

## Vapor-Liquid Critical Properties of Elements and Compounds. 3. Aromatic Hydrocarbons

Constantine Tsionopoulos\*

Exxon Research and Engineering Company, P.O. Box 101, Florham Park, New Jersey 07932

Douglas Ambrose

University College London, 20 Gordon Street, London WC1H 0AJ, England

This is part 3 of a series of contributions by the critical properties group of the IUPAC Commission I.2 on Thermodynamics, Subcommittee on Thermodynamic Data. It presents all known experimental data for the critical constants of aromatic hydrocarbons, which have been divided into four families: normal alkylbenzenes (5 compounds, C<sub>6</sub>-C<sub>10</sub>); other alkylbenzenes (13 compounds, C<sub>8</sub>-C<sub>12</sub>); polyphenyls (5 compounds, C<sub>12</sub>-C<sub>18</sub>); and condensed polycyclics (7 compounds, C<sub>9</sub>-C<sub>14</sub>). Recommendations are given together with uncertainties. Critical temperatures have been converted to ITS-90.

The aromatic hydrocarbons have been divided into four families: (A) normal alkylbenzenes; (B) other alkylbenzenes; (C) polyphenyls; and (D) condensed polycyclics. Except for benzene, there are relatively few experimental data available for aromatic hydrocarbons, and some of these data, especially for the terphenyls, may be unreliable.

The presentation and evaluation of the experimental data follow the guidelines of Ambrose et al. in parts 1 and 2 of this series [95-amb/you; 95-amb/tso]. The recommended values are given in Table 1, while all known data have been collected in Table 2. The references follow Ambrose's format (year-first three letters of first author/first three letters of second author, and, where required, a sequence number).

### (A) Normal Alkylbenzenes

Experimental critical constants are known for only five normal alkylbenzenes: (1) benzene; (2) toluene (methylbenzene); (3) ethylbenzene; (4) propylbenzene; and (5) butylbenzene. Only benzene and (to a lesser extent) toluene have been extensively investigated. The critical densities of toluene, ethylbenzene, propylbenzene, and butylbenzene are based on Simon's 1938 thesis, which was published by Timmermans in 1957 [57-sim].

Hales and Townsend [72-hal/tow] measured liquid densities of benzene, several alkylbenzenes, naphthalene, and 2-methylnaphthalene up to 490 K and obtained values for the critical densities by fitting their results to Riedel's equation. The calculated values for benzene, toluene, ethylbenzene, *o*-xylene, *m*-xylene, and *p*-xylene do not differ from those in Table 1 by more than the uncertainties given. For naphthalene the discrepancy is slightly greater than the uncertainty given in Table 1. There are no experimental critical density data for isopropylbenzene and 2-methylnaphthalene with which to compare the calculated values, 0.279 and 0.308 g·cm<sup>-3</sup>, respectively.

(1) **Benzene.** Kobe and Lynn [53-kob/lyn] reviewed the measurements of Young [10-you], Harand [35-har], Esso Laboratories [41-ano], Gornowski et al. [47-gor/ami], and Bender et al. [52-ben/fur]. They averaged the values from 41-ano, 47-gor/ami, and 52-ben/fur to obtain their recommendations for  $T_c$  and  $p_c$ , while they based  $\rho_c$  on 10-you and 47-gor/ami.

Kudchadker et al. [68-kud/ala] reviewed the measurements of Kreglewski [55-kre], Ambrose and Grant [57-amb/

gra], Simon [57-sim], Ambrose et al. [60-amb/cox], Partington et al. [60-par/row], Connolly and Kandalic [62-con/kan], Ambrose and Townsend [63-amb/tow], and Ambrose et al. [67-amb/bro]. They based their recommendations on the  $T_c$  of 60-amb/cox, the  $p_c$  of 67-amb/bro, and the  $\rho_c$  of 10-you and 57-sim, which were adjusted to accord with the value of  $T_c$  chosen. Kudchadker et al. erroneously included values from Oldenburg [55-old], an engineering paper dealing with the use of liquefied petroleum gas rather than with critical constants.

Of the pre-1910 references, the only one worthy of mention, other than Young [1889-you], is Altschul [1893-alt], who also investigated several other alkylbenzenes. Altschul's method for the determination of critical pressure is described by Kobe and Lynn. His  $T_c$  is nearly 2 K higher than the accepted value, but his  $p_c$  is remarkably close to the recommended value (4.91 vs 4.895 MPa).

The "modern" measurements begin with the work of Bender et al. [52-ben/fur], who determined all three properties on the basis of  $p$ - $V$ - $T$  measurements. Ambrose et al. [57-amb/gra; 60-amb/cox; 63-amb/tow; 67-amb/bro; 87-amb] confirmed the  $T_c$  and  $p_c$  but did not measure  $\rho_c$ . Also very important are the  $T_c$  and  $p_c$  measurements of Connolly and Kandalic [62-con/kan], Ewing et al. [81-ewi/mcgl], and Hugill and McGlashan [81-hug/mcgl], which agree with each other but give slightly lower  $T_c$  and  $p_c$  values than Bender's and Ambrose's 1960 and 1987 results. Averaging these selected values gives

$$T_c = (562.05 \pm 0.07) \text{ K}$$

$$p_c = (4.895 \pm 0.006) \text{ MPa}$$

These values are considered more reliable than the lower  $T_c$  and  $p_c$  recommended by Goodwin [88-goo] or those measured by Chirico and Steele (94-chi/ste;  $T_c$  by DSC and  $p_c$  by extrapolation and thermodynamic analysis). Our recommendation for  $\rho_c$  is the average of all data published since 1952:

$$\rho_c = (0.305 \pm 0.004) \text{ g·cm}^{-3}$$

Of the compounds considered in this paper, benzene is the one that has been studied most extensively, and it is also one that is relatively easy to prepare in a state of high purity. The results for benzene, therefore, provide a

**Table 1. Recommended Values of Critical Properties of Aromatic Hydrocarbons**

	molar mass $M/\text{g}\cdot\text{mol}^{-1}$	$T_c/\text{K}^a$	( $\pm$ ) <sup>b</sup>	$p_c/\text{MPa}$	( $\pm$ ) <sup>b</sup>	$\rho_c/\text{g}\cdot\text{cm}^{-3}$	( $\pm$ ) <sup>b</sup>	$V_c/\text{cm}^3\cdot\text{mol}^{-1}$	$Z_c^c$
normal alkylbenzenes									
benzene	78.11364	562.05	(0.07)	4.895	(0.006)	0.305	(0.004)	256	0.268
toluene	92.14052	591.75	(0.15)	4.108	(0.010)	0.292	(0.004)	316	0.264
ethylbenzene	106.1674	617.15	(0.1)	3.609	(0.010)	0.284	(0.004)	374	0.263
propylbenzene	120.19428	638.35	(0.1)	3.200	(0.010)	0.273	(0.004)	440	0.265
butylbenzene	134.22116	660.5	(0.5)	2.89	(0.04)	0.270	(0.010)	497	0.262
other alkylbenzenes									
<i>o</i> -xylene	106.1674	630.3	(0.5)	3.732	(0.04)	0.287	(0.004)	370	0.263
<i>m</i> -xylene	106.1674	617.0	(0.5)	3.541	(0.04)	0.283	(0.004)	375	0.259
<i>p</i> -xylene	106.1674	616.2	(0.2)	3.511	(0.02)	0.281	(0.004)	378	0.259
isopropylbenzene	120.19428	631.0	(0.5)	3.209	(0.04)				
1,2,3-trimethylbenzene	120.19428	664.5	(0.5)	3.454	(0.04)				
1,2,4-trimethylbenzene	120.19428	649.1	(0.5)	3.232	(0.04)				
1,3,5-trimethylbenzene	120.19428	637.3	(0.5)	3.127	(0.04)				
1-methyl-4-ethylbenzene	120.19428	640.2	(1.0)	3.23	(0.10)				
isobutylbenzene	134.22116	650	(?)	3.05	(?)				
<i>p</i> -cymene	134.22116	652	(?)	2.8	(?)				
1,4-diethylbenzene	134.22116	657.9	(0.5)	2.803	(0.04)				
1,2,4,5-tetramethylbenzene	134.22116	676	(?)	2.9	(?)				
hexamethylbenzene	162.27492	758	(1)						
polyphenyls									
diphenylmethane	168.23828	760	(8)	2.71	(0.3)	0.299	(0.030)	563	0.241
biphenyl	154.2114	773	(3)	3.38	(0.1)	0.310	(0.01)	497	0.262
<i>o</i> -terphenyl	230.30916	857	(5)	2.99	(0.6)	0.315	(0.04)	731	0.307
<i>m</i> -terphenyl	230.30916	883	(10)	2.48	(0.5)	0.318	(0.04)	724	0.245
<i>p</i> -terphenyl	230.30916	908	(10)	2.99	(0.6)	0.316	(0.04)	729	0.289
condensed polycyclics									
indan	118.1784	684.9	(0.5)	3.95	(0.04)				
naphthalene	128.17352	748.4	(0.5)	4.05	(0.05)	0.315	(0.005)	407	0.265
1-methylnaphthalene	142.2004	772	(1)	3.60	(0.1)				
2-methylnaphthalene	142.2004	761	(1)						
2,7-dimethylnaphthalene	156.22728	775	(2)	3.23	(0.2)	0.26 <sup>d</sup>	(0.05)	601 <sup>d</sup>	0.300 <sup>d</sup>
phenanthrene	178.2334	869	(1)						
tetralin	182.20528	720	(1)	3.65	(0.1)	0.324	(0.010)	408	0.249

<sup>a</sup> Temperatures are expressed on ITS-90. <sup>b</sup> The uncertainties ( $\pm$ ) are based on those for benzene, as a minimum, and values given by the investigators. <sup>c</sup>  $Z_c = p_c V_c / RT_c$ , where  $R = 8.31451 \text{ Pa}\cdot\text{m}^3\cdot\text{mol}^{-1}\cdot\text{K}^{-1}$ . <sup>d</sup> The  $\rho_c$  value derived by fitting saturated liquid density data with the Riedel equation was  $0.2965 \text{ g}\cdot\text{cm}^{-3}$  [93-chi/kni-1]; with this value,  $V_c = 527 \text{ cm}^3\cdot\text{mol}^{-1}$  and  $Z_c = 0.264$ .

standard for the aromatic hydrocarbons, and in the assessment of the uncertainties to be attributed to values of the critical properties, it has been assumed that they should not be less than the corresponding ones for benzene.

