.[1,11,22] In addition, in this work we studied methyl-, ethyl-, and butylbenzenes, the critical constants of which are well investigated.[1] By comparing our critical constants with the literature values, we concluded that the uncertainties in the critical temperatures and pressures of *n*-alkylbenzenes were as follows: $0.01T_c$ and $0.03p_c$.

Results and Discussion

The critical temperatures and pressures of *n*-alkylbenzenes from benzene to 1-phenyltridecane measured in this work are given in Tables 2 and 3 together with their uncertainties. These tables also contain the values recommended by Tsonopoulos and Ambrose.[1] All known data for the critical constants of *n*-alkylbenzenes can be found in their paper.

We estimated the critical temperatures and pressures of alkylbenzenes by the well-known group-contribution methods of Lydersen,[17] Joback and Reid,[23] and Constantinou and Gani.[24] The Lydersen and Joback and Reid methods require knowledge of the normal boiling point (T_b) for the estimation of the critical temperature. The values reported by various authors are often rather contradictory. Normal boiling points for benzene to butylbenzene were taken in accordance with the TRC recommendations.[14] For pentyl- and hexylbenzenes, we used the data by Weast and Grasselli,[25] which are in excellent agreement with the values by Růžička et al.[12] For heptyl- and octylbenzenes, we took the average between the data reported by Weast and Grasselli[25] and Aldrich Chemical Co.[26] For decyl- and undecylbenzenes, we used the data by Aldrich Chemical Co.[16,26] Such a choice of normal boiling points gives a smooth dependence of T_b on n. We failed to find in the literature the normal boiling point of tridecylbenzene.

It is seen from Table 2 that for alkylbenzenes the methods of Lydersen and Joback and Reid have approximately equal accuracies. The method of Constantinou and Gani gives in general worse results (underestimates the critical temperatures of alkylbenzenes beginning from butylbenzene), and the difference between the experimental and estimated critical temperatures increases with increasing molar mass. For the critical pressures (Table 3), the Lydersen method gives the best results; the methods of Joback and Reid and Constantinou and Gani underestimate the critical pressures of heavy alkylbenzenes at $n \geq 10$.

The critical constants of *n*-alkylbenzenes were correlated with the carbon number in the side chain n ($3 \leq n \leq 13$):

$$p_c/\mathrm{MPa} = 319.40n^{-3/2} - 1514.4n^{-2} + 2679.4n^{-5/2} - 1670.9n^{-3} \quad (5)$$

$$T_c/\mathrm{K} = 1419.9 - 3797.2n^{-1/2} + 6654.5n^{-1} - 4195.3n^{-3/2} \quad (6)$$

The form of eqs 5 and 6 was obtained by us earlier by analyzing the properties of long chain molecule fluids.[21,27]

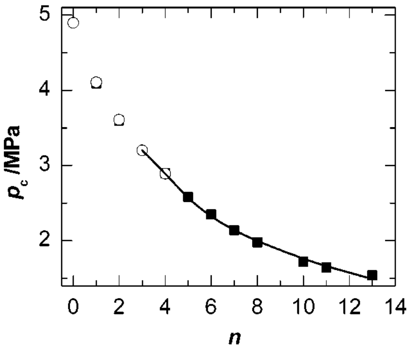

Figure 1. Critical pressures of *n*-alkylbenzenes vs the number of carbon atoms in the side chain: ○, ref 1; ■, this work; the solid line corresponds to eq 5.

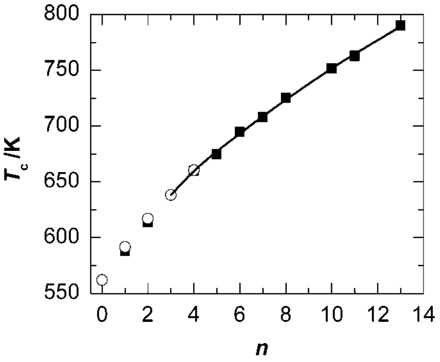

Figure 2. Critical temperatures of *n*-alkylbenzenes vs the number of carbon atoms in the side chain: ○, ref 1; ■, this work; the solid line corresponds to eq 6.

