

PROPERTIES OF ALKYL BENZENES¹

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This paper includes a tabular compilation of the physical properties of all alkylbenzenes described in the literature through 1947, so far as found by the author, together with a critical review of the evidence for identity in several doubtful cases. Tentative identification is suggested for some new hydrocarbons.

Approximate functions of structure in simple form have been found for the properties as follows:

$$d_4^{20} = 0.850 + (0.12/n)(1 + a + b)$$

$$d_4^{20} - 0.854 = 27(n_D^{20} - 1.475)^2$$

$$\text{B.p.} = 18n + 21 - 1800/n^2 \quad (\text{for } n\text{-alkylbenzenes})$$

(similar equations for boiling points of other alkylbenzenes)

$$\text{M.p.} = 19n - 0.3n^2 - 247$$

(for normal and three other classes of alkylbenzenes)

The letter n in the equations is the number of carbon atoms; a is the number of pairs of adjacent alkyl groups; b is 1 for mono-*tert*-alkylbenzenes, and 0 for all other aromatics.

These relations have been used to calculate the properties of most of the alkyl benzenes listed. The calculations of properties not observed are included in the table; and observations differing substantially from the calculations are questioned. Correlations with the observations are shown graphically and discussed.

I. INTRODUCTION

Monocyclic aromatics with saturated side chains, or alkylbenzenes, constitute one of the most important classes of hydrocarbons. This is also one of the largest classes, the number of known members exceeding the known paraffins by over one hundred. This review contains a concise list of 379 alkylbenzenes, with observed properties which are recorded in the literature. It also includes a critical discussion of the evidence for structure in about eighty doubtful cases and, in addition, simple but comprehensive correlations of the properties of all members of this class of hydrocarbons.

Two general compilations of such physical properties have been made in addition to Beilstein (30) (which lists only 175 alkylbenzenes in all three volumes) and others with less than 100 alkylbenzenes (7, 8, 231, 353, 382). Doss (87) selected a single observation for each value, but since the latest edition is four years old, it omits 117 alkylbenzenes which can now be included. Egloff's compilation (95) is more recent and lists several observations on each property when available, but many of the best observations were restricted during the war and so could not be published. About 112 alkylbenzenes now described in the literature are not included in that list. Moreover, for 58 other alkylbenzenes which are listed

¹ The portion of this paper which deals with the calculation of physical properties, together with the graphs, was presented before the Division of Petroleum Chemistry at the 112th Meeting of the American Chemical Society, New York City, September, 1947.

in Egloff's compilation, observed values for one or more additional properties are now available.

Many of the published observations, sometimes the only one on a certain hydrocarbon, are "casual observations", that is, made on impure material, or material of uncertain structure, or, in the case of boiling points, without stem correction or barometer reading. This does not mean careless work, since the investigator was not determining physical properties, and the hydrocarbon may have been an incidental by-product in which he had little interest. For many alkylbenzenes an assumption of an average value of 0.86 for density and 1.49 for refractive index would be less in error than to use the published observations. For example, the *lowest* of the fifteen observations on the density of isobutylbenzene included in Egloff's compilation (95) is 0.8628, although the value now accepted (8) and supported by three recent excellent observations (50, 121, 142) is only 0.8532. Similarly, the *highest* of fifteen previously recorded normal boiling-point observations for it is 171.0°C., compared with the now accepted 172.8°C. (8) (supported by 38b, 50, 121, 328). The explanation may be that most of the older observations were actually made on *tert*-butylbenzene, since they agree fairly well with good values for the latter. Schramm (308) in 1888 was clear on this point, and reported good observations for the density and boiling point of both hydrocarbons. The evidence for structure in some of the other early papers is lacking or inadequate. Even recently, observations on the densities of three alkylbenzenes not higher than C₁₃ in the *Journal of the American Chemical Society* seem to be about 9 per cent too high, judging by other observations on the same or related hydrocarbons.

Nevertheless, observations on so large a number of alkylbenzenes are available that relations are discernible, if some erratic observations are disregarded.

In order to judge the reliability of an observation or to choose between badly discrepant ones, it is desirable to have a comprehensive correlation between the properties and structures of hydrocarbons. Three papers by Corbin, Alexander, and Egloff (70, 71, 72) have already correlated the properties of the simpler types of alkylbenzenes,—namely, the 1- and 2-phenylalkanes,—and some of the dialkylbenzenes, but less than one-seventh of the total number of known alkylbenzenes are included. In a fourth paper (73) the same authors showed the relation of boiling point to pressure for some additional alkylbenzenes. Other more general but less accurate correlations for boiling point are those of Kinney (184) and Klages (200). Curves correlating the properties for certain series of alkylbenzenes were drawn by Schmidt and coworkers (302, 304, 305). Ward and Kurtz (382) have shown relationships between boiling point and other properties for the lower alkylbenzenes.

Since the more complex hydrocarbons are the less common and therefore the more in need of tests of reliability, it was felt that the correlation must be applicable to every member. It should also be as simple as possible, even though empirical. This was the attitude in the analogous correlation of all paraffin hydrocarbons (106, 107) and seems to have been justified by the results. For example, the average deviation of the calculations from the values selected by the Bureau

of Standards (6) two years later for the 35 nonanes, eleven of which were unknown at the time of the calculations, were for the boiling point 0.92°C ., for density 0.0013, and for refractive index 0.0008. Later the Bureau of Standards made calculations (358) by an independent method for all three properties, but applied it only up to the nonanes. Recently Wiener (391) developed still another method by which he calculated boiling points for paraffins up to decanes. The three methods give comparable precision except for paraffins containing two quaternary carbon atoms. The earlier method (106) seems better adapted for this type, but this also gives low values for some paraffins with five or more branches (149a). The calculations have facilitated other researches (for example, 149, 173). The former (and also citation 352, p. 68) confirmed an error of 7°C . in the observed boiling point of one nonane, which had been pointed out in the calculations (106). The present calculations for alkylbenzenes are probably less accurate than those for the paraffins, because the data on which they are based are on the average much older.

II. DESCRIPTION OF TABLE

Table 1 (see Section VIII) lists every alkylbenzene found by the author in the literature for which one or more of its observed physical properties is given. The names of some alkylbenzenes listed in Doss's (87) and Egloff's compilations are reworded or renumbered for consistency with the Bureau of Standards table (8) and usage in *Chemical Abstracts*. However, when used in the name, a phenyl group is listed first and given the smallest possible number, because it is considered the most important radical. Sometimes an alternative name is added in parentheses, which is shorter and acceptable, though less formal. A precise arrangement is used in the table to permit easy location of a hydrocarbon, or a conclusion that it is unknown. The arrangement is substantially the same as that of Beilstein (30) and of Egloff (95). Isomers are listed in order of increasing number of substituents, and of the positions of substituents in the order phenyl, methyl, ethyl, etc., and normal, secondary, iso, and tertiary. "Sec-" is used only for butyl groups (except in a few cases of uncertain structure), and "tert-" is used only for butyl and amyl groups. For these there is no ambiguity. The table includes the 18 unknown C_{11} alkylbenzenes with properties calculated by methods of this review, and also a C_{12} alkylbenzene, described in the literature, but later shown to have a structure different from that assigned. These 19 unknown hydrocarbons and benzene are not counted in the "379 alkylbenzenes" mentioned above.

Observations of the boiling point at pressures of 710–775 mm. were corrected to 760 mm. by the relation applicable to alkylbenzenes (correlated from the values of references 7 and 8):

$$dt/dp = 0.035 + 0.0001t$$

No attempt was made to convert boiling points at low pressures, although this conversion is facilitated by a recent paper (73), because the pressures given are not usually sufficiently accurate. In view of the high thermal stability of aromatic

hydrocarbons, it is unfortunate that normal boiling points were not observed in many more cases. For about 57 alkylbenzenes boiling below 300°C. the only reported boiling points are those at low pressures, which are of little value in identification.

Observations of density and refractive index at temperatures different from 20°C. were corrected to that temperature by the relations of Lipkin and Kurtz (224). Approximately the coefficients are $dd_4^{20}/dt = -0.00075$, and $dn_D^{20}/dt = -0.00045$.

The numbers of theoretically possible isomers in the first column were taken from a recent paper (109).

The properties listed for C_8 to C_{10} hydrocarbons are substantially those chosen by the A. P. I. Hydrocarbon Research Project No. 44 (7, 8), with trifling revisions for more recent publications. Only a few supporting citations are given for each hydrocarbon, since the hundreds of references available would add little in reliability to those given. For example, eighty-three citations have been found prior to 1875 for "cymene", presumably *p*-cymene, many of which agree well with the now accepted values. Wright (393) reviewed some of them, and gave boiling points of material from eight different sources. Gladstone (127) reported good values for density and refractive index for the same samples. There is a still larger number of early references on benzene, toluene, and the xylenes which are of historical interest only.

The properties listed for the alkylbenzenes containing more than ten carbon atoms are selected means when more than one observation is available for any value. The selection was made on the basis of preponderance of agreement of observations, except that in the case of melting and boiling points the higher values are given increased weight because impurities are more likely to cause low results. An error on the low side would result also from neglect of stem correction. Galle's method (117) of correcting boiling points is theoretically sound if not extremely accurate. His corrected value for hexaethylbenzene, 305°C., is higher than those of fourteen other observers, although only 1.6°C. above that of the present author (110).

In making the choices all of the observations cited by Doss (87) and by Egloff (95) were considered and checked, about 90 per cent of them by the use of the original literature, and most of the remainder by the use of abstracts. The book by Thomas (358a) and the chapter by Price (284a) proved fruitful sources of references. Over one thousand additional observations (on alkylbenzenes above C_{10}), including many too recent for those books, were found and considered. These were the source of the data on the additional hydrocarbons. Since Egloff's compilation presents hundreds of citations on the properties, it seems unnecessary to repeat them all here. However, the present bibliography is intended to be complete for observations on the properties of alkylbenzenes above C_{10} which are *not* included in Egloff's book. Two C_{10} hydrocarbons, *o*- and *m-n*-propyltoluenes, also are covered completely in this respect, since the lack of melting-point values, or of decimal points on the boiling-point selections by the Bureau of Standards (8), probably indicates that they have not, like their isomers, been given

recent accurate study. Several of Egloff's citations are repeated in order to cover the most reliable observations on each property, and also some observations not mentioned by him, although included in the citations. Page numbers show the exact location of data except in about twenty-five foreign citations which were not available (indicated by a plus sign after the page number). The abstract reference or other actual source of the data is appended for these and some other citations. Preference is given to *Chemical Abstracts*, or for the earlier papers to *British Chemical Abstracts*, unless some observation is omitted there and included in *Chemisches Zentralblatt* or other source listed. The listing of two secondary sources usually means that each contains pertinent data which are omitted from the other. The spelling of authors' names follows that of *Chemical Abstracts* (or the *British Chemical Abstracts* cumulative index), even in preference to the original spelling in foreign journals.

Question marks are applied in the table to observations far out of line with those of hydrocarbons of similar structure (more than 5°C. in boiling point or melting point, or 0.01 in density, or 0.006 in refractive index, according to the correlations of this paper), and not well established experimentally; and suggested revisions calculated below are included, enclosed in parentheses. The same notation is used also for several values for which no observation has been made. A question mark after the numerals in the name of a hydrocarbon indicates uncertainty in the positions of the groups; and one after the name shows doubt of the whole structure. A question mark after a reference number indicates similar doubt of structure in that reference.

III. DISCUSSION OF IDENTITY

Doubts of the identity of some of the hydrocarbons named in the literature have appeared in the light of other citations, or from the physical properties, or by experience in the reactions. Some of these considerations are as follows: It is generally agreed that in the Fittig and Grignard reactions the alkyl groups remain unchanged and replace the halogens of the ring. In the Friedel-Crafts reaction the resulting alkyl groups above ethyl are rarely primary except from cycloparaffins (132, 166, 324) and primary alcohols (166), and under mild conditions from primary esters or halides (166), especially those with long chains (125a, 312). They are usually secondary from straight-chain olefins and other reagents, and tertiary from reactants having a branch adjacent to the double bond or other functional group. The phenyl group frequently assumes a position different from that occupied by the functional group of the reagent (156, 371); but in the case of secondary alcohols (156) the position can be predicted with good probability by postulating a preliminary decomposition of the alcohol to olefin, followed by addition of the aromatic to one side of the double bond according to Markovnikov's rule.

The positions assumed by the alkyl groups are seldom ortho or vicinal (1,2,3- or 1,2,3,4-) in appreciable amount if it is possible for them to be further apart. The possibility of migration of alkyl groups should be considered. When two or more products are possible and two are found, the higher-melting one is probably

the more symmetrical; and the one with higher boiling point, density, or refractive index is probably the one with more pairs of adjacent alkyl groups, especially if one of the groups is methyl. Gilman and Meals (124) have discussed the evidence of identity in many cases.

Each statement in the following discussion is intended to correct an apparently inaccurate designation (indicated usually by quotation marks) of some alkylbenzene in a compendium or literature article, or to facilitate identification of a hydrocarbon whose structure was incompletely established. On the other hand, the structures assigned tentatively to some of the hydrocarbons not previously listed are admittedly rather speculative.

The possible mistaking of *tert*-butylbenzene for isobutylbenzene has been mentioned already. There is similar confusion in some of the early literature between amyl derivatives, especially normal, iso, and tertiary. The "*o*- and *m*-cymenes" of Claus and coworkers (67) probably contained *n*-propyl groups, in view of their synthesis from propyl bromide by the Fittig reaction and the high boiling point of the ortho isomer, although that of the meta isomer is low.