**(2) Toluene.** Kobe and Lynn reported, with minimal comments, the measurements of Altschul [1893-alt], Krase and Goodman [30-kra/goo], Harand [35-har], and Fischer and Reichel [43-fis/rei]. Kobe and Lynn missed the  $T_c$  value of Pawlewski [1883-paw] and erroneously credited Mathias with measuring the critical density of toluene in 1892; the reported value ( $0.287 \text{ g}\cdot\text{cm}^{-3}$ ) is actually a later estimate based on the liquid density at room temperature [04-mat].

Kudchadker et al. reviewed the work of Ambrose et al. [57-amb/gra; 60-amb/cox; 67-amb/bro], Simon [57-sim], and Partington et al. [60-par/row]. Ambrose [87-amb] published details of the vapor pressure measurements underlying the values in 67-amb/bro and included two similar sets of  $T_c$  and  $p_c$ . If we also consider the results of Partington et al. (who used the same material as Ambrose), Powell et al. [70-pow/swi], and Teja's group [90-tej/ans; 90-tej/ros], then we conclude that

$$T_c = (591.75 \pm 0.15) \text{ K}$$

$$p_c = (4.108 \pm 0.010) \text{ MPa}$$

As in the case of benzene, Altschul's (1893-alt)  $p_c$  is very close to the recommended value. Goodwin's [89-goo] recommendations for  $T_c$  and  $p_c$  are surprisingly high. Apparently they are based on the values of Akhundov and Abdullaev [69-akh/abd], who measured the vapor pressure of toluene from 159 to 320.8 °C. However, Akhundov and

Abdullaev appear not to have observed the critical point and probably took the critical temperature (320.8 °C) from the literature.

Steele et al. [88-ste/chi] and Chirico and Steele [94-chi/ste] determined  $T_c$  with a DSC technique. In addition, they estimated  $\rho_c$  by fitting a corresponding-states equation to their own density measurements and those of Hales and Townsend [72-hal/tow] and derived  $p_c$  either by extrapolating available vapor pressure data [88-ste/chi] or by a fitting procedure utilizing their new vapor pressure and density measurements [94-chi/ste]. The  $T_c$  and  $\rho_c$  values of Steele et al. agree closely with those of Simon [57-sim], while the extrapolated  $p_c$  value, 4.109 MPa [88-ste/chi], is very close to the recommended value. On the other hand, their more recent  $p_c$  result, 4.162 MPa [94-chi/ste], is significantly higher than the measurements of Ambrose and Teja's group.

For  $\rho_c$ , Simon's [57-sim] value was corrected by Kudchadker et al. to conform to the selected  $T_c$ , giving

$$\rho_c = 0.292 \text{ g}\cdot\text{cm}^{-3}$$

to which we assign an uncertainty of  $\pm 0.004 \text{ g}\cdot\text{cm}^{-3}$ .

**(3) Ethylbenzene.** Only Altschul's [1893-alt] results were available at the time of Kobe and Lynn's review. Kudchadker et al. reviewed the measurements of Simon [57-sim] and of Ambrose et al. [60-amb/cox; 67-amb/bro]. The only additional known data are those of Pak and Kay [72-pak/kay], Rätzsch and Strauch [72-rae/str], and the Ambrose [87-amb] supplement to the earlier paper [67-amb/bro].

Table 2. Critical Properties from the Literature

year	values reported in nonstandard units	$T_{90}/\text{K}$	$p/\text{MPa}$	$\rho/\text{gcm}^{-3}$	method <sup>a</sup>	authors
BENZENE: molar mass <sup>b</sup> = 78.11364; CASRN 71-43-2						
$T_{68} - T_{48} = 0.071 \text{ K}; T_{90} - T_{68} = -0.040 \text{ K}; T_{90} - T_{48} = 0.031 \text{ K at } 562 \text{ K}$						
1878-saj	280.6 °C, 49.5 atm	553.8	5.02		?	Sajotschewsky
1881-ram	291.7 °C, (60.4 ± 0.1) atm	564.8	6.12		1	Ramsay
1889-you	288.5 °C, 36395 mmHg	561.6	4.8523		1	Young
1891-sch	296.4 °C	569.6			1	Schmidt
1893-alt	290.5 °C, 50.1 kg·cm <sup>-2</sup>	563.6	4.91		1	Altschul
1899-rad	288.1 °C	561.2			1	Radice
08-sch	288.68 °C, 49.5 atm	561.8	5.02		?	Schamhardt
10-you	288.5 °C, 36395 mmHg	561.6	4.8523	0.3045	1, 7	Young
35-har	290.8 °C	564.0			1	Harand
41-ano	289.45 °C, 48.9 atm	562.6	4.955		?	Esso Laboratories
43-fis/rei	291.2 °C	564.4			1	Fischer and Reichel
47-gor/ami	289.5 °C, 36985 mmHg	562.6	4.9309	0.297	1, 7	Gornowski et al.
52-ben/fur	(288.94 ± 0.05) °C, (48.34 ± 0.03) atm, (0.253 ± 0.03) L·mol <sup>-1</sup>	562.12	4.898	0.309	3	Bender et al.
52-kay/nev	288.71 °C, 707.1 psi	561.89	4.875		1a	Kay and Nevens
55-kre	288.8 °C	562.0			1	Kreglewski
57-amb/gra	(288.8 ± 0.1) °C	562.0			1	Ambrose and Grant
57-kri/kha	290 °C, 260 cm <sup>3</sup> ·mol <sup>-1</sup>	563.2		0.300	1, 7	Krichevskii et al.
57-sim	288.5 °C	561.6		0.3044	1, 7	Simon
60-amb/cox	(288.94 ± 0.01) °C	562.12			1	Ambrose et al.
60-mcc/sto	(553 ± 1) °F, (716 ± 1) psi	562.6	4.94		4	McCracken et al.
60-par/row	(288.7 ± 0.1) °C	561.88			1	Partington et al.
62-con/kan	288.84 °C, 48.28 atm	562.02	4.892		1	Connolly and Kandalic
63-amb/tow	48.36 atm		4.900		1	Ambrose and Townsend
63-che	288.5 °C, 260 cm <sup>3</sup> ·mol <sup>-1</sup>	561.6		0.300	1	Cheng
64-mak/noz	(289 ± 1) °C	562			4	Makhan'ko and Nozdrev
64-ska/kay	289.00 °C, 710.1 psi	562.18	4.896	0.304	1a	Skaates and Kay
67-amb/bro			4.898		1	Ambrose et al.
68-cam/cha	288.95 °C, 48.22 atm	562.13	4.886	0.275(?)	1, 7	Campbell and Chatterjee
69-cam/cha				0.306	7	Campbell and Chatterjee
70-art/shi	288.65 °C	561.8		0.301	2b, 7	Artyukhovskaya et al.
70-cam/mus	(288.0 ± 0.1) °C	561.2			1	Campbell and Musbally
70-kob/mat	(552.0 ± 0.5) °F, (712 ± 2) psi	562.0	4.91	0.316 ± 0.002	3, 7	Kobe and Matthews
72-pak/kay	288.1 °C, 712.1 psi	561.2	4.910		1a	Pak and Kay
72-rae/str		563.3			1	Rätzsch and Strauch
77-akh/abd	(3.32 ± 0.04) cm <sup>3</sup> ·g <sup>-1</sup>	(562.6)		0.301	3	Akhundov and Abdullaev
81-ewi/mcg		562.03 ± 0.05	4.888 ± 0.003		2(?)	Ewing et al.
81-hug/mcg		562.01 ± 0.02	4.889 ± 0.003		2(?)	Hugill and McGlashan
83-hal/gun				0.302	4	Hales and Gundry
83-kay/kre		562.17 ± 0.05	4.897 ± 0.006		1a	Kay and Kreglewski
87-amb		562.12	4.898		1	Ambrose
88-goo	3.90 mol·dm <sup>-3</sup>	561.71	4.87575	0.305	8	Goodwin
88-bru		562.36 ± 0.30	4.894 ± 0.020		2a	Brunner
89-kni/arc		562.2	4.900 ± 0.020		4, 6	Knipmeyer et al.
94-chi/ste		561.8 ± 1.0	4.884 ± 0.050	0.3038 ± 0.0030	4, 6, 7	Chirico and Steele
	recommended values	562.05 ± 0.07	4.895 ± 0.006	0.305 ± 0.004		

Krichevskii et al. [57-kri/kha] also report in their Table 1 a critical pressure (48.6 atm) taken from 23-lan/boe (3rd suppl.).

Makhan'ko and Nozdrev [64-mak/noz] determined the critical temperature by ultrasonic absorption.

Campbell and Chatterjee [69-cam/cha] corrected the critical density they had reported in 68-cam/cha.

year	values reported in nonstandard units	$T_{90}/\text{K}$	$p/\text{MPa}$	$\rho/\text{gcm}^{-3}$	method <sup>a</sup>	authors
TOLUENE (Methylbenzene): molar mass <sup>b</sup> = 92.14052; CASRN 108-88-3						
$T_{68} - T_{48} = 0.075 \text{ K}; T_{90} - T_{68} = -0.040 \text{ K}; T_{90} - T_{48} = 0.035 \text{ K at } 592 \text{ K}$						
1883-paw	320.8 °C	594.0			1	Pawlewski
1893-alt	320.6 °C, 41.6 kg·cm <sup>-2</sup>	593.8	4.08		1	Altschul
30-kra/goo	41.6 atm		4.22		5	Krase and Goodman
35-har	320.8 °C	594.0			1	Harand
43-fis/rei	320.8 °C	594.0			1	Fischer and Reichel
57-amb/gra	(318.6 ± 0.1) °C	591.8			1	Ambrose and Grant
57-sim	319.9 °C	593.0		0.2913	1, 7	Simon
60-amb/cox	(318.57 ± 0.01) °C	591.76			1	Ambrose et al.
60-par/row	(318.8 ± 0.1) °C	591.98			1	Partington et al.
67-amb/bro			4.109		1	Ambrose et al.
69-akh/abd	320.8 °C(?)	594.0	4.2358		3	Akhundov and Abdullaev
70-pow/swi		592.0			1	Powell et al.
72-rae/str		592.4			1	Rätzsch and Strauch
87-amb		591.75	4.1066		1	Ambrose
		591.76	4.1087			
88-ste/chi		593 ± 1	4.109 ± 0.020	0.291 ± 0.005	4, 6, 7	Steele et al.