These equations are the series in powers of n and work better the greater the number of mers in a molecule. Because of a comparatively small number of carbons in the side chain in the *n*-alkylbenzenes studied, we had to use four terms in eqs 5 and 6 and begin the correlation from $n = 3$. We took the data recommended by Tsonopoulos and Ambrose[1] for $n = 3$ and 4 and our data for the rest. The constants of eqs 5 and 6 were calculated using the $1/\delta^2$ weight method, since the critical properties of alkylbenzenes have been measured by various methods with essentially different errors. The correlation coefficients R were $R = 0.999\,66$ and $R = 0.999\,95$ for eqs 5 and 6, respectively. The results of calculation of the critical temperatures and pressures by eqs 5 and 6 are compared with the experimental data in Figures 1 and 2.

The critical pressures of *n*-alkylbenzenes were also correlated with the number of carbons in the side chain n and the molar mass M ($0 \le n \le 13$):

$$\{(M/\text{kg}\cdot\text{mol}^{-1})/(p_c/\text{MPa})\}^{1/2} = 0.12751 + 0.02243n \quad (7)$$

The results of correlation are shown in Figure 3, which demonstrates good self-consistency of the data obtained. A way to check the self-consistency of the critical temperatures is to consider the ratio T_c/T_b as a function of n. Such a correlation is given in Figure 4. The solid line in Figure 4 corresponds to the following equation:

$$\frac{T_c}{T_b} = 1.58424 - 0.03913n + 0.00125n^2 \quad (8)$$

To obtain eqs 7 and 8, we used the critical pressures and temperatures recommended by Tsonopoulos and Ambrose[1] for $n = 0-4$ and our data for the rest. The choice of the normal boiling points was discussed above. The scatter of points in Figure 4 corresponds to the uncertainties in measuring the critical temperatures and the normal boiling points of heavy *n*-alkylbenzenes.

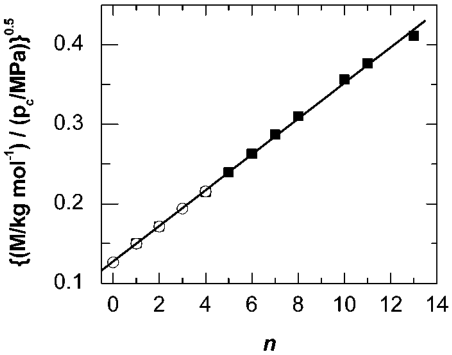

Figure 3. Correlation of the critical pressure of *n*-alkylbenzenes as a function of the number of carbon atoms in the side chain and molar mass: ○, ref 1; ■, this work; the solid line corresponds to eq 7.

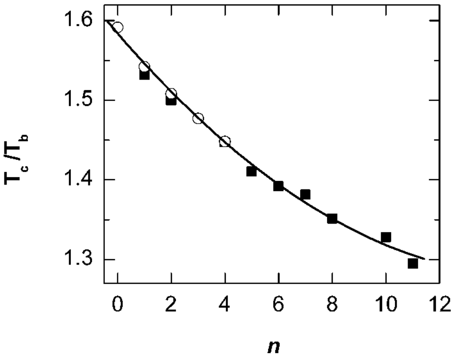

Figure 4. Correlation of the critical temperature of *n*-alkylbenzenes as a function of the number of carbon atoms in the side chain and normal boiling point. Critical temperatures: ○, ref 1; ■, this work; the solid line corresponds to eq 8.