The dimethylethylbenzene of Anschütz and Romig (9a) must have been symmetrical rather than "1-ethyl-2,4-dimethylbenzene" (95), because it gave uvitic acid on oxidation. O'Connor and Sowa (263) made 2-phenylpentane instead of "1-phenyl-2-methylbutane" (95).

The methylbutylbenzenes of Kozak and Novak (207) had *tert*-butyl groups (as they showed) instead of normal ones (95). Similarly, Baur (25) showed that the product which Kelbe and he (180) had called "1-methyl-3-isobutylbenzene" contained a tertiary group. Since Effront (94) considered his product the same, it too can be regarded as 1-methyl-3-*tert*-butylbenzene. Apparently no isobutyltoluene has ever been made and described. The hydrocarbons called "1-methyl-4-isobutylbenzene" (87, 95) were both 1-methyl-4-*sec*-butylbenzene (237, 379). Brun (48a) gave no properties or identification for his "isobutyltoluene." Kelbe and Baur's "*p*-butyltoluene" with a "butyl group of unknown structure", boiled at 176–178°C. Since the only evidence for C₁₁H₁₆ composition was elementary analysis (the difference being slight), the low boiling point makes the substance look like *p*-cymene, as suggested by Tafel (355) and by Noelting (257). For "metaethylpropylbenzene" (288) there is no evidence for the structure assigned to the alkyl groups. Since the propyl groups in Renard's other products were iso, this one too was probably secondary. It might even be 1-methyl-3-*sec*-butylbenzene, but in either case the assigned structure would be unknown.

The evidence of Claus and Eller (66) for the structure of their "isoamylbenzene" is good except for the elementary analysis, which is far too low in hydrogen, as noted by Bygden (56). On the other hand, the isoamylbenzenes of Menshutkin (236) and Stratford (350) probably had that structure rather than "2-phenylpentane" (95). The "trimethylethylbenzene" described by Glattfeld and Milligan (130) was not "1-phenyl-2,2-dimethylpropane" (95) but 2-phenyl-3-methylbutane.

Tilicheev (359) made it clear that almost all of the alkylbenzenes described by him (360) and by him and Kuruindin (361) were secondary (2-phenylalkanes); but

most of them have been listed in one or more compilations (95, 302, 304) as "normal alkylbenzenes" and even the abstracts are not definite. Brochet (47) and Khardin (181) identified their hexylbenzenes as 2-phenylhexane and 1-phenyl-3-methylpentane, respectively, rather than the normal compounds (95). Kruber's heptylbenzene (212) probably was secondary; and Ciamician assigned no structure to his $C_{13}H_{20}$ product (63). The "ethylhexylbenzene" of Hennion and Tous-saint (144) probably had the tertiary structure, 3-phenyl-3-methylheptane.

Tafel (355) found that the monoalkylbenzenes to which he and his coworkers (356, 357) had assigned the structures "1-phenyl-2-methylbutane" and "2-methyl-2-benzylbutane" were probably *n*-amylbenzene and 1-phenyl-3-methylpentane, respectively. The properties and syntheses are more consistent with the latter structures. The second hydrocarbon mentioned must be considered unknown.

The " β -methyl- δ -phenylpentane" of Berman and Lowy (33) may have been a mixture with 3-phenyl-2-methylpentane (*cf.* 156). Huston and Kaye (156) made twenty products, not all of which were identified by name, but it was made clear that some of the others were binary or ternary mixtures of isomers. The probable components include a branched hexyl and five branched heptylbenzenes which are otherwise unknown. These are listed in the present table with appropriate brackets. (One hydrocarbon is slightly out of order to permit bracketing.)

Essner and Gossin's identification (98) of their principal product as *m*-tert-amyltoluene (supported by references 62, 257) seems justified rather than "1-methyl-3-*n*-pentylbenzene" (95). They did not identify their lower-boiling product, which from its synthesis might be 1-methyl-3-(1',2'-dimethylpropyl)benzene (*cf.* 206 for the corresponding amylbenzene). Similarly, the *p*-amyltoluene of Kunckel and Ulex (213) and one of the amyltoluenes of Tsukervanik (371) seem to contain the 1',2'-dimethylpropyl group, assuming the mechanism implied in the papers. The branched "amyltoluene" of Avenarius and Link (17a) was considered by Noelting (257) to be a butyltoluene.

Although Uhlhorn (374) gave evidence for the ortho structure in his diisopropylbenzene, Heise and Töhl (141) claimed that it was para. This would make the ortho isomer unknown until 1947 (235b), although it is listed in several compilations (70, 87, 95, 353). The new low boiling point supports the view of Heise and Töhl. Genvresse (119) and McKenna and Sowa (230) both indicated a para structure for their diisopropylbenzenes rather than meta (95) or ortho (87), respectively.

Nightingale, Radford, and Shanholtzer (253) and also Buu-Hoi and Cagnaint (54) showed that the "1,3-dimethyl-4-*tert*-butylbenzene" of Nightingale and Smith (255) was largely the 1,3,5-isomer. On the other hand both groups of authors confirmed the identity of the former structure for the product made by Smith and Perry (340). The latter investigators' observations of density and refractive index are incredibly high, and no values for these properties were given by Buu-Hoi and Cagnaint (54).

The hydrocarbon of Böseseken and Wildschut (42) was not "*n*-heptylbenzene"

(95), since it was made from 3-ethylpentane. It probably had the otherwise unknown structure, 1-phenyl-3-ethylpentane.

Kirrman and Graves (185) did not identify their diisopropyltoluene. Although they reported largely hemimellitic acid on oxidation of the fraction containing it, the vicinal structure is very improbable considering its synthesis, the low values for density and refractive index, and the analogy in color reaction to that of their 1,2,4-triisopropylbenzene. The structure 1-methyl-2,4-diisopropylbenzene seems most probable.

The only observation on the density of 1-methyl-3-ethyl-6-*n*-butylbenzene—0.6882 at 11°C. (232)—is an obvious typographical error, which is copied in Beilstein (30c) and in three abstracts, though questioned in *Chemisches Zentralblatt*. Doss (87) took the value 0.8882, but the slightly lower value, 0.8862, selected by Egloff (95) seems more probable. The density (0.8550) given by Larsen, Thorpe, and Armfield (217) for hexadecylbenzene was inadvertently assigned to hexaethylbenzene (95); and that assigned to di-*tert*-butylbenzene (95) should apply to the mono derivative (153). The melting points assigned (95) to the 1,2,4- and 1,3,5-triethylbenzenes (333) and to triisopropylbenzene (248) should apply to derivatives.

Barbier (19, 20, 21, 22) made by alkylation six of the ten theoretically possible methylisopropyl-*tert*-butylbenzenes, but assigned structures to only three of them, the 1,4,2- and 1,4,3- (22) and 1,3,5-isomers (21). The others can be identified with fair probability as follows: Three other possible structures (1,2,3-; 1,2,6-; and 1,3,2-) are vicinal trialkylbenzenes, and are very unlikely to result from alkylation. Eliminating these as probabilities, one of the other products, the one boiling at 235°C. under 737 mm. (Barbier's "2") (20, 21), must be the 1,2,5-isomer, since it was made from *m-tert*-butyltoluene and the other possibilities are accounted for. The product boiling at 236°C. under 727 mm. (Barbier's "3") must be the 1,3,6-isomer, since it was made from *p-tert*-butylcumene (22). The remaining product (Barbier's "1"), which boiled at 230°C. under 733 mm., was made from *p-tert*-butyltoluene and could have its isopropyl group in either the 2- or the 3-position. Steric influences favor the former, but the relatively low boiling point favors the isomer with no alkyl group adjacent to the methyl group (1,3,4-).

Timmermans listed a tetraethylbenzene as "1,2,3,4?". The numbering probably should be "1,2,4,5-" because of the high melting point, 11.6°C. (*cf.* 171, 334), since the former freezes below -50°C. (334), also < -20°C. (117, 170). The vicinal structure is copied without a question mark in *Chemical Abstracts* and in compilations (95, 353). Galle (117) considered his tetraethylbenzene to be the 1,2,3,5-isomer, because on oxidation it gave prehnitic acid. The literature on the structure of the latter is equivocal; and Jacobsen (170) showed that Galle had the vicinal derivative. This was confirmed by Smith and Guss (355), who formed only the 1,2,3,4-isomer by the Jacobsen reaction used by Galle (117).

Denisenko (81) used an ingenious method, the catalytic reduction of phenyl- ω -cyclopentylalkanes, to make mixtures of monoalkylbenzenes. Each product

contained presumably the *n*-alkylbenzene and (except for C₁₁) two other 1-phenylalkanes in which the alkyl group had one methyl or one ethyl group side chain, respectively. The products above C₁₁ were incompletely separated. The higher-boiling cuts from the C₁₅ and C₁₆ products are assigned structures of the normal alkylbenzenes, and the lower-boiling cuts are considered to be mixtures of the other two predicted isomers, which should have almost identical properties. The high densities and refractive indices of the products may indicate incomplete rupture of the cyclopentyl ring.

Similarly Fleischer and Melber (102a) obtained a C₁₄ alkylbenzene by Clemmensen reduction of a bicyclic diketone and indicated four possible structures, depending on the point of rupture of the second ring. Reaction probabilities and the high values of the observed density and index both favor the two structures with three alkyl groups, of which one is selected tentatively,—namely, 1,2-dimethyl-3-(2'-ethylbutyl)benzene.

The structure of the "methyloctylbenzene" described by Joukovsky (174) is not given. From its synthesis the most probable structure is 1-methyl-4-(1',5'-dimethylhexyl)benzene (made also by Ruzicka and van Veen (295)), but since Joukovsky showed it to contain double bonds in substantial amount, it must be impure.

The unsymmetrical structure, 1,3,4-, was assigned by de Capeller (59) for his di-*tert*-butyltoluene because the same product resulted on dialkylation by means of aluminum chloride, which according to Baur (25) gives *m-tert*-butyltoluene, or on dialkylation by means of ferric chloride, which Bialobrzewski (37) found to give *p-tert*-butyltoluene. The latter observations were supported by Noelting (257), by Buu-Hoi and Cagnaint (52), and partly by Pajeau (265a), but not by Shoemsmith and McGechee (318). However, this evidence for the structure of the di-*tert*-butyltoluene is not very convincing, in view of the reluctance of branched-chain alkyl groups to assume adjacent positions, of the weakness of directive influence in alkylation (110, 284), and of the facility of rearrangement (213, 306), especially in the nascent state. Noelting (257) proved that his di-*tert*-butyltoluene, similarly made, was symmetrical because it formed a trinitro derivative. The comparatively high melting point, 32°C. (59), also favors the symmetrical structure.

For similar reasons a symmetrical structure is assigned in this compilation, and also in Nightingale's review (250a), to the tri-*tert*-butylbenzene which melts at 128°C. Senkowsky (313) did not indicate the positions; and R. A. Smith (341) gave no evidence for the positions "1,4,6-" by which he designated it (*cf.* 95), although the presumed intermediate, *p*-di-*tert*-butylbenzene, suggests the unsymmetrical arrangement (*cf.* 306 for analogous rearrangement of isopropyl groups). The liquid "tributylbenzene" described by Ipatieff and coworkers (160, 162), which may be the same as that of Koch and Steinbrink (202) and of Kunckel and Ulex (213), is assigned tentatively the 1,2,4- structure, although Legge (218a) has evidence for more complex reactions upon the per-alkylation of benzene with isobutene. Firla's "tributylbenzene" (102) had a boiling point too low for any tributyl- and too high for a dibutylbenzene. His products may be

similar to those of Legge. The properties of some of Legge's fractions (218a) are listed in table 1 after the structures assigned, even though separation was incomplete, because calculated properties for structures comprising a fraction are nearly alike.

The structure 1,3-dimethyltetraethylbenzene is assigned in table 1 to the product of Staudinger and coworkers (345) since they employed "pure xylene", which was probably *m*-xylene. Galle's product (117) was probably the same.

The positions of most of the alkyl groups are not given in the polyalkylbenzenes of Dreisbach (89, 90) and Dreisbach and Heusted (91). The products were probably mixtures, but the structures assigned are preferred for the reasons given. For the ethyldiisopropylbenzene the symmetrical structure is most common in alkylation under vigorous conditions. Similarly, the 2,4,6-positions are assigned tentatively to the three isopropyl groups in derivatives of toluene, ethylbenzene, xylene, and diethylbenzene. No structure is assigned to the diethyldiisopropylbenzenes. The ethyl groups are probably *meta*. One of the ethyltriisopropylbenzenes probably has the structure 1,2,4,5- and the other 1,2,4,6-. The product with the high melting point, 106.9°C., is assigned the more symmetrical structure, 1,2,4,5-, by analogy with durene and the corresponding tetraethyl- and tetraisopropyl-benzenes, all of which have high melting points.

The two triethyldiisopropylbenzenes were both made from "triethylbenzene". Since the symmetrical isomer could give only one diisopropyl derivative, the other product must result from unsymmetrical triethylbenzene (the vicinal isomer being unknown). The lower boiling point is assigned to the product from the symmetrical isomer, because it lacks adjacent ethyl groups. In the tetraisopropyltoluene the positions of the four isopropyl groups are practically determined by analogy with the only known tetraisopropylbenzene (symmetrical).