Table 2 (Continued)

year	values reported in nonstandard units	$T_{90}/\text{K}$	$p/\text{MPa}$	$\rho/\text{g}\cdot\text{cm}^{-3}$	method <sup>a</sup>	authors
TOLUENE (Methylbenzene): molar mass <sup>b</sup> = 92.14052; CASRN 108-88-3						
$T_{68} - T_{48} = 0.075 \text{ K}; T_{90} - T_{68} = -0.040 \text{ K}; T_{90} - T_{48} = 0.035 \text{ K}$ at 592 K						
89-goo	3.15 mol·dm <sup>-3</sup>	593.91	4.2365	0.290	8	Goodwin
90-tej/ans		591.5 ± 0.2			1c	Teja and Anselme
90-tej/ros		591.5 ± 0.6	4.107 ± 0.002		1c	Teja and Rosenthal
94-chi/ste		592.5 ± 1.0	4.162 ± 0.050	0.2910 ± 0.0030	4, 6, 7	Chirico and Steele
	recommended values	591.75 ± 0.15	4.108 ± 0.010	0.292 ± 0.004		
ETHYLBENZENE: molar mass <sup>b</sup> = 106.1674; CASRN 100-41-4						
$T_{68} - T_{48} = 0.077 \text{ K}; T_{90} - T_{68} = -0.041 \text{ K}; T_{90} - T_{48} = 0.036 \text{ K}$ at 617 K						
1893-alt	346.4 °C, 38.1 kg·cm <sup>-2</sup>	619.6	3.74		1	Altschul
57-sim	344.0 °C	617.2		0.2835	1, 7	Simon
60-amb/cox	(343.97 ± 0.02) °C	617.16			1	Ambrose et al.
67-amb/bro	343.92 °C	617.11	3.609		1	Ambrose et al.
72-pak/kay	343.6 °C, 529.2 psi	616.8	3.649		1a	Pak and Kay
72-rae/str		618.2			1	Rätzsch and Strauch
87-amb		617.16	3.6088		1	Ambrose
	recommended values	617.15 ± 0.1	3.609 ± 0.010	0.284 ± 0.004		
PROPYLBENZENE: molar mass <sup>b</sup> = 120.19428; CASRN 103-65-1						
$T_{68} - T_{48} = 0.077 \text{ K}; T_{90} - T_{68} = -0.042 \text{ K}; T_{90} - T_{48} = 0.035 \text{ K}$ at 638 K						
1893-alt	365.6 °C, 32.3 kg·cm <sup>-2</sup>	638.8	3.17		1	Altschul
57-sim	366.0 °C	639.2		0.2727	1, 7	Simon
60-amb/cox	(365.21 ± 0.01) °C	638.40			1	Ambrose et al.
67-amb/bro	365.09 °C	638.28	3.200		1	Ambrose et al.
	recommended values	638.35 ± 0.1	3.200 ± 0.010	0.273 ± 0.004		
BUTYLBENZENE: molar mass <sup>b</sup> = 134.22116; CASRN 104-51-8						
57-sim	387.8 °C	661.0		0.2697	1, 7	Simon
60-amb/cox	(387.3 ± 0.1) °C	660.4			1	Ambrose et al.
67-amb/bro	386.9 °C	660.0	2.887 ± 0.02		1	Ambrose et al.
	recommended values	660.5 ± 0.5	2.89 ± 0.04	0.270 ± 0.010		
o-XYLENE (1,2-Dimethylbenzene): molar mass <sup>b</sup> = 106.1674; CASRN 95-47-6						
$T_{68} - T_{48} = 0.077 \text{ K}; T_{90} - T_{68} = -0.042 \text{ K}; T_{90} - T_{48} = 0.035 \text{ K}$ at 630 K						
1893-alt	358.3 °C, 36.9 kg·cm <sup>-2</sup>	631.4	3.62		1	Altschul
06-bro	362.95 °C	636.1			1	Brown
43-fis/rei	358.5 °C	631.6			1	Fischer and Reichel
57-amb/gra	(357.1 ± 0.1) °C	630.2			1	Ambrose and Grant
57-fra	358 °C	631.0			1	Francis
57-gla/rue	344.3 °C, 31.5 atm	617.4	3.19		3	Glaser and Rüländ
57-sim	357.9 °C	631.0		0.2877	1, 7	Simon
59-ric/row	(356.2 ± 0.1) °C	629.4			1a	Richardson and Rowlinson
67-amb/bro			3.733		1	Ambrose et al.
70-akh/ima	(3.49 ± 0.02) cm <sup>3</sup> ·g <sup>-1</sup>			0.2865	3	Akhundov and Imanov
70-mam/akh	358.44 °C (?)	631.55	3.8081		3	Mamedov et al.
72-pak/kay	356.2 °C, 544.5 psi	629.4	3.754		1a	Pak and Kay
87-amb		630.29	3.7318		1	Ambrose
	recommended values	630.3 ± 0.5	3.732 ± 0.04	0.287 ± 0.004		

Richardson and Rowlinson [59-ric/row] measured (356.1 ± 0.1) °C with a trace of mercury present and (355.8 ± 0.1) °C in the presence of excess mercury.

year	values reported in nonstandard units	$T_{90}/\text{K}$	$P/\text{MPa}$	$\rho/\text{g}\cdot\text{cm}^{-3}$	method <sup>a</sup>	authors
<i>m</i> -XYLENE (1,3-Dimethylbenzene): molar mass <sup>b</sup> = 106.1674; CASRN 108-38-3						
$T_{68} - T_{48} = 0.077 \text{ K}; T_{90} - T_{68} = -0.041 \text{ K}; T_{90} - T_{48} = 0.036 \text{ K}$ at 617 K						
1893-alt	345.6 °C, 35.8 kg·cm <sup>-2</sup>	618.8	3.51		1	Altschul
06-bro	349.0 °C	622.2			1	Brown
57-amb/gra	(343.3 ± 0.1) °C	616.4			1	Ambrose and Grant
57-fra	347 °C	620.2			1	Francis
57-gla/rue	344.3 °C, 33.0 atm	617.4	3.34		3	Glaser and Rüländ
57-sim	343.6 °C	616.8		0.2822	1, 7	Simon
67-amb/bro	343.82 °C	617.01	3.541		1	Ambrose et al.
68-akh/asa	3.51 cm <sup>3</sup> ·g <sup>-1</sup>			0.2849	3	Akhundov and Asadullaeva
87-amb		617.01	3.5412		1	Ambrose
	recommended values	617.0 ± 0.5	3.541 ± 0.04	0.283 ± 0.004		

Table 2 (Continued)

year	values reported in nonstandard units	$T_{90}/\text{K}$	$p/\text{MPa}$	$\rho/\text{gcm}^{-3}$	method <sup>a</sup>	authors
<i>p</i> -XYLENE (1,4-Dimethylbenzene): molar mass <sup>b</sup> 106.1674; CASRN 106-42-3						
$T_{68} - T_{48} = 0.077 \text{ K}; T_{90} - T_{68} = -0.041 \text{ K}; T_{90} - T_{48} = 0.036 \text{ K}$ at 616 K						
1893-alt	344.4 °C, 35.0 kgcm <sup>-2</sup>	617.6	3.43		1	Altschul
06-bro	348.5 °C	621.6			1	Brown
43-fis/rei	345.0 °C	618.2			1	Fischer and Reichel
57-amb/gra	(343.0 ± 0.1) °C	616.2			1	Ambrose and Grant
57-fra	346 °C	619.2			1	Francis
57-gla/rue	344.3 °C, 33.0 atm	617.4	3.34		3	Glaser and Rüländ
57-sim	342.75 °C	615.9		0.2807	1, 7	Simon
67-amb/bro			3.511		1	Ambrose et al.
70-akh/ima	(3.54 ± 0.02) cm <sup>3</sup> ·g <sup>-1</sup>			0.2825	3	Akhundov and Imanov
70-mam/akh	354 °C(?)	618.2	3.6175		3	Mamedov et al.
70-pow/swi		616.2			1	Powell et al.
87-amb		616.19	3.5107		1	Ambrose
	recommended values	616.2 ± 0.2	3.511 ± 0.02	0.281 ± 0.004		
ISOPROPYLBENZENE [(1-Methylethyl)benzene, Cumene]: molar mass <sup>b</sup> = 120.19428; CASRN 98-82-8						
$T_{68} - T_{48} = 0.077 \text{ K}; T_{90} - T_{68} = -0.041 \text{ K}; T_{90} - T_{48} = 0.036 \text{ K}$ at 631 K						
1893-alt	362.7 °C, 32.2 kgcm <sup>-2</sup>	635.8	3.16		1	Altschul
57-amb/gra	(357.9 ± 0.1) °C	631.0			1	Ambrose and Grant
67-amb/bro			3.209		1	Ambrose et al.
	recommended values	631.0 ± 0.5	3.209 ± 0.04			
1,2,3-TRIMETHYLBENZENE: molar mass <sup>b</sup> = 120.19428; CASRN 526-73-8						
$T_{68} - T_{48} = 0.076 \text{ K}; T_{90} - T_{68} = -0.046 \text{ K}; T_{90} - T_{48} = 0.030 \text{ K}$ at 665 K						
60-amb/cox	(391.35 ± 0.01) °C	664.53			1	Ambrose et al.
67-amb/bro	391.24 °C	664.42	3.454		1	Ambrose et al.
80-kay/pak		665.50	3.4426		1a	Kay and Pak
	recommended values	664.5 ± 0.5	3.454 ± 0.04			
1,2,4-TRIMETHYLBENZENE (Pseudocumene): molar mass <sup>b</sup> = 120.19428; CASRN 95-63-6						
$T_{68} - T_{48} = 0.077 \text{ K}; T_{90} - T_{68} = -0.044 \text{ K}; T_{90} - T_{48} = 0.033 \text{ K}$ at 650 K						
1893-alt	381.2 °C, 33.2 kgcm <sup>-2</sup>	654.4	3.26		1	Altschul
57-gla/rue	337 °C, 19 atm	610.2	1.9		3	Glaser and Rüländ
60-amb/cox	(375.87 ± 0.01) °C	649.05			1	Ambrose et al.
67-amb/bro	375.94 °C	649.12	3.232		1	Ambrose et al.
80-kay/pak		(a) 650.51 (b) 650.31	3.2771 3.2695		1a	Kay and Pak
	recommended values	649.1 ± 0.5	3.232 ± 0.04			
Kay and Pak [80-kay/pak] made determinations with both (a) gallium and (b) mercury.						
year	values reported in nonstandard units	$T_{90}/\text{K}$	$p/\text{MPa}$	$\rho/\text{gcm}^{-3}$	method <sup>a</sup>	authors
1,3,5-TRIMETHYLBENZENE (Mesitylene): molar mass <sup>b</sup> = 120.19428; CASRN 108-67-8						
$T_{68} - T_{48} = 0.077 \text{ K}; T_{90} - T_{68} = -0.042 \text{ K}; T_{90} - T_{48} = 0.035 \text{ K}$ at 638 K						
1893-alt	367.7 °C, 33.2 kgcm <sup>-2</sup>	640.8	3.26		1	Altschul
06-bro	370.5 °C	643.6			1	Brown
60-amb/cox	(364.14 ± 0.01) °C	637.32			1	Ambrose et al.
67-amb/bro	364.12 °C	637.30	3.127		1	Ambrose et al.
70-pow/swi		637.1			1	Powell et al.
80-kay/pak		638.61	3.1619		1a	Kay and Pak
	recommended values	637.3 ± 0.5	3.127 ± 0.04			
1-METHYL-4-ETHYLBENZENE ( <i>p</i> -Ethyltoluene): molar mass <sup>b</sup> = 120.19428; CASRN 622-96-8						
$T_{68} - T_{48} = 0.077 \text{ K}; T_{90} - T_{68} = -0.043 \text{ K}; T_{90} - T_{48} = 0.034 \text{ K}$ at 640 K						
85-lyo		640.2	3.173		1a	Lyons
87-dau/jal	(367.08 ± 0.5) °C	640.19	3.233 ± 0.004		1a	Daubert et al.
	recommended values	640.2 ± 1.0	3.23 ± 0.1			
ISOBUTYLBENZENE [(2-Methylpropyl)benzene]: molar mass <sup>b</sup> = 134.22116; CASRN 538-93-2						
1893-alt	377.1 °C, 31.1 kgcm <sup>-2</sup>	650.2	3.05		1	Altschul
	recommended values	650	3.05			
<i>p</i> -CYMENE [1-Methyl-4-(1-methylethyl)benzene, 1-Methyl-4-isopropylbenzene]: molar mass <sup>b</sup> = 134.22116; CASRN 99-87-6						
1893-alt	378.6 °C, 28.6 kgcm <sup>-2</sup>	651.8	2.805		1	Altschul
06-bro	(385.15 ± 2) °C	658.3			1	Brown
	recommended values	652	2.8			
Brown [06-bro] reported 385.15 °C as the mean of measurements ranging from 384 to 387 °C. He reported the normal boiling point as 177.0 °C, but he also noted that his sample was "not sufficiently pure". See also discussion in text.						