Equation 5 describes the experimental critical pressures of alkylbenzenes with the average absolute percent error (AAPE) equal to 1.09%; the AAPE for eq 7 is higher, namely, 1.84% ($3 \le n \le 13$). For very long chains ($n \gg 1$), eq 5 predicts that the critical pressure will decrease as $p_c \propto n^{-3/2}$, whereas eq 7 gives $p_c \propto n^{-1}$. A detailed discussion of the asymptotic ($n \to \infty$) behavior of the critical constants is not the goal of the present paper. In our opinion, it is the law $p_c \propto n^{-3/2}$ that is correct,[21,27−29] although this problem is not to be considered as conclusively solved. Taking into account the foregoing, we recommend eqs 5 and 6 for the calculation of the critical constants of heavy alkylbenzenes. Equation 7 may also be used for a prudent extrapolation, but eq 8 is difficult to use for the prediction of the critical temperatures of alkylbenzenes because their normal boiling points for $n \ge 12$ are unknown.

Conclusion

The critical temperatures and pressures of 10 *n*-alkylbenzenes have been measured using the pulse-heating technique. Our data for methyl-, ethyl-, and butylbenzenes are in good agreement with the data recommended by Tsonopoulos and Ambrose.[1] Equations 5 and 6 adequately reproduce the results of measuring the critical pressures and temperatures of *n*-alkylbenzenes and give, in our opinion, correct asymptotics at $n \to \infty$. We recommend these equations for calculating the critical pressures and temperatures of heavy *n*-alkylbenzenes. Equation 7 may also be used for prudent extrapolation of the critical pressures of alkylbenzenes.

Acknowledgment

The authors are grateful to Dr. V. Růžička for sending reprints of his papers and Dr. B. Taylor for the information about NIST Technical Note 1297.

Literature Cited

(1) Tsonopoulos, C.; Ambrose, D. Vapour-Liquid Critical Properties of Elements and Compounds. 3. Aromatic Hydrocarbons. *J. Chem. Eng. Data* **1995**, *40*, 547−558.

(2) Ambrose, D.; Cox, J. D.; Townsend, R. The Critical Temperatures of Forty Organic Compounds. *Trans. Faraday Soc.* **1960**, *56*, 1452−1459.

(3) Nikitin, E. D.; Pavlov, P. A.; Skripov, P. V. Measurement of the Critical Properties of Thermally Unstable Substances and Mixtures by the Pulse-Heating Method. *J. Chem. Thermodyn.* **1993**, *25*, 869−880.

(4) Nikitin, E. D.; Pavlov, P. A.; Popov, A. P. Critical Temperatures and Pressures of 1-Alkanols with 13 to 22 Carbon Atoms. *Fluid Phase Equilib.* **1998**, *149*, 223−232.

(5) Nikitin, E. D.; Pavlov, P. A.; Skutin, M. G. Acoustic Method of Measuring Critical Properties of Thermally Unstable Substances. *Fluid Phase Equilib.* **1999**, *161*, 119−134.

(6) Skripov, V. P. *Metastable Liquids*; Wiley: New York, 1974.

(7) Skripov, V. P.; Sinitsyn, E. N.; Pavlov, P. A.; Ermakov, G. V.; Muratov, G. N.; Bulanov, N. V.; Baidakov, V. G. *Thermophysical Properties of Liquids in the Metastable (Superheated) State*; Gordon and Breach: London, New York, 1988.

(8) Debenedetti, P. G. *Metastable Liquids: Concepts and Principles*; Princeton University Press: Princeton, 1996.

(9) Nikitin, E. D.; Pavlov, P. A.; Bessonova, N. V. Critical Constants of *n*-Alkanes with from 17 to 24 Carbon Atoms. *J. Chem. Thermodyn.* **1994**, *26*, 177−182.

(10) Filippov, L. P. *Podobie Svoist Veshchestv (Similarity of Substance Properties)*; Moscow University Press: Moscow, 1978.

(11) Vargaftik, N. B. *Tables on the Thermophysical Properties of Liquids and Gases*, 2nd ed.; Wiley: New York, 1975.

(12) Růžička, V., Jr.; Zábranský, M.; Růžička, K.; Majer, V. Vapor pressures for a group of high-boiling alkylbenzenes under environmental conditions. *Thermochim. Acta* **1994**, *245*, 121−144.

(13) Kasehgari, H.; Mokbel, I.; Viton, C.; Jose, J. Vapor Pressure of 11 Alkylbenzenes in the Range $10^{-3} - 280$ Torr. Correlation by Equation of State. *Fluid Phase Equilib.* **1993**, *87*, 133−152.