Tilicheev's *m*-diamylbenzene (360) probably had *sec*-amyl groups, and the Sharples product (316) might be the same, or it might contain tertiary groups; but the amylbenzenes of Austin (10) and Costa (75) were probably *m*-di-*tert*-amylbenzene, because they were made from optically active amyl alcohol.

The two "triamylbenzenes" of Ipatieff, Corson, and Pines (160) showed very different boiling points, and had perhaps secondary and tertiary radicals, respectively. The Sharples product (316) may be the same as the higher-boiling one (*sec*-), although there are 920 possible triamylbenzenes (*cf.* 109). The dioctyl- and dinonyl-benzenes (160) and Tilicheev's diheptylbenzene (360) probably had secondary groups.

The hydrocarbon of Schaeffer and Stirton (297a) is assigned the structure 9-phenyloctadecane, since it would result from either 9- or 10-phenyloctadecanol in their mixture.

Two hydrocarbons, bombicestane, C₂₇H₄₈, and inagostane, C₂₉H₅₂, listed by Egloff (95) are omitted from this compilation, since they probably are not alkylbenzenes but tetracyclics, because of their close similarity to cholestane (178a, b).

The following hydrocarbons listed in a compilation or abstract must be considered unknown, since the names apply to alkylbenzenes described apparently correctly by the original authors under different names: "1,2-di-*n*-propylbenzene"

(95, 137); "3-methyl-4-phenylhexane" (4); "2-*p*-tolylhexane" (95, 344); "1-propyl-2-*n*-pentylbenzene" (43, 95); "1,3,5-trimethyl-2-(2'-methylbutyl)benzene" (95, 199); "1-methyl-3,5-di-*n*-butylbenzene" (95, 257); "3-propyl-3-phenylheptane" (95, 138); "1-methyl-5-undecylbenzene" (87, 140); "1,4-di-*sec*-hexylbenzene" (95, 344); "2,8-dimethyl-3-propylnonane" (95, 138); "5-phenyl-2,8-dimethyl-8-isobutylnonane" (87, 138). This would apply also to "2-phenyl-3-methylhexane" (87, 138), except that it was probably present in one of the products of Huston and Kaye (156). Some of these names are doubtless typographical errors.

Typographical errors in the original literature include observations on density: 0.0834 (380), 0.959 (124), 8.0638 (174), and observations on refractive index: 4.92 (185), 2.522 (247). These values probably should be 0.8834, 0.859, 0.8638, 1.492, and 1.522, respectively.

IV. CALCULATION OF DENSITY

A tentative plot of density against number of carbon atoms for the alkylbenzenes showed that (1) the density decreases slightly with increasing carbon content; (2) the mono-*tert*-alkylbenzenes have consistently higher densities than other monoalkylbenzenes and most polyalkylbenzenes; (3) *o*-dialkylbenzenes and polyalkylbenzenes with two adjacent alkyl groups have a similar exaltation in density; (4) polyalkylbenzenes with more than one pair of adjacent alkyl groups have a further increase in density proportional to the number of such pairs. Thus 1,2,3-trialkyl- and 1,2,4,5-tetraalkyl-benzenes have twice as much increase in density; 1,2,3,4-tetraalkylbenzenes have three times as much, etc.

All of these effects are correlated by the following simple equation:

$$d_4^{20} = 0.850 + (0.12/n)(1 + a + b)$$

in which n is the number of carbon atoms, a is the number of pairs of adjacent alkyl groups, and b is 1 for mono-*tert*-alkylbenzenes and zero for other aromatics, even including those with tertiary alkyl groups.

Ninety-six of the more reliable observations of density are plotted in figure 1 with the densities adjusted for a and b (when applicable). This group includes the selections of the Bureau of Standards for hydrocarbons up to C_{10} (7, 8); several for higher aromatics accompanied by precise melting points, a property which is considered a criterion of purity; and also some others with concordant observations by different investigators. For clarity the points are represented by letters suggestive of the type of hydrocarbon, as shown in the legend. The less reliable observations show a similar distribution of points, but are omitted to avoid too great congestion of the graph.

The curve is the plot of the equation, $d = 0.850 + 0.12/n$, the base line being the asymptote. No reliable observation on density of an alkylbenzene disagrees with the values thus calculated by more than 0.01, and none for a n -alkylbenzene by more than 0.002. No further consistent deviation of a sub-class (same letter) is apparent. On the other hand, when many more accurate data become available, further refinement in the calculations will be possible. Values of density

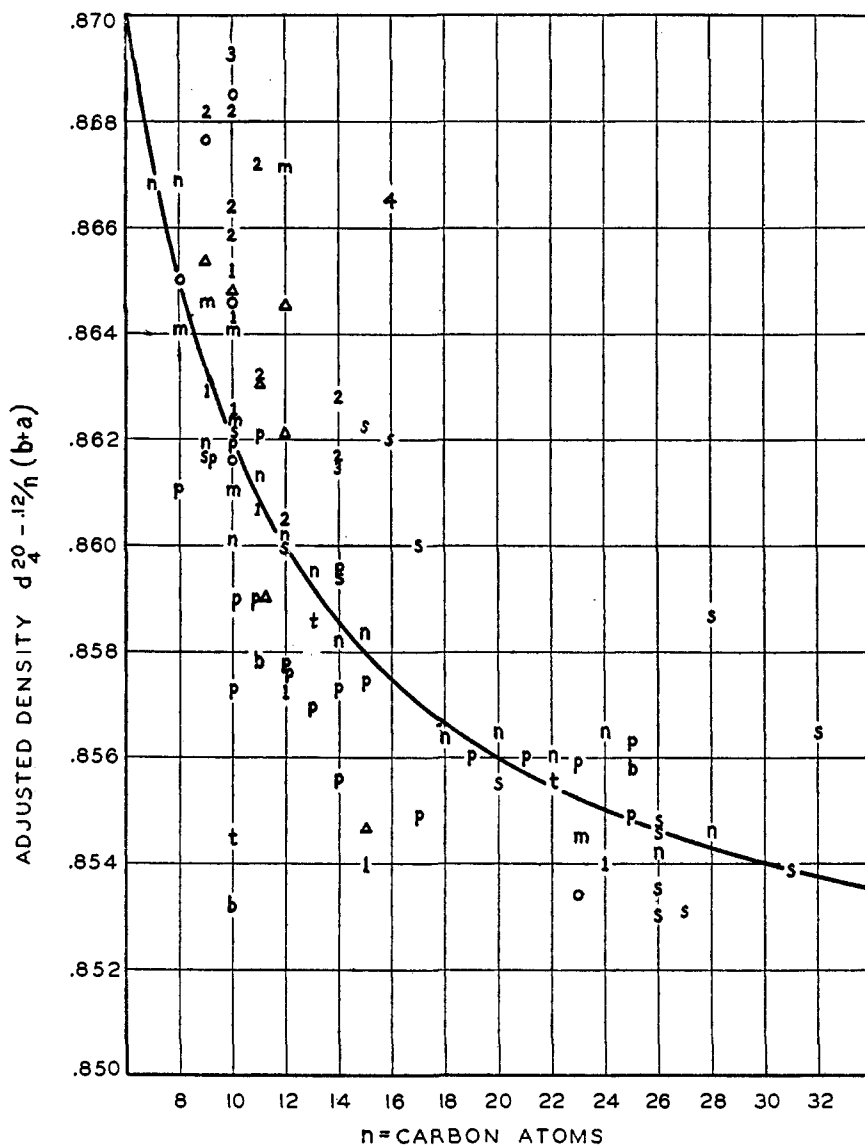


FIG. 1. Density

b, branched-chain primary monoalkylbenzenes
 m, *m*-dialkylbenzenes
 n, *n*-monoalkylbenzenes
 o, *o*-dialkylbenzenes
 p, *p*-dialkylbenzenes
 s, *sec*-monoalkylbenzenes
 t, *tert*-monoalkylbenzenes
 Δ, 1,3,5-trialkylbenzenes

1, polyalkylbenzenes with one pair of adjacent alkyl groups
 2, polyalkylbenzenes with two pairs of adjacent alkyl groups
 3, polyalkylbenzenes with three pairs of adjacent alkyl groups (vicinal tetraalkyl)
 4, polyalkylbenzenes with four pairs of adjacent alkyl groups (pentaalkyl)

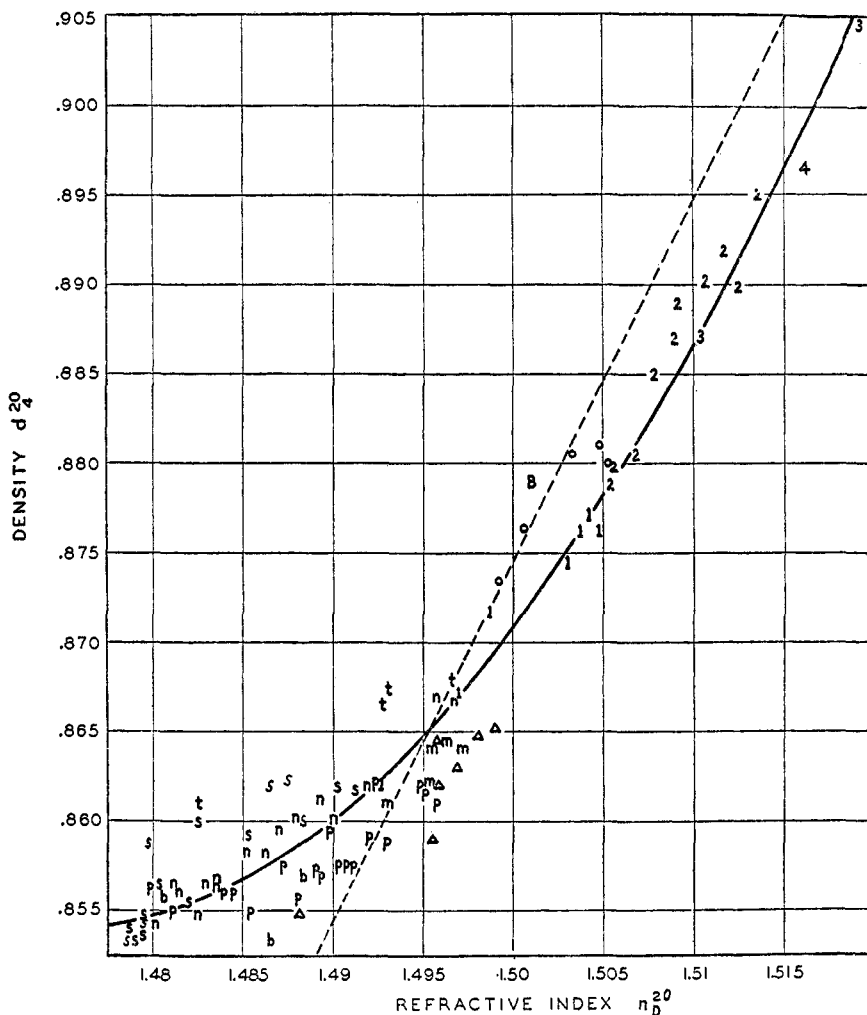


FIG. 2. Density versus refractive index

- | | |
|---|---|
| <p>B, benzene b, branched-chain primary monoalkyl benzenes m, <i>m</i>-dialkylbenzenes n, <i>n</i>-monoalkylbenzenes o, <i>o</i>-dialkylbenzenes p, <i>p</i>-dialkylbenzenes s, <i>sec</i>-monoalkylbenzenes t, <i>tert</i>-monoalkylbenzenes Δ, 1,3,5-trialkylbenzenes</p> | <p>1, polyalkylbenzenes with one pair of adjacent alkyl groups 2, polyalkylbenzenes with two pairs of adjacent alkyl groups 3, polyalkylbenzenes with three pairs of adjacent alkyl groups (vicinal tetraalkyl) 4, polyalkylbenzenes with four pairs of adjacent alkyl groups (pentaalkyl)</p> |
|---|---|

calculated by this relation are listed in the table when the observations are missing for both density and refractive index, or when they differ from the calculations by more than 0.01 and 0.006, respectively.