Table 2 (Continued)

year	values reported in nonstandard units	$T_{90}/\text{K}$	$p/\text{MPa}$	$\rho/\text{g}\cdot\text{cm}^{-3}$	method <sup>a</sup>	authors
1,4-DIETHYLBENZENE: molar mass <sup>b</sup> = 134.22116; CASRN 105-05-5						
60-amb/cox	$T_{68} - T_{48} = 0.077 \text{ K}$ ; $T_{90} - T_{68} = -0.045 \text{ K}$ ; $T_{90} - T_{48} = 0.032 \text{ K}$ at 658 K (384.72 ± 0.03) °C	657.90			1	Ambrose et al.
67-amb/bro	384.74 °C	657.92	2.803		1	Ambrose et al.
	recommended values	657.9 ± 0.5	2.803 ± 0.04			
Ambrose et al. [60-amb/cox] had mistakenly reported the compound as isobutylbenzene.						
year	values reported in nonstandard units	$T_{90}/\text{K}$	$p/\text{MPa}$	$\rho/\text{g}\cdot\text{cm}^{-3}$	method <sup>a</sup>	authors
1,2,4,5-TETRAMETHYLBENZENE (Durene): molar mass <sup>b</sup> = 134.22116; CASRN 95-93-2						
01-guy/mal, 02-guy/mal	402.5 °C, 28.6 atm	675.6	2.90		1	Guye and Mallet
	recommended values	676	2.9			
Guye and Mallet [02-guy/mal] reported that the compound decomposed at 400 °C.						
year	values reported in nonstandard units	$T_{90}/\text{K}$	$p/\text{MPa}$	$\rho/\text{g}\cdot\text{cm}^{-3}$	method <sup>a</sup>	authors
HEXAMETHYLBENZENE: molar mass <sup>b</sup> = 162.27492; CASRN 87-85-4						
02-guy/mal	> 478.0 °C	> 751			1	Guye and Mallet
13-ano	494 °C	767.2			?	Societe Francaise de Physique
74-amb/bro		758 ± 1			1	Ambrose et al.
	recommended values	758 ± 1				
DIPHENYLMETHANE: molar mass <sup>b</sup> = 168.23828; CASRN 101-81-5						
1899-rad	497.0 °C	770.2			1	Radice
01-guy/mal, 02-guy/mal	28.2 atm		2.86		1	Guye and Mallet
80-wie/kob, 81-wil/joh		(760)	2.71		6	Wieczorek and Kobayashi, Wilson et al.
85-smi	(494 ± 1) °C	767			1c	Smith
92-ste		760 ± 2		0.2994 ± 0.015	4, 7	Steele
	recommended values	760 ± 8	2.71 ± 0.3	0.299 ± 0.030		
BIPHENYL: molar mass <sup>b</sup> = 154.2114; CASRN 92-52-4						
01-guy/mal, 02-guy/mal	495.6 °C, (31.80 ± 0.04) atm	768.8	3.222		1	Guye and Mallet
30-cor	528 °C, 31400 mmHg	801.2	4.19	0.343	1, 6, 7	Cork
57-gla/rue	496 °C, 30.8 atm	769.2	3.12		3	Glaser and Rütland
60-man/ewb	960 °F, 551 psi	788.7	3.80	0.307	1, 6, 7	Mandel and Ewbank
63-ell/yan	(500 ± 2) °C, 485.3 psi	773	3.346	0.310	2, 3	Ellard and Yanko
63-rei	(504 ± 3) °C, 34.5 atm	777	3.50	0.322	1, 6, 7	Reiter
89-chi/kni		772.5 ± 2.0	3.380 ± 0.025	0.313 ± 0.003	4, 6, 7	Chirico et al.
	recommended values	773 ± 3	3.38 ± 0.1	0.310 ± 0.01		
<i>o</i> -TERPHENYL (1,2-Diphenylbenzene): molar mass <sup>b</sup> = 230.30916; CASRN 84-15-1						
60-man/ewb	1144 °F, 566 psi	891	3.90	0.306	1, 6, 7	Mandel and Ewbank
63-rei	(584 ± 5) °C, (29.5 ± 5.9) atm	857	2.99	0.315 ± 0.02	1, 6, 7	Reiter
	recommended values	857 ± 5	2.99 ± 0.6	0.315 ± 0.04		
<i>m</i> -TERPHENYL (1,3-Diphenylbenzene): molar mass <sup>b</sup> = 230.30916; CASRN 92-06-8						
60-man/ewb	1205 °F, 508 psi	925	3.5	0.300	1, 6, 7	Mandel and Ewbank
63-rei	(610 ± 10) °C, (24.5 ± 4.9) atm	883	2.48	0.318 ± 0.02	1, 6, 7	Reiter
	recommended values	883 ± 10	2.48 ± 0.5	0.318 ± 0.04		
<i>p</i> -TERPHENYL (1,4-Diphenylbenzene): molar mass <sup>b</sup> = 230.30916; CASRN 92-94-4						
60-man/ewb	1207 °F, 483 psi	926	3.33	0.302	1, 6, 7	Mandel and Ewbank
63-rei	(635 ± 10) °C, (29.5 ± 5.9) atm	908	2.99	0.316 ± 0.02	1, 6, 7	Reiter
	recommended values	908 ± 10	2.99 ± 0.6	0.316 ± 0.04		
INDAN: molar mass <sup>b</sup> = 118.1784; CASRN 496-11-7						
74-amb/bro		684.9 ± 0.3	3.95 ± 0.01		1	Ambrose et al.
	recommended values	684.9 ± 0.5	3.95 ± 0.04			
Ambrose et al. reported a 0.2 K·h <sup>-1</sup> rise in critical temperature.						

Table 2 (Continued)

year	values reported in nonstandard units	$T_{90}/\text{K}$	$p/\text{MPa}$	$\rho/\text{g}\cdot\text{cm}^{-3}$	method <sup>a</sup>	authors
NAPHTHALENE: molar mass <sup>b</sup> = 128.17352; CASRN 91-20-3						
$T_{68} - T_{48} = 0.076 \text{ K}$ ; $T_{90} - T_{68} = -0.070 \text{ K}$ ; $T_{90} - T_{48} = 0.006 \text{ K}$ at 749 K						
01-guy/mal, 02-guy/mal	468.2 °C, (39.23 ± 0.09) atm	741.4	3.975		1	Guye and Mallet
37-zhu	476.5 °C	749.6		0.3148	1, 7	Zhuraviev
41-sch	480 °C, 42.0 kg $\cdot$ cm <sup>-2</sup>	753	4.12	0.314	1	Schröer
60-amb/cox	(475.2 ± 0.05) °C	748.36			1	Ambrose et al.
62-che/mcc		748.0			1	Cheng et al.
63-che	473.4 °C, 408 cm <sup>3</sup> ·mol <sup>-1</sup>	746.6		0.314	1	Cheng
67-amb/cox	475.20 °C	748.36	4.051		1	Ambrose et al.
80-kay/pak		(a) 749.38 (b) 748.78 (c) 749.38	4.0976 4.0645		1a	Kay and Pak
93-chi/kni-1		749 ± 1	4.105	0.310 ± 0.015	4, 6, 7	Chirico et al.
	recommended values	748.4 ± 0.5	4.05 ± 0.05	0.315 ± 0.005		
Kay and Pak [80-kay/pak] made determinations with both (a) gallium and (b) mercury, as well as with (c) a sealed tube. Chirico et al. [93-chi/kni] used $T_c = 748.4 \text{ K}$ in fitting their vapor pressure data with the Wagner equation to derive $p_c$ ; a similar fitting of their saturated liquid density data (from 373 to 548 K) with the Riedel equation gave a critical density of 0.320 g $\cdot$ cm <sup>-3</sup> .						
year	values reported in nonstandard units	$T_{90}/\text{K}$	$p/\text{MPa}$	$\rho/\text{g}\cdot\text{cm}^{-3}$	method <sup>a</sup>	authors
1-METHYLNAPHTHALENE: molar mass <sup>b</sup> = 142.2004; CASRN 90-12-0						
60-amb/cox	> 495 °C	> 768			1	Ambrose et al.
63-amb	(499 ± 1) °C	772			1	Ambrose
81-wil/joh		(772)	3.60		5	Wilson et al.
	recommended values	772 ± 1	3.60 ± 0.1			
2-METHYLNAPHTHALENE: molar mass <sup>b</sup> = 142.2004; CASRN 91-57-6						
63-amb	(488 ± 1) °C	761			1	Ambrose
	recommended values	761 ± 1				
2,7-DIMETHYLNAPHTHALENE: molar mass <sup>b</sup> = 156.22728; CASRN 582-16-1						
93-chi/kni-1		775 ± 2	3.234	0.255 ± 0.030	4, 6, 7	Chirico et al.
	recommended values	775 ± 2	3.23 ± 0.2	0.26 ± 0.05		
Chirico et al. [93-chi/kni-1] fitted their vapor pressure data with the Wagner equation to derive $p_c$ ; a fitting of their saturated liquid density with the Riedel equation gave a critical density of 0.2965 g $\cdot$ cm <sup>-3</sup> .						
year	values reported in nonstandard units	$T_{90}/\text{K}$	$p/\text{MPa}$	$\rho/\text{g}\cdot\text{cm}^{-3}$	method <sup>a</sup>	authors
PHENANTHRENE: molar mass <sup>b</sup> = 178.2334; CASRN 85-01-8						
63-che	596.1 °C	869.2			1	Cheng
	recommended values	869 ± 1				
TETRALIN (1,2,3,4-Tetrahydronaphthalene): molar mass <sup>b</sup> = 132.20528; CASRN 119-64-2						
88-ste/chi		721 ± 1	3.75 ± 0.05	0.300 ± 0.005	4, 6, 7	Steele et al.
90-tej/ans-1		719.9 ± 1.0		0.324 ± 0.005	1c	Teja and Anselme
91-gud/tej		719.5 ± 0.4	3.63 ± 0.02		1c	Gude and Teja
	recommended values	720 ± 1	3.65 ± 0.1	0.324 ± 0.010		