(14) Thermodynamic Research Center, NIST Boulder Laboratories, M. Frenkel director. Thermodynamic Source Database. In *NIST Chemistry WebBook*; Lindstrom, P. J., Mallard, W. G., Eds.; NIST Standard Reference Database Number 69; National Institute of Standards and Technology: Gaithersburg, MD, July 2001; 20899 (http://webbook.nist.gov).

(15) Morton, A. A.; Davidson, J. B.; Best, R. J. Condensation by Sodium. XXI. *n*-Octyl- and *n*-Decylsodium. *J. Am. Chem. Soc.* **1942**, *64*, 2239−2240.

(16) *Catalog Handbook of Fine Chemicals*; Aldrich Chemical Co., Inc.: Milwaukee, WI, 1994−1995.

(17) Reid, R. C.; Prausnitz, J. M.; Sherwood, T. K. *The Properties of Gases and Liquids*, 3rd ed.; McGraw-Hill: New York, 1977.

(18) Nikitin, E. D.; Pavlov, P. A.; Popov, A. P. (Gas + Liquid) Critical Temperatures and Pressures of Polyethene Glycols from $HOCH_2$-CH_2OH to $H(OCH_2CH_2)_{\nu=13.2}OH$. *J. Chem. Thermodyn.* **1995**, *27*, 43−51.

(19) Woodward, A. E.; Mesborian, R. B. Low-temperature autoxidation of hydrocarbons. The kinetics of tetralin oxidation. *J. Am. Chem. Soc.* **1953**, *75*, 6189−6195.

(20) Pavlov, P. A. *Dinamika Vskipaniya Sil'no Peregretykh Zhidkostei (Dynamics of Boiling of Highly Superheated Liquids)*; Ural Branch of the Russian Academy of Sciences Pub.: Sverdlovsk, 1988.

(21) Nikitin, E. D.; Pavlov, P. A.; Popov, A. P. Vapour-Liquid Critical Temperatures and Pressures of Normal Alkanes with from 19 to 36 Carbon Atoms, Naphthalene and m-Terphenyl determined by the Pulse-Heating Technique. *Fluid Phase Equilib.* **1997**, *141*, 155−164.

(22) Ambrose, D.; Tsonopoulos, C. Vapor-Liquid Critical Properties of Elements and Compounds. 2. Normal Alkanes. *J. Chem. Eng. Data* **1995**, *40*, 531−546.

(23) Joback, K. G.; Reid, R. C. Estimation of Pure-Component Properties from Group-Contributions. *Chem. Eng. Commun.* **1987**, *57*, 233−243.

(24) Constantinou, L.; Gani, R. New Group Contribution Method for Estimating Properties of Pure Compounds. *AIChE J.* **1994**, *40*, 1697−1710.

(25) *CRC Handbook of Data on Organic Compounds*, 2nd ed.; Weast, R. C., Grasselli, J. G., Eds.; CRC Press: Boca Raton, FL, 1989; p 1.

(26) *Catalog Handbook of Fine Chemicals*; Aldrich Chemical Co., Inc.: Milwaukee, WI, 1990.

(27) Nikitin, E. D.; Pavlov, P. A. Van der Waals Chain-Molecule Fluid in Self-Consistent Field Approximation: Some Thermal Properties. *High Temp.* **2000**, *38*, 690−697.

(28) Nikitin, E. D.; Pavlov, P. A.; Skripov, P. V. Estimation of the Critical Constants of Long-Chain Normal Alkanes. *Int. J. Thermophys.* **1996**, *17*, 455−469.

(29) Nikitin, E. D. Asymptotic Behavior of the Critical Properties of Substances Consisting of Long Chain Molecules. *High Temp.* **2000**, *38*, 317−319.

Received for review February 12, 2002. Accepted April 19, 2002. This study was supported by the Russian Foundation for Basic Research under Grants N 01-02-17025 and 00-15-96719.

JE025514N