V. RELATION BETWEEN DENSITY AND REFRACTIVE INDEX

Figure 2 is the plot of refractive index against density for the same group of 96 aromatics by classes as in figure 1. The points seem to be clustered to some extent about the parabola which is the plot of the equation,

$$d_4^{20} - 0.854 = 27(n_D^{20} - 1.475)^2$$

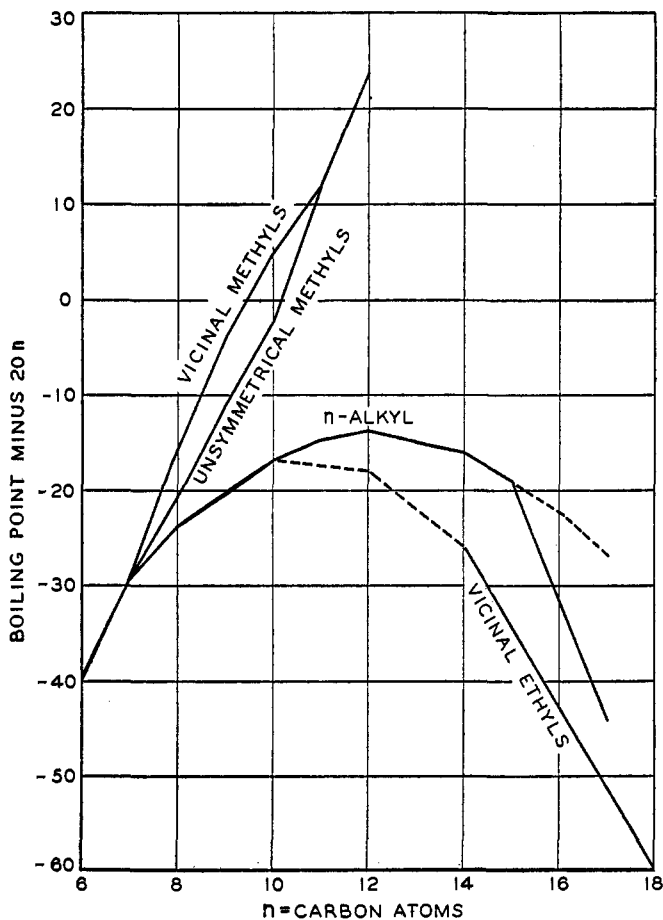


FIG. 3. Boiling point

especially if added weight is assigned to the *n*-alkylbenzenes, as before. However, the more symmetrical hydrocarbons, the 1,3,5-trialkylbenzenes, and the *p*- and to a less extent the *m*-dialkylbenzenes, have densities lower by 0.002 to 0.004 than the others. On the other hand, several branched-chain monoalkylbenzenes have reported densities about 0.01 higher than the curve, but are not shown because the values are not supported by other studies and are not consistent among themselves. The "refractivity intercept" line (dotted line in the

figure) of Ward and Kurtz (382) holds well except for those hydrocarbons of low refractive index, which include mostly those of high boiling point.

The curve is used to calculate values of refractive index in the table when observations are missing or questionable (deviating more than 0.006 from the calculations). It is used also to calculate density values from observed refractive index values when the former are missing or questionable and the latter are more consistent.

VI. BOILING POINTS

A plot of boiling point against number of carbon atoms, such as used by Schmidt (302) for *n*-alkylbenzenes only, is necessarily on such a small scale that moderate discrepancies are not apparent. In order to accentuate them, figures 3 to 5 are plotted with the ordinates "boiling point minus kn ", a procedure which permits a much larger scale. Straight lines connecting the observations are used instead of smooth curves, thus identifying the points and making it unnecessary to have several different kinds of points. When observations are lacking, or so far out of line that their reliability is questioned, dotted lines are used connecting calculated (interpolated or extrapolated) values.

Figure 3 shows convex "curves" for normal alkylbenzenes, and for the ethylbenzenes with all ethyl groups adjacent (1,2,3-triethylbenzene is not reported in the literature). The boiling point reported for *n*-hendecylbenzene is 17°C. lower than that extrapolated. The observed boiling points of the *n*-alkylbenzenes agree well with the equation

$$\text{b.p.} = 18n + 21 - 1800/n^2$$

as shown in the following table:

| <i>n</i> | BOILING POINT | | <i>n</i> | BOILING POINT | |
|----------|---------------|----------|----------|---------------|----------|
| | Calculated | Observed | | Calculated | Observed |
| 6 | 79.0 | 80.1 | 11 | 204.1 | 205.3 |
| 7 | 110.3 | 110.6 | 12 | 224.5 | 226.2 |
| 8 | 136.9 | 136.2 | 13 | 244.35 | 244 |
| 9 | 160.8 | 159.2 | 14 | 263.8 | 264 |
| 10 | 183.0 | 183.3 | 15 | 283.0 | 282 |

For extrapolation above C₁₅ it may be necessary to revise the equation to contain an n^2 term. For the vicinal ethylbenzenes no equation is satisfactory, partly because of the small number of reliable points.

The polymethylbenzenes show nearly a straight line:

$$\text{b.p.} = 30n - 100$$

It is curious that toluene and pentamethylbenzene have boiling points a little low for the vicinal series, and a little high for the unsymmetrical series. They can be considered to belong to both classes. The symmetrical polymethylbenzenes, *p*-xylene, mesitylene, and durene (not shown), would have points just below the line for unsymmetrical isomers.

Boiling points of four other series of monoalkylbenzenes are plotted in figure 4. The "C₂ chain" series includes ethylbenzene, cumene, and *tert*-butylbenzene, each of which has two carbon atoms in the longest arrangement of its side chain. The lines agree fairly well with the following equations:

| | |
|---|------------------|
| C ₂ chain..... | b.p. = 16.5n + 4 |
| Isoalkyl..... | b.p. = 21n - 37 |
| 2-Phenylalkane (secondary)..... | b.p. = 20n - 27 |
| 2-Phenyl-2-methylalkane (tertiary)..... | b.p. = 19n - 21 |

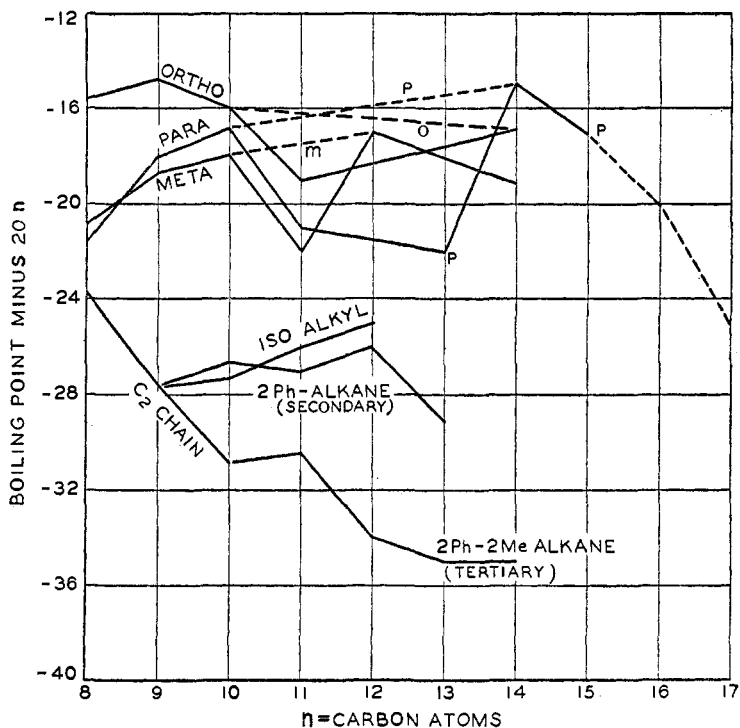


FIG. 4. Boiling points of monoalkylbenzenes and methyl-*n*-alkylbenzenes

In view of the large scale it is uncertain whether discrepancies from straight lines are real or due to inaccuracies. For more highly branched monoalkylbenzenes it seems advisable to deduct 3°C. for each additional branch from the estimates by the above equations.

Figure 4 also shows the three series of methyl-*n*-alkylbenzenes. Dips in the "curves" seem to indicate that the reported boiling points for the C₁₁ and C₁₃ members are about 4°C. low. There is very little difference between the *m*- and *p*-isomers, and the *o*-isomer also differs only when the second alkyl group is methyl or ethyl. The equation for an average corrected curve for this series is

$$\text{b.p.} = 17n + 33 - 1800/n^2$$

Figure 5 includes other meta and para di-*n*-alkylbenzenes. An upward revision of about 5°C. is suggested for the boiling point of "1-ethyl-3-*n*-propylbenzene"

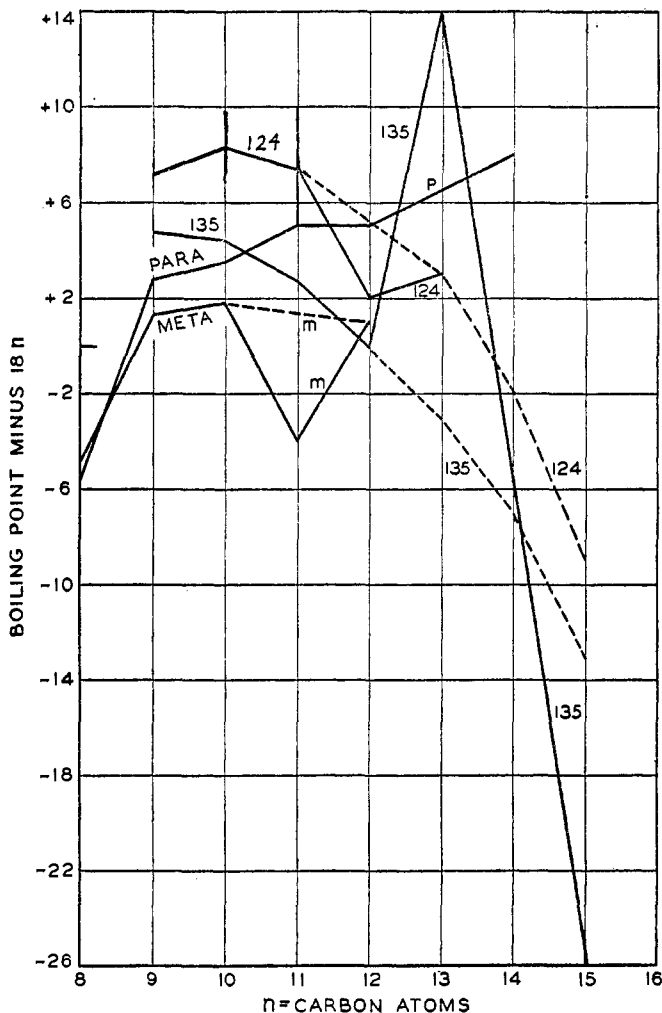


FIG. 5. Boiling points of di- and tri-*n*-alkylbenzenes

(probably wrong structure). These series are represented approximately by the equation:

$$\text{b.p.} = 17n + 31 - 1800/n^2$$

The symmetrical series (1,3,5-tri-*n*-alkylbenzenes) shows much more violent fluctuations, which can be smoothed out by an adjustment for the C₁₃ and C₁₅ members. The unsymmetrical series (1,2,4-) requires only one slight adjustment (C₁₂). The short vertical lines at C₁₀ and C₁₁ are drawn to indicate three

and four isomers, respectively, included in the class. The "curve" is drawn through the average boiling point of such isomers. The following equations are applicable:

| | |
|--|--------------------------------|
| 1,3,5-Tri- <i>n</i> -alkylbenzene..... | b.p. = $12.5n + 78 - 1800/n^2$ |
| 1,2,4-Tri- <i>n</i> -alkylbenzene..... | b.p. = $12.5n + 82 - 1800/n^2$ |

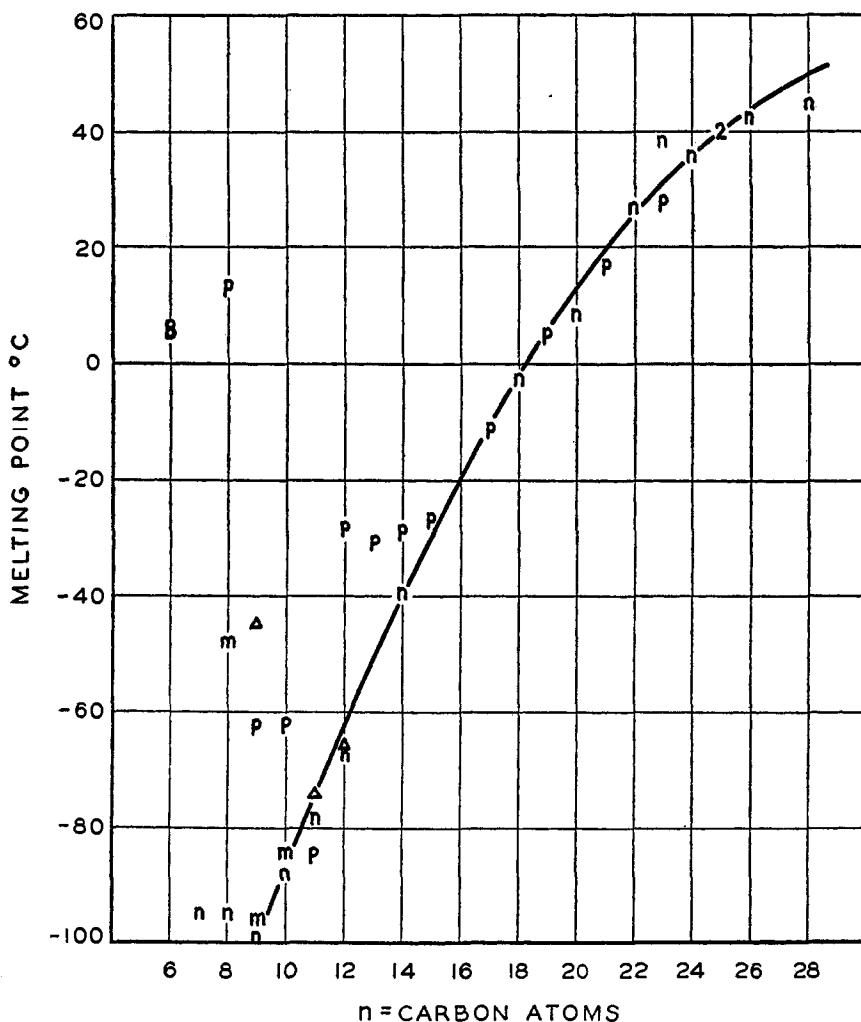


FIG. 6. Melting point. B, benzene; m, *m*-di-*n*-alkylbenzenes; p, *p*-methyl-*n*-alkylbenzenes; Δ, 1,3,5-tri-*n*-alkylbenzenes; 2, hexadecylmesitylene.