<sup>a</sup> See Table 3. <sup>b</sup> Molar masses based on carbon 12.011, hydrogen 1.00794.

The recommended values for  $T_c$  and  $p_c$  are based entirely on Ambrose's results, while Simon's  $\rho_c$  value has been rounded up:

$$T_c = (617.15 \pm 0.1) \text{ K}$$

$$p_c = (3.609 \pm 0.010) \text{ MPa}$$

$$\rho_c = (0.284 \pm 0.004) \text{ g}\cdot\text{cm}^{-3}$$

**(4) Propylbenzene.** As in the case of ethylbenzene, only Altschul's [1893-alt] results were available at the time of Kobe and Lynn's review, while Kudchadker et al. also reported Simon's [57-sim] and Ambrose's [60-amb/cos; 67-amb/bro] more reliable values. The recommended  $T_c$  and

$p_c$  values are based on the work of Ambrose, while  $\rho_c$  is from Simon's study, with one less significant figure:

$$T_c = (638.35 \pm 0.1) \text{ K}$$

$$p_c = (3.200 \pm 0.010) \text{ MPa}$$

$$\rho_c = (0.273 \pm 0.004) \text{ g}\cdot\text{cm}^{-3}$$

**(5) Butylbenzene.** The only pre-1960 results are those of Simon [57-sim], who measured the  $T_c$  and  $\rho_c$ . Ambrose et al. [60-amb/cox] found this compound to be unstable at its critical temperature: the rate of change of the apparent critical temperature was -1.3 K/h. The value given in Table 2 was obtained by extrapolating the apparent critical

**Table 3. Keys to Methods of Critical Point Determination (Reprinted with permission from 95-amb/you. Copyright 1995 American Chemical Society)**

1. visual—in glass tube
  2. visual—in cell with windows
  3. nonvisual— $pVT$  measurements
  4. other nonvisual methods
  5. critical pressure measurements combined with vapor pressure measurements up to the critical point
  6. critical pressure by extrapolation of vapor pressure curve
  7. orthobaric density measurements
  8. equation of state, thermodynamic study
  9. calculation from another physical property
  10. literature survey
- (a) with stirring  
 (b) instrumental detection of critical point  
 (c) special feature of apparatus

temperatures to zero time. Because of this instability, Ambrose et al. [67-amb/bro] estimated the uncertainty in their  $p_c$  value to be  $\pm 0.02$  MPa and also considered their earlier [60-amb/cox] value for  $T_c$  to be more reliable.

The recommended values have larger estimated uncertainties because of butylbenzene's instability:

$$T_c = (660.5 \pm 0.5) \text{ K}$$

$$p_c = (2.89 \pm 0.04) \text{ MPa}$$

$$\rho_c = (0.270 \pm 0.010) \text{ g}\cdot\text{cm}^{-3}$$

### (B) Other Alkylbenzenes

Experimental critical constants are available for 13 other alkylbenzenes: (1) *o*-xylene (1,2-dimethylbenzene); (2) *m*-xylene (1,3-dimethylbenzene); (3) *p*-xylene (1,4-dimethylbenzene); (4) isopropylbenzene [(1-methylethyl)benzene, cumene]; (5) 1,2,3-trimethylbenzene; (6) 1,2,4-trimethylbenzene (pseudocumene); (7) 1,3,5-trimethylbenzene (mesitylene); (8) 1-methyl-4-ethylbenzene (*p*-ethyltoluene); (9) isobutylbenzene [(2-methylpropyl)benzene]; (10) *p*-cymene [1-methyl-4-(1-methylethyl)benzene, 1-methyl-4-isopropylbenzene]; (11) 1,4-diethylbenzene; (12) 1,2,4,5-tetramethylbenzene (durene); (13) hexamethylbenzene. Kobe and Lynn [53-kob/lyn] reported critical temperatures from Prud'homme [20-pru] for 1,2,3,5-tetramethylbenzene (isodurene) and pentamethylbenzene. However, these values were based on a rough approximation; namely, that  $(T_c - T_b)/T_c$  is constant for higher members of a homologous series. Prud'homme's estimates are not included in Tables 1 and 2.

Glaser and Rüländ [57-gla/rue] measured vapor pressures using a pressure gauge attached to a heated steel autoclave and identified the critical point for each compound by the break in the curve when pressure was plotted against temperature, an insensitive method. Their values are included in Table 2 for the three xylenes, 1,2,4-trimethylbenzene, and biphenyl. Their values for other aromatic hydrocarbons are not included in Table 2, because the critical temperatures were calculated from equations based on the principle of corresponding states (and the critical pressures were estimated by extrapolating the vapor pressure curves to the critical temperature).

As in the case of the normal alkylbenzenes, Ambrose's  $T_c$  and  $p_c$  data provide the most reliable information. Also useful are the data of Altschul [1893-alt] and of Guye and Mallet [01-guy/mal; 02-guy/mal], because they are the only data available for isobutylbenzene and 1,2,4,5-tetramethylbenzene, respectively.

**(1–3) Xylenes.** The values in Table 1 for  $T_c$  and  $p_c$  for all three xylenes are based on the results of Ambrose et al. [57-amb/gra; 67-amb/bro; 87-amb], while the  $\rho_c$  values are the averages of Simon's [57-sim] results and those of

Akhundov et al. [68-akh/asa; 70-akh/ima]. In the case of *p*-xylene, Ambrose's  $T_c$  is supported by the value of Powell et al. [70-pow/swi]. On the other hand, the critical pressures of Mamedov et al. [70-mam/akh], possibly at critical temperatures taken from the literature (see earlier discussion of toluene data from [69-akh/abd]), are significantly higher than Ambrose's results. Richardson and Rowlinson [59-ric/row] observed a lower  $T_c$  for *o*-xylene, which was lower still in the presence of trace or excess mercury (see Table 2). The uncertainty given in Table 1 for *o*- and *m*-xylene reflects the difference between the  $T_c$  values for *m*-xylene in 57-amb/gra and 67-amb/bro. Lower uncertainties are given for *p*-xylene, which is easier to prepare in a pure state than the other two xylenes.

**(4–8)  $C_9$  Alkylbenzenes.** Ambrose's [57-amb/gra; 60-amb/cox; 67-amb/bro] measurements once again establish the  $T_c$  and  $p_c$ , but no experimental  $\rho_c$  data are available. For the three trimethylbenzenes, we also have the  $T_c$  and  $p_c$  data of Kay and Pak [80-kay/pak]. Powell's [70-pow/swi]  $T_c$  for 1,3,5-trimethylbenzene agrees very well with Ambrose's values, but Kay's  $T_c$  values are 1.2–1.4 K higher than Ambrose's.

Kay and Pak [80-kay/pak] made determinations with both gallium and mercury for 1,2,4-trimethylbenzene (they report two slightly different  $p_c$  values with mercury) and examined the effect of the temperature of the mercury-to-hydrocarbon interface: the results with the interface at room temperature, especially for  $p_c$ , were preferable to those with it at the sample temperature.

Daubert and his students used a Kay-type visual apparatus to measure the critical temperature and pressure of 1-methyl-4-ethylbenzene (*p*-ethyltoluene). Lyons [85-lyo] made his measurements on a sample that was only 98% pure. Later work by Daubert et al. [87-dau/jal] on the same sample confirmed the  $T_c$  of Lyons but determined a slightly higher  $p_c$ . Because of the low purity of the sample, the uncertainty for  $T_c$  was assumed to be twice that given by Daubert et al., while the uncertainty for  $p_c$  was raised to make it consistent with that for  $T_c$ .

**(9–12)  $C_{10}$  Alkylbenzenes.** The only modern data have been reported by Ambrose et al. [60-amb/cox; 67-amb/bro] for 1,4-diethylbenzene, which had originally been reported mistakenly as isobutylbenzene. For the other isomers, the recommended values should be used with caution, although Altschul's [1893-alt] data for isobutylbenzene and those of Guye and Mallet [01-guy/mal; 02-guy/mal] for 1,2,4,5-tetramethylbenzene may be of relatively good quality, if it can be assumed that the measurements were made on reasonably pure samples.

Altschul [1893-alt] and Brown [06-bro] reported values for cymene. The latter author also reported values of critical temperature for a number of alkanols, acids, and esters in addition to the aromatics given in Table 2. For all of the compounds that other investigators have studied (i.e., all except the esters), Brown's values have been found to be too high. The difference for the three xylenes and 1,3,5-trimethylbenzene in Table 2 exceeds 5 K. We therefore recommend Altschul's value for the critical temperature together with his (rounded) value for the critical pressure. As was noted by Kobe and Lynn [53-kob/lyn], neither Altschul nor Brown stated which isomer was investigated, but the reason would have been that at that time cymol (in German) or cymene was the name normally used for the para isomer, which is a natural product occurring, for example, in oil of eucalyptus.