Still another series, the hexaalkylbenzenes, is not shown because it would require an individual graph. The members with reliable observations, those with

12, 17, 18, and 24 carbon atoms, have observed boiling points consistent with the equation:

$$\text{b.p.} = 5n + 216 - 1800/n^2$$

Estimates for boiling points of alkylbenzenes not so far included are based on the following approximate relations, which are superposed on results from the most appropriate equations for di- or tri-*n*-alkylbenzenes (tetra- and penta-alkylbenzenes are derived from the latter):

(1) The boiling points of isomeric poly-*n*-alkylbenzenes are nearly alike except for a correction for adjacent methyl and ethyl groups. Each such pair of methyl groups adds about 7°C., and an adjacent methyl and ethyl group add about 4°C. to the boiling point.

(2) One branch in any alkyl group lowers the boiling point about 10°C.; a second branch lowers it about half as much; a third branch, half as much again, etc.

Estimates are listed in table 1 for boiling points when the observations are missing or differ from the calculations by more than 5°C., for all known alkylbenzenes up to C₁₆ and a few beyond, and for the 18 unknown C₁₁ alkylbenzenes.

VII. MELTING POINTS

Melting points of organic compounds are usually extremely sensitive to structure, so that comparatively few of the observations on 138 of the alkylbenzenes can be correlated quantitatively. In figure 6 are plotted the "best" observations on all the known members of four series of *n*-alkylbenzenes. A single curve, a parabola, which is the plot of the equation,

$$\text{m.p.} = 19n - 0.3n^2 - 247$$

agrees well with the values for mono-*n*-alkyl and the *m*-di-*n*-alkyl series above C₈, the symmetrical series above C₉, and the methyl-*p*-*n*-alkylbenzenes above C₁₄. Most of the latter were observed by Schmidt and Schoeller (305), who were aware of the discrepancies for the members with 12, 13, and 14 carbon atoms, so that they are probably real as are those for the members below C₁₁. Single observations on melting points of *n*-octylbenzene (3) and 1-methyl-4-*n*-octylbenzene (223) are questionable because they are about 30°C. higher than those of other observers which are consistent with the curve.

The apparent validity of one curve for those series has permitted the estimation of twelve melting points not yet observed. For the other observations the only correlation now possible seems to be the qualitative one that high symmetry, as in hexaalkylbenzenes, results in high melting points.

VIII. SUMMARY

Table 1 presents a summary of data on the boiling points, density, refractive index, and melting points of benzene and alkylbenzenes.

The author is indebted to Dr. C. F. Feasley, who checked the section dealing with the discussion of identity, and to other colleagues for helpful suggestions.

TABLE 1
Properties of benzene and alkylbenzenes

| FORMULA | HYDROCARBON | BOILING POINT | | d_4^{20} | n_D^{20} | MELTING POINT | REFERENCES |
|-------------------------------------|---|---------------|-----|-----------------------|------------|----------------------------|--|
| | | °C. | mm. | | | °C. | |
| C_6H_6 | Benzene..... | 80.103 | 760 | 0.87903 | 1.50110 | 5.53 | (7, 78, 103, 120, 128, 328, 392) |
| | | | | 1.015 (solid at 0°C.) | | | |
| C_7H_8 | Toluene..... | 110.623 | 760 | 0.86683 | 1.49682 | -95.00 | (7, 103, 120, 128, 328, 392) |
| C_8H_{10} (4 possible) | Ethylbenzene..... | 136.187 | 760 | 0.86696 | 1.49580 | -95.00 | (7, 103, 120, 128, 311, 328, 392) |
| | <i>o</i> -Xylene..... | 144.414 | 760 | 0.88005 | 1.50524 | -25.15 | (7, 103, 120, 121, 128, 329, 392) |
| | <i>m</i> -Xylene..... | 139.102 | 760 | 0.86412 | 1.49715 | -47.87 | (7, 103, 128, 329, 392) |
| | <i>p</i> -Xylene..... | 138.348 | 760 | 0.86100 | 1.49580 | 13.27 | (7, 78, 103, 120, 121, 128, 329, 392) |
| C_9H_{12} (8 possible; all known) | <i>n</i> -Propylbenzene..... | 159.216 | 760 | 0.86198 | 1.4919 | -99.50 (I) -101.53 (II) | (7, 103, 120, 128, 147, 271, 302, 304, 328, 351, 372, 392) |
| | Isopropylbenzene (cumene).... | 152.393 | 760 | 0.86175 | 1.4913 | -96.00 | (7, 103, 120, 128, 147, 271, 328, 362, 392) |
| | 1-Methyl-2-ethylbenzene..... | 165.23 | 760 | 0.8810 | 1.5048 | -80.84 (I) -86.53 (II) | (7, 121, 147, 351) |
| | 1-Methyl-3-ethylbenzene..... | 161.29 | 760 | 0.8645 | 1.4961 | -95.59 (I) -97.0 (II) | (7, 121, 147, 351, 372) |
| | 1-Methyl-4-ethylbenzene..... | 161.94 | 760 | 0.8616 | 1.4952 | -62.36 | (7, 121, 147, 291, 351, 372) |
| | 1,2,3-Trimethylbenzene (hemimellitene)..... | 176.10 | 760 | 0.8951 | 1.5139 | -25.39 | (7, 128, 147, 329, 351) |

| | | | | | | | |
|--|---|--------|-----|--------|--------|---|--|
| C ₁₀ H ₁₄ (22 possible; all known) | 1,2,4-Trimethylbenzene (pseudocumene)..... | 169.18 | 760 | 0.8762 | 1.5048 | -43.79 (I) -48.98 (II) | (7, 128, 131a, 147, 267, 271, 329, 351) |
| | 1,3,5-Trimethylbenzene (mesitylene)..... | 164.64 | 760 | 0.8653 | 1.4990 | -44.73 (I) -49.80 (II) -51.68 (III) | (7, 128, 147, 271, 329, 351) |
| | <i>n</i> -Butylbenzene..... | 183.26 | 760 | 0.8601 | 1.4900 | -87.97 | (8, 38B, 45, 50, 93, 121, 128, 131a, 142, 204, 267, 302, 304, 328, 344, 350, 352) |
| | <i>sec</i> -Butylbenzene..... | 173.30 | 760 | 0.8618 | 1.4900 | -75.47 | (8, 23, 38B, 50, 128, 131a, 142, 188, 189, 204, 221, 237, 326, 328, 349, 352, 362, 368) |
| | Isobutylbenzene..... | 172.80 | 760 | 0.8532 | 1.4865 | -51.48 | (8, 38b, 50, 121, 128, 142, 308, 328, 352) |
| | <i>tert</i> -Butylbenzene..... | 169.10 | 760 | 0.8662 | 1.4925 | -57.85 | (8, 32, 38b, 50, 57, 128, 131a, 142, 143, 153, 218, 237, 267, 308, 322, 323, 325, 326, 328, 343, 352, 368) |
| | 1-Methyl-2- <i>n</i> -propylbenzene.... | 184 | 760 | 0.8736 | 1.4993 | | (8, 12, 15, 38b, 67, 93, 96, 174, 227) |
| | 1-Methyl-3- <i>n</i> -propylbenzene.... | 182 | 760 | 0.8623 | 1.4951 | | (8, 12, 15, 38b, 67, 96, 227, 320?, 372) |
| | 1-Methyl-4- <i>n</i> -propylbenzene.... | 183.45 | 760 | 0.8588 | 1.4930 | -62 | (8, 12, 15, 38b, 93, 96, 161 227, 305, 320?, 372) |
| | 1-Methyl-2-isopropylbenzene (<i>o</i> -cymene)..... | 178.5 | 760 | 0.8766 | 1.5006 | -71.6 | (8, 12, 38b, 82, 96, 227, 297) |

TABLE 1—Continued

| FORMULA | HYDROCARBON | BOILING POINT | | n_D^{20} | n_D^{20} | MELTING POINT | REFERENCES |
|---|---|---------------|-----|-------------------------|------------|---------------|---|
| | | °C. | mm. | | | | |
| C ₁₀ H ₁₄ (continued) | 1-Methyl-3-isopropylbenzene (<i>m</i> -cymene)..... | 175.2 | 760 | 0.8610 | 1.4930 | -63.8 | (8, 12, 38b, 96, 119, 227, 297, 320?) |
| | 1-Methyl-4-isopropylbenzene (<i>p</i> -cymene..... | 177.23 | 760 | 0.8567 | 1.4908 | -68.17 | (8, 12, 38b, 96, 120, 127, 143, 201, 204, 215, 218, 227, 237, 245, 267, 271, 287, 297, 306, 326, 329, 379, 381, 384, 393) |
| | <i>o</i> -Diethylbenzene..... | 183.5 | 760 | 0.8790 | 1.5034 | -32.07 | (8, 38b, 114, 137, 178) |
| | <i>m</i> -Diethylbenzene..... | 181.62 | | 0.8641 | 1.4955 | -84.09 | (8, 38b, 69, 120, 245, 258, 350, 372) |
| | <i>p</i> -Diethylbenzene..... | 183.8 | 760 | 0.8620 | 1.4950 | -42.95 | (8, 15, 38b, 161, 178, 193, 213, 222, 245) |
| | 1,2-Dimethyl-3-ethylbenzene... | 193.91 | 760 | 0.8921 | 1.5117 | -49.5 | (8) |
| | 1,2-Dimethyl-4-ethylbenzene... | 189.75 | | 0.8745 | 1.5031 | -67.0 | (8, 17?, 211, 373, 381) |
| | 1,3-Dimethyl-2-ethylbenzene... | 190.01 | | 0.8904 | 1.5107 | -16.3 | (8, 77a, 337) |
| | 1,3-Dimethyl-4-ethylbenzene... | 188.41 | | 0.8763 | 1.5038 | -63.0 | (8, 193, 260, 282, 337) |
| | 1,3-Dimethyl-5-ethylbenzene... | 183.75 | | 0.8648 | 1.4981 | -84.2 | (8, 118, 260, 261, 287) |
| | 1,4-Dimethyl-2-ethylbenzene... | 186.91 | | 0.8772 | 1.5043 | -53.7 | (8, 111, 193, 287, 337) |
| | 1,2,3,4-Tetramethylbenzene (prehnitene)..... | 205.04 | | 0.9053 | 1.52013 | -6.25 | (8, 68, 229, 233, 267, 329, 331, 332, 337, 338, 339) |
| | 1,2,3,5-Tetramethylbenzene (isodurene)..... | 197.92 | 760 | 0.8899 | 1.5125 | -23.97 | (8, 68, 229, 267, 329, 331, 339) |
| | 1,2,4,5-Tetramethylbenzene (durene)..... | 196 | 760 | 0.889† 1.032 (solid) | 1.512† | 79.3 | (8, 68, 85, 100, 112, 113, 211, 229, 245, 267, 329, 331, 339) |

| | | | | | | | |
|---|---|--------|----------|----------|----------|----------------|---|
| C ₁₁ H ₁₆ (51 possible; 33 known) | <i>n</i> -Amylbenzene | 205.3 | 760 | 0.8613 | 1.4892 | -78.25 | (38a, 45, 49, 79, 81, 93, 123, 125, 167, 175, 176, 204, 217, 227, 272, 285, 302, 304, 307, 317, 321, 328, 347, 350, 355, 356, 357, 394) |
| | 2-Phenylpentane | 193 | 760 | 0.8597 | 1.4856 | | (79, 81, 112, 155, 156, 163, 167, 188, 189, 263, 315, 322, 349, 353, 360, 361, 368) |
| | 3-Phenylpentane | 191 | 760 | 0.8649 | 1.4880 | | (76, 81, 156, 167, 190, 225, 322?, 343) |
| | 1-Phenyl-2-methylbutane (benzylbutane) | 194 | 760 | 0.8617 | 1.4880 | | (43, 92, 123, 129, 167, 220, 293, 347, 355, 356, 357) |
| | 1-Phenyl-3-methylbutane (isoamylbenzene) | 196 | 760 | 0.8558 | 1.4847 | | (38, 64, 66?, 93, 123, 167, 191, 236, 296, 307, 314, 315, 328, 350, 367?) |
| | 2-Phenyl-2-methylbutane (<i>tert</i> -amylbenzene) | 189.6 | 760 | 0.8675 | 1.4930 | | (9, 10, 55, 97, 112, 143, 150, 153, 156, 159, 165, 167, 206, 217, 227, 245, 263, 283, 308, 322, 323, 343, 361, 370) |
| | 2-Phenyl-3-methylbutane | 189 | 760 | 0.8641 | 1.4913 | | (130, 155, 165, 167, 190, 206, 283, 308?) |
| | 1-Phenyl-2,2-dimethylpropane (neopentylbenzene) | 186 | 760 | 0.8569 | 1.4884 | | (56, 57, 167, 183, 283, 364) |
| | 1-Methyl-2- <i>n</i> -butylbenzene | 201 | 760 | 0.8721 | 1.4958 | | (227, 250) |
| | 1-Methyl-3- <i>n</i> -butylbenzene | 198? | 760 | 0.8640 | 1.4924 | (-74)‡ | (59, 137, 227, 250) |
| | | (203)‡ | | | | | |
| | 1-Methyl-4- <i>n</i> -butylbenzene | 199? | 760 | 0.8590 | 1.4920 | -85? | (227, 234, 250, 305, 319) |
| | | (204)‡ | | | | (-74)‡ | |
| | (1-Methyl-2- <i>sec</i> -butylbenzene)§. | (193)‡ | 760 | (0.872)‡ | (1.501)‡ | | Unknown |
| 1-Methyl-3- <i>sec</i> -butylbenzene . . . | 197 | | (0.865)‡ | 1.4957 | | (23, 131, 318) | |