**(13) Hexamethylbenzene.** The rapid decomposition of the sample did not allow Guye and Mallet [02-guy/mal] to make an accurate determination. Ambrose et al. [74-amb/



bro] determined a value for  $T_c$  but could not measure  $p_c$  because hexamethylbenzene was "markedly unstable" at its critical temperature (2 K/h rise).

### (C) Polyphenyls

Experimental critical constants are known for the following polyphenyls: (1) diphenylmethane; (2) biphenyl; (3) *o*-terphenyl (1,2-diphenylbenzene); (4) *m*-terphenyl (1,3-diphenylbenzene); (5) *p*-terphenyl (1,4-diphenylbenzene). Only biphenyl has been investigated extensively. It is also the only polyphenyl that is stable at its critical point. In addition, Nikitin et al. [93-nik/pav] investigated a mixture of isomers of dicumylmethane.

**(1) Diphenylmethane.** Steele [92-ste] determined  $T_c = 760$  K with a DSC technique and  $\rho_c = 0.2994$  gcm<sup>-3</sup> with the rectilinear diameter method; see 89-chi/kni for details on this approach. Steele's  $T_c$  is preferred over Smith's [85-smi] measurement with a sealed ampule method, which was reported only in his thesis. Extrapolation of the vapor pressure data of Wiczorek and Kobayashi [80-wie/kob] and Wilson et al. [81-wil/joh] to 760 K gave  $p_c = 2.71$  MPa.

**(2) Biphenyl.** Chirico et al. [89-chi/kni] determined  $T_c$  with a DSC technique,  $\rho_c$  with the rectilinear diameter method, and  $p_c$  by extrapolating available vapor pressure data. The latter may be the least certain result, but Chirico's values, which are supported by the measurements of Ellard and Yanko [63-ell/yan], are the recommended critical constants for biphenyl (with larger uncertainties than those given by Chirico et al.). Reiter's [63-rei] results are also in reasonable agreement with the selected values. On the other hand, the  $T_c$  and  $p_c$  of Mandel and Ewbank [60-man/ewb] are significantly higher than the selected values.

No critical properties could be found in Carnelley [1880-car], who is credited by Kudchadker et al. [68-kud/ala] with measuring the  $T_c$  of biphenyl.

**(3-5) Terphenyls.** Reiter [63-rei] used the meniscus disappearance method to determine the critical temperature of the three terphenyls. Reiter analyzed the terphenyl (and biphenyl) samples after the measurements and found their purities to be 97.0% for *o*-terphenyl, 83.3% for *m*-terphenyl, and 65.2% for *p*-terphenyl (and 100% for biphenyl). The major impurities were quaterphenyls and quinquephenyls. Reiter corrected the measured critical temperatures for the presence of all other components. He then estimated the critical pressures by extrapolating available vapor pressure data to  $T_c$  and the critical density by use of the law of the rectilinear diameter. Reiter estimated the error in  $p_c$  to be 20% and in  $\rho_c$  5%. The latter estimate may be too optimistic, because the vapor density was based on the ideal gas law (up to the normal boiling point).

The results of Reiter [63-rei] are recommended over those of Mandel and Ewbank [60-man/ewb], who claimed  $\pm 2\%$  uncertainty for *o*-terphenyl and  $\pm 3-4\%$  for *m*- and *p*-terphenyl. Ellard and Yanko [63-ell/yan] could not determine the critical constants of the terphenyls (because of their rapid decomposition), but their  $P-V-T$  measurements for *o*- and *m*-terphenyl supported Reiter's results.

Nikitin et al. [93-nik/pav] measured the critical temperature and pressure of a mixture of isomers of dicumylmethane [bis(1-methylethyl)phenyl]methane with a method in which the time of attainment of the critical temperature is from  $10^{-5}$  to  $3 \times 10^{-3}$  s. This method is based on measuring the temperature of the attainable superheat by means of a thin wire probe that is heated with electric current pulses. With increasing pressure, the temperature of the attainable superheat tends to the critical temperature.

Nikitin et al. tested their method with stable substances (pentane, hexane, heptane, and water) and found that they were underestimating the  $T_c$  by 1% and the  $p_c$  by 1-4%. Their measurements on a mixture of isomers of dicumylmethane, which was thermally stable at times less than  $10^{-3}$  s (but decomposes above 630 K in longer time exposure), resulted in the following values:  $T_c = 795$  K and  $p_c = 1.55$  MPa. These values are not included in Tables 1 and 2 because the sample used by Nikitin et al. was a mixture of isomers whose boiling point was from 608 to 618 K. The purity of the main substance was 98 mass % (method of determination not stated). The authors did not make clear if the main substance was the mixture of isomers, but that is inferred from the boiling point range.

### (D) Condensed Polycyclics

Experimental critical constants have been reported for the following seven condensed polycyclic hydrocarbons: (1) indan; (2) naphthalene; (3) 1-methylnaphthalene; (4) 2-methylnaphthalene; (5) 2,7-dimethylnaphthalene; (6) phenanthrene; (7) tetralin (1,2,3,4-tetrahydronaphthalene). In addition, Chirico et al. [93-chi/kni] estimated the critical constants of two partially hydrogenated pyrenes with equations based on the principle of corresponding states.

Naphthalene is very stable and can easily be purified. Its critical constants have been measured by several investigators, including Ambrose et al. [60-amb/cox; 67-amb/bro]. Ambrose's  $T_c$  and  $p_c$  are recommended, although the more recent investigation of Kay and Pak [80-kay/pak] has produced a  $T_c$  that is 1.1 K higher than Ambrose's. A similar discrepancy was noted earlier for the three trimethylbenzenes. Zhuravlev's [37-zhu]  $\rho_c$  has apparently been confirmed by the measurements of Schröer [41-sch] and Cheng [63-che]. The recommended value was calculated at the selected  $T_c$  with Zhuravlev's rectilinear diameter equation. Chirico et al. [93-chi/kni-1] determined the critical temperature of naphthalene and 2,7-dimethylnaphthalene with a DSC technique. Graphical fitting of density data in the critical region also made it possible to derive the critical densities:

	$T_c$ /K	$\rho_c$ /kgm <sup>-3</sup>
naphthalene	749 $\pm$ 1	310 $\pm$ 15
2,7-dimethylnaphthalene	775 $\pm$ 2	255 $\pm$ 30

The critical density for 2,7-dimethylnaphthalene was very much lower than that derived by fitting saturated liquid density data with the Riedel equation (296.5 kgm<sup>-3</sup>), and this difference was attributed to decomposition near  $T_c$ .

Chirico et al. [93-chi/kni-1] also derived the critical pressure by fitting their vapor pressure data (up to 539 K for naphthalene and 586 K for 2,7-dimethylnaphthalene) with the Wagner equation. In the fitting procedure, Chirico et al. used Ambrose's [60-amb/cox; 67-amb/bro]  $T_c$  of 748.4 K for naphthalene. However, the calculated  $p_c$ , 4.105 MPa, was slightly higher than Ambrose's (4.051 MPa). Finally, fitting of the saturated liquid density (from 373 to 548 K) with the Riedel equation resulted in a critical density for naphthalene of 320.0 kgm<sup>-3</sup> (and the previously mentioned value of 296.5 kgm<sup>-3</sup> for 2,7-dimethylnaphthalene).

For the unstable 1- and 2-methylnaphthalenes, we recommend the  $T_c$  values of Ambrose [60-amb/cox; 63-amb]. Wilson et al. [81-wil/joh] measured the vapor pressure of 1-methylnaphthalene up to 900 °F (755.4 K): 439 psia (3.027 MPa). Extrapolation of these data to Ambrose's  $T_c$  (772 K) gives  $p_c = 3.60$  MPa, which is our recommended value. Considering the 1 K uncertainty in  $T_c$ , the uncertainty in  $p_c$  should be about 0.1 MPa (3 times the uncertainty in the experimental vapor pressures).

Cheng [63-che] determined the  $T_c$  of phenanthrene by extrapolating data on benzene + phenanthrene mixtures with only up to 30 mol % phenanthrene. Another source of uncertainty is phenanthrene's instability at its critical temperature. (The temperature of meniscus disappearance rose with time for mixtures with more than 15 mol % phenanthrene.) Cheng also calculated the  $T_c$  of anthracene (873 K) by assuming that its  $T_b/T_c$  is equal to that of phenanthrene and the  $\rho_c$  of both phenanthrene and anthracene (he estimated them with Lydersen's method).

The critical properties of tetralin, which is unstable at its critical point, had not been measured until recently. Steele et al. [88-ste/chi] determined the  $T_c$  with a DSC technique, the  $\rho_c$  by fitting a corresponding-states equation to their own density data, and the  $p_c$  by extrapolating their vapor pressure data. More reliable are believed to be the results for  $\rho_c$  and  $p_c$  from Teja's group with a sealed ampule method [90-tej/ans-1] and a flow method [91-gud/tej]. Gude and Teja [91-gud/tej] recommended the value  $T_c = 719.6$  K, but  $(720 \pm 1)$  K is a more reasonable average of all three results:  $(721 \pm 1)$  K [88-ste/chi];  $(719.9 \pm 1.0)$  K [90-tej/ans-1];  $(719.5 \pm 0.4)$  K [91-gud/tej].

**Tetrahydro- and Hexahdropyrene.** Chirico et al. [93-chi/kni] made extensive thermodynamic property measurements on THP (4,5,9,10-tetrahydropyrene) and HHP (1,2,3,6,7,8-hexahdropyrene). Their vapor pressure measurements extended up to 659.5 (THP) and 639.0 K (HHP), where some sample decomposition was noted. They also measured the two-phase heat capacities up to 700 K and the saturated liquid densities from 423.15 to 523.15 K.