TABLE 1—Continued

| FORMULA | HYDROCARBON | BOILING POINT | | d_4^{20} | n_D^{20} | MELTING POINT | REFERENCES |
|---|---|---------------|----------|------------|------------|----------------|--|
| | | °C. | mm. | | | | |
| C ₁₁ H ₁₆ (continued) | 1-Methyl-4- <i>sec</i> -butylbenzene . . . | 200 | | 0.8650 | 1.4932 | | (23, 143, 237, 318, 326, 379, 384) |
| | (1-Methyl-2-isobutylbenzene)§.. | (193)‡ | 760 | (0.872)‡ | (1.501)‡ | | Unknown |
| | (1-Methyl-3-isobutylbenzene)§.. | (195)‡ | | (0.861)‡ | (1.492)‡ | | (94; unknown, see text) |
| | (1-Methyl-4-isobutylbenzene)§.. | (193)‡ | 760 | (0.861)‡ | (1.492)‡ | | Unknown, see text |
| | 1-Methyl-2- <i>tert</i> -butylbenzene . . . | 171? | | (0.863)‡ | 1.4930 | | (207) |
| | | (188)‡ | | | | | |
| | 1-Methyl-3- <i>tert</i> -butylbenzene . . . | 188 | 760 | (0.863)‡ | 1.4928 | | (25, 133, 180, 205, 257, 318, 370) |
| | 1-Methyl-4- <i>tert</i> -butylbenzene . . . | 193 | | 0.8621 | 1.4921 | | (11, 31, 37, 58, 143, 150, 205, 207, 213, 215, 218, 237, 257, 265a, 323, 326, 371, 377, 384) |
| | (1-Ethyl-2- <i>n</i> -propylbenzene)§... | (204)‡ | 760 | (0.872)‡ | (1.501)‡ | | Unknown |
| | 1-Ethyl-3- <i>n</i> -propylbenzene? . . . | 194? | | 0.8580 | (1.487)‡ | | (288); probably unknown, see text |
| | | (199)‡ | | | | | |
| | 1-Ethyl-4- <i>n</i> -propylbenzene | 203 | 760 | 0.866 | (1.496)‡ | (-74)‡ | (29, 161, 390) |
| | (1-Ethyl-2-isopropylbenzene)§.. | (193)‡ | | (0.872)‡ | (1.501)‡ | | Unknown |
| | 1-Ethyl-3-isopropylbenzene | 195 | | 0.8616 | (1.492)‡ | < -20 | (29, 108, 353) |
| | 1-Ethyl-4-isopropylbenzene | 197 | | 0.8625 | 1.4927 | < -20 | (29, 193, 287, 353, 379, 384) |
| | (1,2-Dimethyl-3- <i>n</i> -propylbenzene)§. | (215)‡ | 760 | (0.883)‡ | (1.508)‡ | | Unknown |
| | 1,2-Dimethyl-4- <i>n</i> -propylbenzene | 204 | | 0.8670 | 1.4972 | < -20 | (17, 373) |
| (1,3-Dimethyl-2- <i>n</i> -propylbenzene)§. | (208)‡ | | (0.883)‡ | (1.508)‡ | | Unknown | |
| 1,3-Dimethyl-4- <i>n</i> -propylbenzene | 208 | | 0.8778 | 1.5010 | < -20 | (36, 251, 373) | |

| | | | | | | |
|--|--------|-----|----------|----------|--------|----------------------------------|
| 1,3-Dimethyl-5- <i>n</i> -propylbenzene..... | 209 | | (0.861)‡ | 1.4933 | | (168, 251, 373) |
| 1,4-Dimethyl-2- <i>n</i> -propylbenzene..... | 207 | | (0.872)‡ | (1.501)‡ | < -20 | (373) |
| (1,2-Dimethyl-3-isopropylbenzene)§..... | (203)‡ | | (0.883)‡ | (1.508)‡ | | Unknown |
| 1,2-Dimethyl-4-isopropylbenzene..... | 199 | | 0.8710 | 1.4980 | -41 | (179, 192, 198, 211) |
| (1,3-Dimethyl-2-isopropylbenzene)§..... | (198)‡ | | (0.883)‡ | (1.508)‡ | | Unknown |
| 1,3-Dimethyl-4-isopropylbenzene.. | 195 | | 0.869 | 1.5018 | < -80 | (179, 251, 373) |
| 1,3-Dimethyl-5-isopropylbenzene..... | 191 | | 0.859 | 1.4955 | -55.3 | (179, 213?, 251, 380) |
| (1,4-Dimethyl-2-isopropylbenzene)§..... | (196)‡ | | (0.872)‡ | (1.501)‡ | | Unknown |
| (1-Methyl-2,3-diethylbenzene)§..... | (208)‡ | | (0.883)‡ | (1.508)‡ | | Unknown |
| (1-Methyl-2,4-diethylbenzene)§..... | (205)‡ | | (0.872)‡ | (1.501)‡ | | Unknown |
| 1-Methyl-2,5-diethylbenzene... | 207 | | (0.872)‡ | (1.501)‡ | | (232) |
| (1-Methyl-2,6-diethylbenzene)§..... | (209)‡ | | (0.883)‡ | (1.508)‡ | | Unknown |
| 1-Methyl-3,4-diethylbenzene... | 203 | | (0.872)‡ | (1.501)‡ | | (213) |
| 1-Methyl-3,5-diethylbenzene... | 200.70 | | 0.8631 | 1.4969 | -74.12 | (108?, 118, 120, 261, 353, 372?) |
| (1,2,3-Trimethyl-4-ethylbenzene)§..... | (223)‡ | 760 | (0.894)‡ | (1.514)‡ | | Unknown |
| (1,2,3-Trimethyl-5-ethylbenzene)§..... | (219)‡ | | (0.883)‡ | (1.508)‡ | | Unknown |
| 1,2,4-Trimethyl-3-ethylbenzene..... | 216 | | 0.899 | 1.5133 | < -50 | (336, 337) |

TABLE 1—Continued

| FORMULA | HYDROCARBON | BOILING POINT | | d_4^{20} | n_D^{20} | MELTING POINT | REFERENCES |
|--|---|----------------|-----|---------------------------------------|----------------------|---------------|--|
| | | °C. | mm. | | | | |
| C ₁₁ H ₁₆ (continued) | 1,2,4-Trimethyl-5-ethylbenzene | 210 | | 0.885 | 1.5079 | -13.6 | (12, 15, 17, 193, 287?, 336, 353, 365) |
| | (1,2,4-Trimethyl-6-ethylbenzene)§ | (216)‡ | 760 | (0.883)‡ | (1.508)‡ | | Unknown |
| | 1,3,5-Trimethyl-2-ethylbenzene | 210 | | 0.8856 | 1.5090 | -15.56 | (12, 15, 77a, 115, 172, 187, 193, 287, 336, 353, 366) |
| | Pentamethylbenzene | 231.9 | 760 | 0.921†? (0.9045)‡ 1.011 (solid) | 1.5287†? (1.519)‡ | 54.3 | (2, 17, 45a, 68, 85, 99, 100, 113, 169, 229, 269, 329, 338, 339, 378, 395) |
| | <i>n</i> -Hexylbenzene | 226.2 | 760 | 0.8602 | 1.4879 | -66.8 | (45, 78a, 80, 81, 123, 124, 175, 176, 182, 272, 296, 302, 304, 317, 321, 328, 385) |
| C ₁₂ H ₁₈ (136 possible; 55 known) | 2-Phenylhexane | 214 | 760 | 0.8600 | 1.4882 | | (47, 124, 156, 221, 349, 361) |
| | 3-Phenylhexane | 211 | | 0.8609 | 1.4877 | | (4, 124, 221, 344) |
| | 1-Phenyl-2-methylpentane | 215 | | 0.8624 | 1.4847 | | (39, 92, 348) |
| | 1-Phenyl-3-methylpentane | 221 | | 0.8605 | 1.4876 | | (181, 195, 293, 348, 355, 357) |
| | 1-Phenyl-4-methylpentane | 218 | | 0.8536 | (1.48)‡ | | (307, 347) |
| | 2-Phenyl-2-methylpentane | 206 | | 0.8717 | 1.4938 | | (153, 156, 309) |
| | 2-Phenyl-3-methylpentane | 211 | | 0.8798? (0.860)‡ | 1.4973? (1.490)‡ | | (156, mixture with 3-phenyl-3-methylpentane) |
| | 2-Phenyl-4-methylpentane | 198? (210)‡ | 760 | 0.8592 | 1.4856 | | (33?, 156, 191) |

| | | | | | | |
|---|---------|-----|----------|----------|-------|----------------------------------|
| 3-Phenyl-2-methylpentane..... | 209 | 760 | 0.8678 | 1.4912 | | (4, 157) |
| 3-Phenyl-3-methylpentane..... | 206 | | 0.8755 | 1.4958 | | (153, 309) |
| 1-Phenyl-2-ethylbutane (3-benzylpentane)..... | 218 | | (0.860)‡ | (1.490)‡ | | (347) |
| (1-Phenyl-2,2-dimethyl- butane)§..... | 215 | 760 | 0.8592 | 1.4878 | | (355, 357; unknown, see text) |
| 1-Phenyl-2,3-dimethylbutane... | 217 | | 0.8718 | (1.501)‡ | | (64) |
| 2-Phenyl-2,3-dimethylbutane... | 210 | | 0.8814? | 1.4988 | | (153) |
| | | | (0.870)‡ | | | |
| 2-Phenyl-3,3-dimethylbutane... | 206 | 760 | 0.8803? | 1.4962 | | (156) |
| | | | (0.866)‡ | | | |
| 1-Methyl-2- <i>n</i> -amylbenzene..... | (224)‡ | 760 | 0.8725 | (1.501)‡ | | (227) |
| 1-Methyl-3- <i>n</i> -amylbenzene..... | 223 | | 0.8593 | 1.4911 | | (60, 227) |
| 1-Methyl-4- <i>n</i> -amylbenzene..... | 99 | 12 | 0.8569 | 1.4904 | -28 | (227, 305) |
| | (224)‡ | 760 | | | | |
| 1-Methyl-4-(1'-methylbutyl)- benzene..... | 95 | 20 | 0.8631 | 1.4920 | | (384) |
| | (214)‡ | 760 | | | | |
| 1-Methyl-4-(ethylpropyl)ben- zene..... | 85 | 13 | 0.8694 | 1.4940 | | (143) |
| | (214)‡ | 760 | | | | |
| 1-Methyl-2-isoamylbenzene..... | (213)‡ | | 0.8675 | (1.497)‡ | | (227) |
| 1-Methyl-3-isoamylbenzene..... | (211)‡ | | 0.8565 | (1.484)‡ | | (227) |
| 1-Methyl-4-isoamylbenzene..... | 211 | | 0.8629 | 1.4950 | < -20 | (38, 227, 319) |
| 1-Methyl-3- <i>tert</i> -amylbenzene.... | 209 | | 0.8673 | (1.497)‡ | < -20 | (213?, 371) |
| 1-Methyl-4- <i>tert</i> -amylbenzene... | 208 | | 0.8711 | 1.4952 | | (122, 143, 371) |
| 1-Methyl-3-(1', 2'-dimethyl- propyl)benzene..... | 200-205 | 760 | (0.860)‡ | (1.490)‡ | | (98) |
| 1-Methyl-4-(1', 2'-dimethyl- propyl)?-benzene..... | 207 | 760 | 0.8661 | 1.4951 | | (213?, 371) |
| 1-Ethyl-4- <i>sec</i> -butylbenzene..... | 86 | 16 | 0.8629 | 1.4921 | | (384) |
| | (212)‡ | 760 | | | | |
| 1-Ethyl-3- <i>tert</i> -butylbenzene.... | 205 | | (0.860)‡ | (1.490)‡ | | (25, 27) |