Chirico et al. estimated the critical temperatures by using equations based on the corresponding-states principle to fit simultaneously the vapor pressure and two-phase heat capacity data for a range of fixed  $T_c$  values with  $p_c$  included as a variable. Then with the selected  $T_c$  values, they estimated critical densities by fitting their density data to Riedel's equation, following the example of Hales and Townsend [72-hal/tow]. The resulting estimated critical constants, which are not included in Tables 1 and 2, are

	$T_c$ /K	$p_c$ /kPa	$\rho_c$ /kgm <sup>-3</sup>
THP	900	3000	324.3
HHP	920	3610	313.7

Although Chirico et al. estimate the uncertainty in  $T_c$  to be  $\pm 5$  K (and give no uncertainties for  $p_c$  and  $\rho_c$ ), it may be more realistic to assume an uncertainty of  $\pm 20$  K. The uncertainty in  $p_c$  may exceed 20%, especially if we consider that HHP should probably have a lower  $p_c$  (and  $T_c$ ) than the less hydrogenated THP. Compare the values given here for naphthalene and tetralin with those for *cis*-decalin [72-pak/kay]: 705.0 K and 3.21 MPa.

The corresponding-states correlations Chirico et al. used should not be expected to provide an exact fit of the properties of THP and HHP. More extensive investigation, along the lines suggested by Chirico et al., is warranted to determine whether the simultaneous fitting of vapor pressure and two-phase heat capacity data can actually lead to reliable estimates of  $T_c$  and  $p_c$ .

### Overview of the Recommendations (Table 1)

Table 1 summarizes the recommended critical values given in Table 2. It also includes, where appropriate, the critical volume,  $V_c$ , and the critical compressibility factor,  $Z_c = p_c V_c / RT_c$  ( $R = 8.31451$  Pa·m<sup>3</sup>·mol<sup>-1</sup>·K<sup>-1</sup>).  $Z_c$  is remarkably invariant for the five normal alkylbenzenes, the three xylenes, biphenyl, and naphthalene (0.259–0.268); this would also be true of 2,7-dimethylnaphthalene,

if the  $\rho_c$  value calculated with the Riedel equation is used in place of the experimental result. On the other hand, the  $Z_c$  for *o*- and *p*-terphenyl is most likely too high. This is probably due to a much too high critical pressure. An analysis of the vapor pressure data for the terphenyls may resolve this question.

### Acknowledgment

This work is a product of the IUPAC Commission I.2 on Thermodynamics, Subcommittee on Thermodynamic Data, critical properties group, under the leadership of C. L. Young (University of Melbourne, Melbourne, Australia). The following members commented on the preliminary draft of the paper: K. M. de Reuck (Imperial College, London, England), J. H. Dymond (University of Glasgow, Glasgow, Scotland), and C. L. Young. C.T. is grateful to Exxon Research and Engineering Co. for permission to publish this paper.

**Registry No. Supplied by the Author:** Benzene, 71-43-2; toluene, 108-88-3; ethylbenzene, 100-41-4; propylbenzene, 103-65-1; butylbenzene, 104-51-8; 1,2-dimethylbenzene, 95-47-6; 1,3-dimethylbenzene, 108-38-3; 1,4-dimethylbenzene, 106-42-3; (1-methylethyl)benzene, 98-82-8; 1,2,3-trimethylbenzene, 526-73-8; 1,2,4-trimethylbenzene, 95-63-6; 1,3,5-trimethylbenzene, 108-67-8; 1-methyl-4-ethylbenzene, 622-96-8; (2-methylpropyl)benzene, 538-93-2; 1-methyl-4-(1-methylethyl)benzene, 99-87-6; 1,4-diethylbenzene, 105-05-5; 1,2,4,5-tetramethylbenzene, 95-93-2; hexamethylbenzene, 87-85-4; diphenylmethane, 101-81-5; biphenyl, 92-52-4; 1,2-diphenylbenzene, 84-15-1; 1,3-diphenylbenzene, 92-06-8; 1,4-diphenylbenzene, 92-94-4; indan, 496-11-7; naphthalene, 91-20-3; 1-methylnaphthalene, 90-12-0; 2-methylnaphthalene, 91-57-6; 2,7-dimethylnaphthalene, 582-16-1; phenanthrene, 85-01-8; 1,2,3,4-tetrahydronaphthalene, 119-64-2.

### Literature Cited

- 1878-saj Sajotschewsky, W. *Kiewer Univ. Unters.* **1878**, No. 4 and 8; abstract in *Beibl.* **1879**, 3, 741 (benzene); see *Landolt-Börnstein* [23-lan/boe].
- 1880-car Carnelley, T. J. *Chem. Soc.* **1880**, 37, 701–720.
- 1881-ram Ramsay, W. *Proc. R. Soc. London* **1881**, 31, 194–205 (benzene).
- 1883-paw Pawlewski, B. *Ber. Dtsch. Chem. Ges.* **1883**, 16, 2633–2636 (toluene).
- 1889-you Young, S. J. *Chem. Soc.* **1889**, 55, 486–521 (benzene).
- 1891-sch Schmidt, G. C. *Justus Liebigs Ann. Chem.* **1891**, 266, 266–292 (benzene).
- 1893-alt Altschul, M. Z. *Phys. Chem.* **1893**, 11, 577–597 (benzene, toluene, ethylbenzene, propylbenzene, *o*-xylene, *m*-xylene, *p*-xylene, isopropylbenzene, 1,2,4-trimethylbenzene, 1,3,5-trimethylbenzene, isobutylbenzene, *p*-cymene).
- 1899-rad Radice, G. (benzene, diphenylmethane); see *Landolt-Börnstein* [23-lan/boe]; complete results on p 40 of Guye and Mallet [02-guy/mal].
- 01-guy/mal Guye, P. A.; Mallet, E. *Compt. Rend.* **1901**, 133, 1287–1290 (1,2,4,5-tetramethylbenzene, diphenylmethane, biphenyl, naphthalene).
- 02-guy/mal Guye, P. A.; Mallet, E. *Arch. Sci. Phys. Nat.* **1902**, 13, 30–40, 129–143, 274–296, 462–489 (1,2,4,5-tetramethylbenzene, hexamethylbenzene, diphenylmethane, biphenyl, naphthalene).
- 04-mat Mathias, E. *Le Point Critique des Corps Pure*; C. Naud: Paris, 1904.
- 06-bro Brown, J. C. J. *Chem. Soc.* **1906**, 89, 311–315 (*o*-xylene, *m*-xylene, *p*-xylene, 1,3,5-trimethylbenzene, *p*-cymene).
- 08-sch Schamhardt (benzene); see *Landolt-Börnstein* [23-lan/boe].