TABLE 1—Continued

| FORMULA | HYDROCARBON | BOILING POINT | | d_4^{20} | n_D^{20} | MELTING POINT | REFERENCES |
|---|--|---------------|-----------|---------------------|---------------------|---------------|--|
| | | °C. | mm. | | | °C. | |
| C ₁₂ H ₁₈ (continued) | 1-Ethyl-4- <i>tert</i> -butylbenzene..... | 211 | | 0.8635 | 1.4950 | | (31, 77, 257, 265a) |
| | 1,3-Di- <i>n</i> -propylbenzene..... | 217 | | 0.9124? (0.862)‡ | 1.4928 | (-62)‡ | (18, 132?, 179, 372) |
| | 1,4-Di- <i>n</i> -propylbenzene..... | 221 | 760 | 0.8564 | 1.4914 | | (16, 18, 101, 132?, 179, 203, 287a, 324?) |
| | 1- <i>n</i> -Propyl-4-isopropylbenzene..... | 215 | 760 | 0.8614 | 1.4972 | | (35, 101, 270) |
| | 1,2-Diisopropylbenzene..... | 203.75 | 760 | 0.87007 | 1.49603 | -56.68 | (141?, 235b, 353?, 374?) |
| | 1,3-Diisopropylbenzene..... | 203.18 | | 0.85593 | 1.48883 | -63.13 | (34, 88, 119, 177, 248, 320, 353, 374) |
| | 1,4-Diisopropylbenzene..... | 210.37 | 760 | 0.85676 | 1.48983 | -17.07 | (58?, 141, 160, 163, 185, 230, 235b, 237, 248, 263, 326, 327, 368, 374?) |
| | 1,3-Dimethyl-4- <i>n</i> -butylbenzene..... | 96 (219)‡ | 8 760 | 0.8718 | 1.4992 | | (255) |
| | 1,3-Dimethyl-4- <i>sec</i> -butylbenzene..... | 84 (210)‡ | 8 760 | 0.8650 | 1.4959 | | (253, 255) |
| | 1,3-Dimethyl-5- <i>sec</i> -butylbenzene..... | 98 (206)‡ | 15 760 | 0.8621 | 1.4940 | | (255) |
| | 1,3-Dimethyl-4-isobutylbenzene..... | 96 (210)‡ | 15 760 | 0.8694 | 1.4994 | | (255) |
| | 1,2-Dimethyl-4- <i>tert</i> -butylbenzene..... | 210 | | (0.867)‡ | 1.4970 | | (252, 257) |
| | 1,3-Dimethyl-4- <i>tert</i> -butylbenzene..... | 213 | | 0.9452? (0.870)‡ | 1.5098? (1.499)‡ | | (54, 255, 340) |

| | | | | | | |
|--|----------------|-----------|------------------|-------------------|--------|--|
| 1,3-Dimethyl-5- <i>tert</i> -butylbenzene..... | 206 | 760 | 0.8645 | 1.4958 | -21.5 | (25, 26, 40, 53, 58, 78a, 218, 228, 253, 255, 256, 257, 261, 262, 265a, 340) |
| 1,4-Dimethyl-2- <i>tert</i> -butylbenzene..... | 210 | 760 | (0.870)‡ | (1.499)‡ | | (257) |
| 1-Methyl-3-ethyl-6- <i>n</i> -propylbenzene..... | 215? (219)‡ | | 0.8762 | (1.503)‡ | | (232) |
| 1-Methyl-2-ethyl-4-isopropylbenzene..... | 214 | 760 | 0.8673 | 1.4969 | | (44, 65, 192, 198, 376) |
| 1-Methyl-3-ethyl-4-isopropylbenzene..... | 213 | 760 | 0.8722 | 1.5006 | | (13) |
| 1,2,4-Triethylbenzene..... | 217.72 | | 0.8791 | 1.4982 | < -70 | (87, 186, 193, 353) |
| 1,3,5-Triethylbenzene..... | 215.92 | | 0.8621 | 1.4958 | -66.48 | (84, 108?, 118, 120, 131a, 134, 164, 186, 193, 194, 214, 258, 259, 260, 261, 287, 333, 342, 372?, 381) |
| 1,2,4-Trimethyl-5- <i>n</i> -propylbenzene..... | 228 | 760 | 0.887 | 1.5095 | | (148) |
| 1,3,5-Trimethyl-2- <i>n</i> -propylbenzene..... | 221 | | 0.8782 | 1.5033 | < -20 | (187, 199, 366) |
| 1,2,4-Trimethyl-5-isopropylbenzene..... | 223 | | 0.8802 | 1.5069 | 21 | (14, 179) |
| 1,3-Dimethyl-4,6-diethylbenzene..... | 105 (224)‡ | 15 760 | (0.880)‡ | (1.506)‡ | < -20 | (282) |
| 1,4-Dimethyl-2,5-diethylbenzene..... | 105 (224)‡ | 15 760 | 0.8803 | 1.5091 | | (111) |
| Hexamethylbenzene..... | 263.8 | | 1.042 (solid) | 1.5032 (solid) | 165.3 | (2, 28, 77a, 85, 113, 132, 147a, 169, 226, 229, 245, 267, 268, 269, 280, 329, 332, 338, 339, 363, 395) |

TABLE 1—Continued

| FORMULA | HYDROCARBON | BOILING POINT | | d_4^{20} | n_D^{20} | MELTING POINT | REFERENCES |
|--|--|---------------|-----------|---------------------|---------------------|---------------|---|
| | | °C. | mm. | | | | |
| C ₁₃ H ₂₀ (335 possible; 58 known) | <i>n</i> -Heptylbenzene..... | 244 | 760 | 0.8595 | 1.4875 | (-51)‡ | (45, 96, 124, 175, 176, 208, 227, 287, 296, 302, 304, 317, 353, 375, 385) |
| | 2-Phenylheptane..... | 231 | 760 | 0.8610 | 1.4863 | -32 | (86, 212, 360, 361) |
| | 3-Phenylheptane..... | 227 | | 0.8607 | 1.4862 | | (86, 139, 221, 293) |
| | 4-Phenylheptane..... | 224 | | 0.8665 | 1.4872 | | (86, 156) |
| | 2-Phenyl-2-methylhexane..... | 225 | | 0.8737 | 1.4943 | | (153, 156) |
| | 2-Phenyl-3-methylhexane..... | 225 | | 0.8804? (0.866)‡ | 1.4961 | | (156, binary mixture with 3-phenyl-3-methylhexane) |
| | 2-Phenyl-5-methylhexane..... | 223 | 760 | 0.8659 | (1.496) | | (188) |
| | 3-Phenyl-2-methylhexane} ? | 225 | 760 | 0.8691 | 1.4895 | | {(156, ternary mixture with 2-phenyl-5-methylhexane) |
| | 3-Phenyl-5-methylhexane} ? | | | | | | |
| | 3-Phenyl-3-methylhexane..... | 226 | 760 | 0.8776 | 1.4980 | | (138, 153, 156) |
| | 1-Phenyl-2-ethylpentane (3-benzylhexane)..... | 120 (236)‡ | 24 760 | (0.859)‡ | (1.488)‡ | | (92) |
| | 1-Phenyl-3-ethylpentane..... | 110 (226)‡ | 10 760 | (0.859)‡ | (1.488)‡ | | (42, 81?) |
| | 3-Phenyl-3-ethylpentane..... | 226 | | 0.8679 | 1.4965 | | (55, 57, 153, 309) |
| | 1-Phenyl-4,4-dimethylpentane.. | 115 (233)‡ | 9 760 | 0.9443? (0.859)‡ | 1.5274? (1.488)‡ | | (146) |
| | 2-Phenyl-2,3-dimethylpentane.. | 223 | 760 | 0.8801? (0.867)‡ | 1.4966 | | (153) |
| | 2-Phenyl-2,4-dimethylpentane.. | 218 | 760 | 0.869 | 1.4926 | | (152, 153, 309) |
| | 2-Phenyl-4,4-dimethylpen- tane?..... | 223 | 760 | 0.8757? (0.863)‡ | 1.4934 | | (156, mixture) |
| | 3-Phenyl-2,2-dimethylpen- tane?..... | | | | | | |

| | | | | | | |
|---|-------------------|------------|---------------------|--------------------|-------|--|
| 3-Phenyl-2,3-dimethylpentane.. | 226 | 760 | 0.8803? (0.868)‡ | 1.4974 | | (153) |
| 3-Phenyl-2,4-dimethylpentane.. | 225 | 760 | 0.8747? (0.859)‡ | 1.507? (1.489)‡ | | (247) |
| 2-Phenyl-2,3,3-trimethylbutane | 226 | 760 | 0.8867? (0.874)‡ | 1.5019 | | (153) |
| 1-Methyl-2- <i>n</i> -hexylbenzene.... | 238 | 760 | (0.868)‡ | (1.498)‡ | | (243) |
| 1-Methyl-3- <i>n</i> -hexylbenzene.... | 238 | | (0.859)‡ | (1.489)‡ | | (243) |
| 1-Methyl-4- <i>n</i> -hexylbenzene.... | 238? (243)‡ | | 0.8569 | 1.4890 | -30.5 | (243, 305) |
| 1-Methyl-4-(1'-ethylbutyl)benzene (3- <i>p</i> -tolylhexane)..... | 165 (233)‡ | 135 760 | 0.8575 | 1.4910 | | (344) |
| 1-Ethyl-4(1'-methylbutyl)benzene..... | 97 (231)‡ | 11 760 | 0.8626 | 1.4910 | | (384) |
| 1-Ethyl-4- <i>tert</i> -amylbenzene.... | 200-230 (226)‡ | | (0.859)‡ | (1.489)‡ | | (122) |
| 1- <i>n</i> -Propyl-3- <i>n</i> -butylbenzene... | 238 | | (0.856)‡ | 1.4837 | | (244) |
| 1-Isopropyl-2- <i>tert</i> -butylbenzene. | 210? (225)‡ | | (0.868)‡ | (1.498)‡ | | (22) |
| 1-Isopropyl-3- <i>tert</i> -butylbenzene. | 222 | | 0.8512 | 1.4832 | | (22, 218a, contains about 9 per cent mono- <i>tert</i> -heptylbenzene) |
| 1-Isopropyl-4- <i>tert</i> -butylbenzene. | 224 | | 0.8610 | 1.4928 | | (20, 21, 22) |
| 1,3-Dimethyl-4- <i>n</i> -amylbenzene | 124 (234)‡ | 16 760 | (0.868)‡ | 1.4972 | | (254) |
| 1,3-Dimethyl-5- <i>n</i> -amylbenzene | 106 (230)‡ | 10 760 | (0.859)‡ | (1.489)‡ | | (254) |
| 1,3-Dimethyl-4-(1'-methylbutyl)benzene..... | 103 (224)‡ | 11 760 | (0.866)‡ | 1.4959 | | (254) |
| 1,3-Dimethyl-4-(ethylpropyl)benzene..... | 106 (224)‡ | 13 760 | (0.868)‡ | 1.4973 | | (254) |
| 1,3-Dimethyl-4-(2'-methylbutyl)benzene..... | 111 (224)‡ | 13 760 | (0.864)‡ | 1.4942 | | (254) |

TABLE 1—Continued

| FORMULA | HYDROCARBON | BOILING POINT | | d_4^{20} | n_D^{20} | MELTING POINT | REFERENCES |
|---|---|-----------------|-----------|--------------------|----------------------|---------------|-------------|
| | | °C. | mm. | | | | |
| C ₁₃ H ₂₀ (continued) | 1,3-Dimethyl-5-(2'-methyl-butyl)benzene | 108 (220) ‡ | 15 760 | (0.859) ‡ | (1.488) ‡ | | (254) |
| | 1,3-Dimethyl-4-isoamylbenzene. | 232 | | 0.8867? (0.867) | 1.4966 | | (38, 254) |
| | 1,3-Dimethyl-5-isoamylbenzene. | 108 (223) ‡ | 15 760 | (0.859) ‡ | (1.488) ‡ | | (254) |
| | 1,3-Dimethyl-4- <i>tert</i> -amylbenzene..... | 94 (219) ‡ | 14 760 | (0.868) ‡ | (1.498) ‡ | | (254) |
| | 1,3-Dimethyl-5- <i>tert</i> -amylbenzene..... | 103 (215) ‡ | 14 760 | (0.868) ‡ | 1.4982 | | (253, 254) |
| | 1,3-Dimethyl-4-(1',2'-dimethylpropyl)benzene | 102 (219) ‡ | 13 760 | (0.874) ‡ | 1.5022 | | (254) |
| | 1,3-Dimethyl-4-neopentylbenzene..... | 98 (219) ‡ | 10 760 | (0.868) ‡ | 1.5081? (1.498) ‡ | | (254) |
| | 1-Methyl-3-ethyl-6- <i>n</i> -butylbenzene..... | 237 | | 0.8795 | (1.506) ‡ | | (232) |
| | 1-Methyl-3-ethyl-6-isobutylbenzene..... | 229 | | 0.8795 | (1.506) ‡ | | (232) |
| | 1-Methyl-3,5-di- <i>n</i> -propylbenzene..... | 248? (230) ‡ | | (0.859) ‡ | (1.489) ‡ | (-51) ‡ | (168, 372?) |
| | 1-Methyl-2- <i>n</i> -propyl-4-isopropylbenzene | 225.2 | | 0.8650 | 1.4937 | | (66, 192) |
| | 1-Methyl-2,4-diisopropylbenzene..... | 225 | 760 | 0.8664 | 1.499 | | (83, 185?) |

| | | | | | | | |
|--|---|--------|----------|----------|----------|---|-----------------------|
| C ₁₄ H ₂₂ (871 possible; 57 known) | 1-Methyl-2,6-diisopropylbenzene..... | 228 | | 0.8768 | 1.5032 | | (82) |
| | 1-Methyl-3,5-diisopropylbenzene..... | 218 | | 0.8668 | 1.4955 | | (108, 215, 306, 326?) |
| | 1,3-Diethyl-4-isopropylbenzene..... | 226 | | | | | (105) |
| | 1,3?-Diethyl-5?-isopropylbenzene..... | 256? | 760 | (0.868)‡ | (1.498)‡ | | (213) |
| | | (228)‡ | | (0.868)‡ | (1.498)‡ | | |
| | 1,3,5-Trimethyl-2- <i>n</i> -butylbenzene..... | 241 | | (0.878)‡ | (1.505)‡ | | (187) |
| | 1,3,5-Trimethyl-2-isobutylbenzene..... | 230 | | 0.8767 | 1.4995 | | (199) |
| | 1,2,3-Trimethyl-5- <i>tert</i> -butylbenzene..... | 115 | 17 | (0.880)‡ | 1.5049 | | (115) |
| | | (226)‡ | 760 | | | | |
| | 1,2,4-Trimethyl-6- <i>tert</i> -butylbenzene..... | 92 | 3.5 | 0.878)‡ | (1.505)‡ | 32.5 | (61) |
| | | (226)‡ | 760 | | | | |
| | 1,3,5-Trimethyl-2,4-diethylbenzene..... | 236? | | (0.896)‡ | (1.515)‡ | | (281) |
| | | (246)‡ | | | | | |
| | Pentamethylethylbenzene..... | (270)‡ | | (0.915)‡ | (1.524)‡ | 125 | (68) |
| <i>n</i> -Octylbenzene..... | 264 | 760 | 0.8572 | 1.4849 | -37.0 | (3, 81?, 93, 96, 266, 279, 290, 296, 300, 302, 304, 310, 383) | |
| 2-Phenyloctane..... | 125 | 20 | 0.8580 | 1.4850 | -38.9 | (144, 274, 275, 300, 359, 360, 361, 368) | |
| | (253)‡ | 760 | | | | (221) | |
| 4-Phenyloctane..... | 119 | 18 | 0.859 | (1.488)‡ | | (221) | |
| | (253)‡ | 760 | | | | | |
| 1-Phenyl-2-methylheptane..... | 130 | 16 | (0.859)‡ | (1.488)‡ | | (43) | |
| | (257)‡ | 760 | | | | | |