- 10-you Young, S. *Sci. Proc. R. Dublin Soc.* **1909-10**, 12, 374-443 (benzene).
- 13-ano Société Française de Physique. Recueil des constantes physiques, 1913 (hexamethylbenzene); ref 10 in 53-kob/lyn.
- 20-pru Prud'homme, M. *J. Chim. Phys.* **1920**, 18, 94-102.
- 23-lan/boe *Landolt-Börnstein. Physikalisch-Chemische Tabellen*, 5th ed.; Springer: Berlin, 1923; pp 253-266 (review); 3rd suppl. 1936; p 2545 (benzene).
- 30-cor Cork, J. M. *Rev. Sci. Instrum.* **1930**, 1, 563-568 (biphenyl).
- 30-kra/goo Krase, N. W.; Goodman, J. B. *Ind. Eng. Chem.* **1930**, 22, 13 (tolene).
- 35-har Harand, J. *Monatsh. Chem.* **1935**, 65, 153-184 (benzene, toluene).
- 37-zhu Zhuravlev, D. I. *Zh. Fiz. Khim.* **1937**, 9, 875-882 (naphthalene).
- 41-ano Esso Laboratories, 1941 (benzene); quoted in 47-gor/ami.
- 41-sch Schröer, E. *Z. Phys. Chem. B.* **1941**, 49, 271-278 (naphthalene).
- 43-fis/rei Fischer, R.; Reichel, T. *Mikrochemie* **1943**, 31, 102-108 (benzene, toluene, *o*-xylene, *p*-xylene).
- 47-gor/ami Gornowski, E. J.; Amick, E. H., Jr.; Hixson, A. N. *Ind. Eng. Chem.* **1947**, 39, 1348-1352 (benzene).
- 52-ben/fur Bender, P.; Furukawa, G. T.; Hyndman, J. R. *Ind. Eng. Chem.* **1952**, 44, 387-390 (benzene).
- 52-kay/nev Kay, W. B.; Nevens, T. D. *Chem. Eng. Prog. Symp. Ser.* **1952**, 48 (3), 108-114 (benzene).
- 53-kob/lyn Kobe, K. A.; Lynn, R. E., Jr. *Chem. Rev.* **1953**, 52, 117-236 (review).
- 55-kre Kreglewski, A. *Rocz. Chem.* **1955**, 29, 754-762 (benzene).
- 55-old Oldenburg, G. *Erdoel Kohle* **1955**, 8, 445-449.
- 57-amb/gra Ambrose, D.; Grant, D. G. *Trans. Faraday Soc.* **1957**, 53, 771-778 (benzene, toluene, *o*-xylene, *m*-xylene, *p*-xylene, isopropylbenzene).
- 57-fra Francis, A. W. *Ind. Eng. Chem.* **1957**, 49, 1787-1788 (*o*-, *m*-, *p*-xylene).
- 57-gla/rue Glaser, F.; Rüländ, H. *Chem.-Ing.-Tech.* **1957**, 29, 772-775 (*o*-, *m*-, *p*-xylene, 1,2,4-trimethylbenzene, biphenyl).
- 57-kri/kha Krichevskii, I. R.; Khazanova, N. E.; Linshits, L. R. *Zh. Fiz. Khim.* **1957**, 31, 2711-2716 (benzene).
- 57-sim Simon, M. *Bull. Soc. Chim. Belg.* **1957**, 66, 375-381 (benzene, toluene, ethylbenzene, propylbenzene, butylbenzene, *o*-xylene, *m*-xylene, *p*-xylene).
- 59-ric/row Richardson, M. J.; Rowlinson, J. S. *Trans. Faraday Soc.* **1959**, 55, 1333-1337 (*o*-xylene).
- 60-amb/cox Ambrose, D.; Cox, J. D.; Townsend, R. *Trans. Faraday Soc.* **1960**, 56, 1452-1459 (benzene, toluene, ethylbenzene, propylbenzene, butylbenzene, 1,2,3-trimethylbenzene, 1,2,4-trimethylbenzene, 1,3,5-trimethylbenzene, isobutylbenzene (corrected to 1,4-diethylbenzene), naphthalene, 1-methylnaphthalene).
- 60-man/ewb Mandel, H.; Ewbank, N. Critical Constants of Diphenyl and the Terphenyls. NAA-SR-5129, 1960 (biphenyl, *o*-, *m*-, *p*-terphenyl).
- 60-mcc/sto McCracken, P. G.; Storvick, T. S.; Smith, J. M. *J. Chem. Eng. Data* **1960**, 5, 130-132 (benzene).
- 60-par/row Partington, E. J.; Rowlinson, J. S.; Weston, J. F. *Trans. Faraday Soc.* **1960**, 56, 479-485 (benzene, toluene).
- 62-che/mcc Cheng, D. C-H.; McCoubrey, J. C.; Phillips, D. G. *Trans. Faraday Soc.* **1962**, 58, 224-229 (naphthalene).
- 62-con/kan Connolly, J. F.; Kandalic, G. A. *J. Chem. Eng. Data* **1962**, 7, 137-139 (benzene).
- 63-amb Ambrose, D. *Trans. Faraday Soc.* **1963**, 59, 1988-1993 (1-methylnaphthalene, 2-methylnaphthalene).
- 63-amb/tow Ambrose, D.; Townsend, R. *J. Chem. Soc.* **1963**, 3614-3625 (benzene).
- 63-che Cheng, D. C-H. *Chem. Eng. Sci.* **1963**, 18, 715-724 (benzene, naphthalene, phenanthrene).
- 63-ell/yan Ellard, J. A.; Yanko, W. H. Thermodynamic Properties of Biphenyl and the Isomeric Terphenyls. US AEC IDO-11008, 1963 (biphenyl).
- 63-rei Reiter, F. W. Kritische Daten von Diphenyl und den Terphenylisomeren. EUR 302 d, 1963 (biphenyl, *o*-, *m*-, and *p*-terphenyl).
- 64-mak/noz Makhan'ko, I. G.; Nozdrev, V. F. *Sov. Phys. Acoust.* **1964**, 10, 207-208 (benzene).
- 64-ska/kay Skaates, J. M.; Kay, W. B. *Chem. Eng. Sci.* **1964**, 19, 431-444 (benzene).
- 67-amb/bro Ambrose, D.; Broderick, B. E.; Townsend, R. *J. Chem. Soc. A* **1967**, 633-641 (benzene, toluene, ethylbenzene, propylbenzene, butylbenzene, *o*-xylene, *m*-xylene, *p*-xylene, isopropylbenzene, 1,2,3-trimethylbenzene, 1,2,4-trimethylbenzene, 1,3,5-trimethylbenzene, 1,4-diethylbenzene, naphthalene).
- 68-akh/asa Akhundov, T. S.; Asadullaeva, N. N. *Izv. Vyssh. Uchebn. Zaved., Neft Gaz* **1968**, 11 (6), 83-86 (*m*-xylene).
- 68-cam/cha Campbell, A. N.; Chatterjee, R. M. *Can. J. Chem.* **1968**, 46, 575-581 (benzene).
- 68-kud/ala Kudchadker, A. P.; Alani, G. H.; Zwolinski, B. J. *Chem. Rev.* **1968**, 68, 659-735 (review).
- 69-akh/abd Akhundov, T. S.; Abdullaev, F. G. *Izv. Vyssh. Uchebn. Zaved., Neft Gaz* **1969**, 12 (9), 44-48 (toluene).
- 69-cam/cha Campbell, A. N.; Chatterjee, R. M. *Can. J. Chem.* **1969**, 47, 3893-3898 (benzene).
- 70-akh/ima Akhundov, T. S.; Imanov, Sh. Yu. *Teplofiz. Svoistva Zhidk.* **1970**, 48-55 (*o*-, *p*-xylene).
- 70-art/shi Artyukhovskaya, L. M.; Shimanskaya, E. T.; Shimanskii, Yu. I. *Ukr. Fiz. Zh. (Russ. Ed.)* **1970**, 15, 1974-1981 (benzene).
- 70-cam/mus Campbell, A. N.; Musbally, G. M. *Can. J. Chem.* **1970**, 48, 3173-3184 (benzene).
- 70-kob/mat Kobe, K. A.; Mathews, J. F. *J. Chem. Eng. Data* **1970**, 15, 182-186 (benzene).
- 70-mam/akh Mamedov, A. M.; Akhundov, T. S.; Imanov, Sh. Yu. *Russ. J. Phys. Chem.* **1970**, 44, 877-878 (*o*-, *p*-xylene).
- 70-pow/swi Powell, R. J.; Swinton, F. L.; Young, C. L. *J. Chem. Thermodyn.* **1970**, 2, 105-115 (toluene, *p*-xylene, 1,3,5-trimethylbenzene).
- 72-hal/tow Hales, J. L.; Townsend, R. *J. Chem. Thermodyn.* **1972**, 4, 763-772.
- 72-pak/kay Pak, S. C.; Kay, W. B. *Ind. Eng. Chem. Fundam.* **1972**, 11, 255-267 (benzene, ethylbenzene, *o*-xylene).
- 72-rae/str Rätzsch, M. T.; Strauch, G. Z. *Phys. Chem. (Leipzig)* **1972**, 243-252 (benzene, toluene, ethylbenzene).
- 74-amb/bro Ambrose, D.; Broderick, B. E.; Townsend, R. *J. Appl. Chem. Biotechnol.* **1974**, 24, 359-372 (hexamethylbenzene, indan).
- 77-akh/abd Akhundov, T. S.; Abdullaev, F. G. *Izv. Vyssh. Uchebn. Zaved., Neft Gaz* **1977**, 20 (2), 73-77 (benzene).
- 80-kay/pak Kay, W. B.; Pak, S. C. *J. Chem. Thermodyn.* **1980**, 12, 673-681 (1,2,3-trimethylbenzene, 1,2,4-trimethylbenzene, 1,3,5-trimethylbenzene, naphthalene).
- 80-wie/kob Wieczorek, S. A.; Kobayashi, R. *J. Chem. Eng. Data* **1980**, 25, 302-305 (diphenylmethane).
- 81-ewi/mcg Ewing, M. B.; McGlashan, M. L.; Tzias, P. *J. Chem. Thermodyn.* **1981**, 13, 527-535 (benzene).
- 81-hug/mcg Hugill, J. A.; McGlashan, M. L. *J. Chem. Thermodyn.* **1981**, 13, 429-436 (benzene).
- 81-wil/joh Wilson, G. M.; Johnston, R. H.; Hwang, S.-C.; Tsonopoulos, C. *Ind. Eng. Chem. Process Des. Dev.* **1981**, 20, 94-104 (diphenylmethane, 1-methylnaphthalene).
- 83-hal/gun Hales, J. L.; Gundry, H. A. *J. Phys. E.: Sci. Instrum.* **1983**, 16, 91-95 (benzene).
- 83-kay/kre Kay, W. B.; Kreglewski, A. *Fluid Phase Equilib.* **1983**, 11, 251-265 (benzene).

- 85-lyo Lyons, R. L. M.S. Thesis, The Pennsylvania State University, 1985 (1-methyl-4-ethylbenzene).
- 85-smi Smith, R. L., Jr. Ph.D. Thesis, Georgia Institute of Technology, 1985 (diphenylmethane).
- 87-amb Ambrose, D. *J. Chem. Thermodyn.* **1987**, *19*, 1007–1008 (benzene, toluene, ethylbenzene, *o*-, *m*-, *p*-xylene).
- 87-dau/jal Daubert, T. E.; Jalowka, J. W.; Goren, V. *AIChE Symp. Ser.* **1987**, *83* (No. 256), 128–156 (1-methyl-4-ethylbenzene).
- 88-bru Brunner, E. *J. Chem. Thermodyn.* **1988**, *20*, 1397–1409 (benzene).
- 88-goo Goodwin, R. D. *J. Phys. Chem. Ref. Data* **1988**, *17*, 1541–1636 (benzene).
- 88-ste/chi Steele, W. V.; Chirico, R. D.; Knipmeyer, S. E.; Smith, N. K. High-Temperature Heat-Capacity Measurements Using a DSC. NIPER-395, Nov 1988 (toluene, tetralin).
- 89-chi/kni Chirico, R. D.; Knipmeyer, S. E.; Nguyen, A.; Steele, W. V. *J. Chem. Thermodyn.* **1989**, *21*, 1307–1331 (biphenyl).
- 89-goo Goodwin, R. D. *J. Phys. Chem. Ref. Data* **1989**, *18*, 1565–1636 (toluene).
- 89-kni/arc Knipmeyer, S. E.; Archer, D. G.; Chirico, R. D.; Gammon, B. E.; Hossenlopp, I. A.; Nguyen, A.; Smith, N. K.; Steele, W. V.; Strube, M. M. *Fluid Phase Equilib.* **1989**, *52*, 185–192 (benzene).
- 90-tej/ans Teja, A. S.; Anselme, M. J. *AIChE Symp. Ser.* **1990**, *86* (No. 279), 115–121 (toluene).
- 90-tej/ans-1 Teja, A. S.; Anselme, M. J. *AIChE Symp. Ser.* **1990**, *86* (No. 279), 122–127 (tetralin).
- 90-tej/ros Teja, A. S.; Rosenthal, D. J. *AIChE Symp. Ser.* **1990**, *86* (No. 279), 133–137 (toluene).
- 91-gud/tej Gude, M. T.; Teja, A. S. DIPPR Project 851: Final Report for 1990; 1991 (tetralin).
- 92-ste Steele, W. V. Private communication, 1992 (diphenylmethane).
- 93-chi/kni Chirico, R. D.; Knipmeyer, S. E.; Nguyen, A.; Smith, N. K.; Steele, W. V. *J. Chem. Thermodyn.* **1993**, *25*, 729–761.
- 93-chi/kni-1 Chirico, R. D.; Knipmeyer, S. E.; Nguyen, A.; Steele, W. V. *J. Chem. Thermodyn.* **1993**, *25*, 1461–1494 (naphthalene, 2,7-dimethylnaphthalene).
- 93-nik/pav Nikitin, E. D.; Pavlov, P. A.; Skripov, P. V. *J. Chem. Thermodyn.* **1993**, *25*, 869–880.
- 94-chi/ste Chirico, R. D.; Steele, W. V. *Ind. Eng. Chem. Res.* **1994**, *33*, 157–167 (benzene, toluene).
- 95-amb/tso Ambrose, D.; Tsonopoulos, C. *J. Chem. Eng. Data* **1995**, *40*, 531–546.
- 95-amb/you Ambrose, D.; Young, C. L. *J. Chem. Eng. Data* **1995**, *40*, 345–360.

Received for review March 14, 1994. Revised November 9, 1994.  
Accepted December 18, 1994.\*

JE940043T

\* Abstract published in *Advance ACS Abstracts*, February 15, 1995.