TABLE 1—Continued

| FORMULA | HYDROCARBON | BOILING POINT | | d_4^{20} | n_D^{20} | MELTING POINT | REFERENCES |
|---|--|---------------|-----------|------------|--------------|---------------|------------|
| | | °C. | mm. | | | °C. | |
| C ₁₄ H ₂₂ (continued) | 1-Phenyl-6-methylheptane | 250 | | (0.859) ‡ | (1.488) ‡ | < -20 | (264) |
| | 2-Phenyl-2-methylheptane | 244 | | 0.8756 | 1.4951 | | (154) |
| | 3-Phenyl-3-methylheptane | 121 | 17 | 0.8738 | 1.4932 | | (144, 151) |
| | | (245) ‡ | 760 | | | | |
| | 4-Phenyl-4-methylheptane | 243 | | 0.8704 | 1.4920 | | (138, 151) |
| | 3-Phenyl-3-ethylhexane | 239 | | 0.875 | 1.4943 | | (138, 151) |
| | 3-Phenyl-4-ethylhexane | 206? | 760 | (0.859) ‡ | (1.488) ‡ | | (4, 286) |
| | | (250) ‡ | | | | | |
| | 2-Phenyl-2,3-dimethylhexane | 237 | 760 | 0.8861? | 1.4961 | | (154) |
| | | | | (0.866) ‡ | | | |
| | 2-Phenyl-2,4-dimethylhexane | 239 | 760 | 0.8729 | 1.4920 | | (154) |
| | 2-Phenyl-2,5-dimethylhexane | 238 | | 0.8749 | 1.4939 | | (138, 154) |
| | 3-Phenyl-2,3-dimethylhexane | 238 | | 0.8763 | 1.4958 | | (151) |
| | 3-Phenyl-3,4-dimethylhexane | 114 | 10 | 0.8757 | 1.4929 | | (151) |
| | | (242) ‡ | 760 | | | | |
| | 3-Phenyl-3,5-dimethylhexane | 116 | 10 | 0.8750 | 1.4918 | | (151) |
| | | (242) ‡ | 760 | | | | |
| | 1-Phenyl-2- <i>n</i> -propylpentane (4-benzylheptane) | 244 | | 0.8496? | 1.4844 | | (246) |
| | | | | (0.856) ‡ | | | |
| | 2-Phenyl-2-methyl-3-ethyl- pentane | 237 | 760 | 0.8782? | 1.4942 | | (154) |
| | | | (0.864) ‡ | | | | |
| 3-Phenyl-2-methyl-3-ethyl- pentane | 239 | 760 | 0.8816? | 1.4981 | (151) | | |
| | | | (0.868) ‡ | | | | |
| 2-Phenyl-2,3,3-trimethyl- pentane | 235 | 760 | 0.8939? | 1.5031? | (154) | | |
| | | | (0.867) ‡ | (1.497) ‡ | | | |
| 2-Phenyl-2,4,4-trimethyl- pentane | 235 | 760 | 0.8803? | 1.4938 | (154, 218a?) | | |
| | | | (0.863) ‡ | | | | |

| | | | | | | |
|--|-----------------|-------------|---------------------|---------------------|--------|---|
| 3-Phenyl-2,2,3-trimethyl-pentane..... | 259? (239)‡ | 760 | (0.867)‡ | (1.497)‡ | | (151) |
| 3-Phenyl-2,3,4-trimethyl-pentane..... | 237 | | 0.8808? (0.867)‡ | 1.4970 | | (151, 152) |
| 1-Methyl-2- <i>n</i> -heptylbenzene.... | 263 | 760 | 0.8717 | 1.4951 | | (96) |
| 1-Methyl-3- <i>n</i> -heptylbenzene.... | 261 | | 0.8615 | 1.4913 | (-40)‡ | (96) |
| 1-Methyl-4- <i>n</i> -heptylbenzene.... | 265 | | 0.8573 | 1.4891 | -28.5 | (96, 305) |
| 1,4-Di- <i>n</i> -butylbenzene..... | 260 | | 0.8556 | 1.4881 | -24 | (142, 235, 241) |
| 1- <i>n</i> -Butyl-4- <i>sec</i> -butylbenzene... | 251 | | 0.8570 | 1.4885 | | (142) |
| 1- <i>n</i> -Butyl-4- <i>isobutyl</i> benzene.... | 252 | | 0.8508 | 1.4858 | | (142) |
| 1- <i>n</i> -Butyl-4- <i>tert</i> -butylbenzene.. | 249 | | 0.8595 | 1.4898 | -46 | (142) |
| 1,3-Di- <i>sec</i> -butylbenzene..... | 90 (245)‡ | 3 760 | (0.859)‡ | 1.4890 | | (23) |
| 1,4-Di- <i>sec</i> -butylbenzene..... | 239 | 760 | 0.8590 | 1.4892 | -58 | (51, 102?, 142, 160, 230, 237, 368, 384) |
| 1- <i>sec</i> -Butyl-4- <i>isobutyl</i> benzene.. | 242 | 760 | 0.8511 | 1.4856 | | (142) |
| 1- <i>sec</i> -Butyl-4- <i>tert</i> -butylbenzene. | 236 | | 0.8607 | 1.4892 | | (142) |
| 1,4-Diisobutylbenzene..... | 243 | | 0.8456? (0.859)‡ | 1.4834? (1.488)‡ | -21 | (142) |
| 1-Isobutyl-4- <i>tert</i> -butylbenzene.. | 239 | 760 | 0.8457? (0.859)‡ | 1.4875 | | (142) |
| 1,3-Di- <i>tert</i> -butylbenzene..... | 106.5 (241)‡ | 18.2 760 | (0.858)‡ | 1.4870 | 10.6 | (48?, 172a, 213?, 313?) |
| 1,4-Di- <i>tert</i> -butylbenzene..... | 237 | | (0.860)‡ | 1.4904‡ | 77.8 | (26, 41, 52, 142, 143, 153, 160, 162, 202, 204, 213, 230, 235a, 237, 294, 313, 322, 323, 325, 326, 341, 368, 377) |
| 1,3-Dimethyl-4- <i>n</i> -hexylbenzene. | 133 (248)‡ | 13 760 | 0.886? (0.867)‡ | 1.4972 | | (104) |
| 1,3-Dimethyl-4-(1'-ethylbutyl)-benzene..... | 102 238 | 3 760 | 0.8645 | 1.493 | | (344) |

TABLE 1—Continued

| FORMULA | HYDROCARBON | BOILING POINT | | d_4^{20} | n_D^{20} | MELTING POINT | REFERENCES |
|---|--|----------------|-----------|----------------------|------------|---------------|---------------|
| | | °C. | mm. | | | | |
| C ₁₄ H ₂₂ (continued) | 1,2?-Dimethyl-3?(2'-ethyl-butyl)benzene | 113 (259) ‡ | 12 760 | 0.9022? (0.884) ‡ | 1.5082 | | (102a) |
| | 1-Methyl-3-ethyl-6-isoamylbenzene | 246 | | 0.8733 | (1.502) ‡ | | (232) |
| | 1-Methyl-4-isopropyl-2- <i>n</i> -butylbenzene | 235 | | 0.8897? (0.867) ‡ | (1.497) ‡ | | (66) |
| | 1-Methyl-4-isopropyl-2-iso-butylbenzene | 230 | 760 | 0.9136? (0.867) ‡ | (1.497) ‡ | | (66) |
| | 1-Methyl-2-isopropyl-5- <i>tert</i> -butylbenzene | 236 | 760 | (0.867) ‡ | (1.497) ‡ | | (20, 21) |
| | 1-Methyl-3?-isopropyl-4- <i>tert</i> -butylbenzene | 231 | 760 | (0.867) ‡ | (1.497) ‡ | | (20, 21) |
| | 1-Methyl-3-isopropyl-5- <i>tert</i> -butylbenzene | 228 | 760 | 0.8660 | 1.4950 | | (19, 21) |
| | 1-Methyl-3-isopropyl-6- <i>tert</i> -butylbenzene | 238 | 760 | (0.867) ‡ | (1.497) ‡ | | (20, 21) |
| | 1-Methyl-4-isopropyl-2- <i>tert</i> -butylbenzene | 238 | 760 | (0.867) ‡ | (1.497) ‡ | | (19, 22) |
| | 1-Methyl-4-isopropyl-3- <i>tert</i> -butylbenzene | 228 | 760 | 0.8839? (0.867) ‡ | 1.4972 | | (19, 22, 126) |
| | 1-Ethyl-3,5?-diisopropylbenzene | 228 | 760 | 0.8610 | 1.4918 | | (90) |
| | 1,3,5-Trimethyl-2-(3'-methyl-butyl)benzene | 243 | | 0.8776 | 1.4992 | | (199) |

| | | | | | | | |
|---|--|---------------|-----------|---------------------|---------------------|--------|---|
| C ₁₆ H ₂₄ (2217 possible; 23 known) | 1,3-Dimethyl-2-ethyl-5- <i>tert</i> -butylbenzene..... | 125 (237)‡ | 20 760 | (0.877)‡ | 1.5044 | | (115) |
| | 1-Methyl-2,6-diethyl-4-isopropylbenzene | 245 | | 0.8810? (0.868)‡ | 1.498 | | (369) |
| | 1,2,3,4-Tetraethylbenzene..... | 254 | 760 | 0.8873 | 1.5101 | < -50 | (117, 170, 271, 334, 335) |
| | 1,2,3,5-Tetraethylbenzene..... | 249 | | 0.8799 | 1.5056 | -21 | (333, 334) |
| | 1,2,4,5-Tetraethylbenzene..... | 248 | | 0.8788 | 1.5054 | 10 | (164? 171, 193, 333, 334, 353, 362, 372?) |
| | <i>n</i> -Nonylbenzene..... | 282 | 760 | 0.8584 | 1.4863 | (-29)‡ | (81?, 175, 176, 204, 242, 296, 317, 328, 385) |
| | 2-Phenylnonane..... | 147 (273)‡ | 19 760 | 0.8627 | 1.4875 | | (359, 360, 361) |
| | 5-Phenylnonane..... | 127 (273)‡ | 12 760 | 0.8586 | 1.4868 | | (275) |
| | 1-Phenyl-5-methyloctane } ?..... | 271 | | 0.8857? (0.858)‡ | 1.5020? (1.487)‡ | | (81, mixture) |
| | 1-Phenyl-5-ethylheptane } | | | | | | |
| | 4-Phenyl-4-ethylheptane..... | 128 (264)‡ | 15 760 | 0.8698 | 1.4900 | | (138) |
| | 3-Phenyl-3,6-dimethylheptane.. | 123 (261)‡ | 14 760 | 0.8760 | 1.4959 | | (138) |
| | 3-Phenyl-5-methyl-3-ethylhexane..... | 242 | | 0.8696 | 1.4888 | | (138) |
| | 3-Phenyl-2,4-dimethyl-3-ethylpentane?..... | 253 | 760 | 0.8746 | 1.4940 | | (152) |
| | 1-Methyl-4- <i>n</i> -octylbenzene..... | 283 | 760 | 0.8574 | 1.4872 | -23 | (223, 291, 292, 305) |
| | 1-Methyl-4-(1'-methylheptyl)benzene..... | 116 (270)‡ | 7 760 | 0.8607 | 1.4877 | | (384) |
| | 1-Methyl-4-(1',5'-dimethylhexyl)benzene (2-methyl-6- <i>p</i> -tolylheptane) .. | 136 (265)‡ | 15 760 | 0.8488 | 1.4815 | | (174?, 295) |

TABLE 1—Continued

| FORMULA | HYDROCARBON | BOILING POINT | | d_4^{20} | n_D^{20} | MELTING POINT | REFERENCES | |
|---|---|------------------------------|----------------|---------------------|---------------------|---------------------|--|----------------------|
| | | °C. | mm. | | | | | °C. |
| C ₁₅ H ₂₄ (continued) | 1-Isopropyl-4-(3'-methylamyl) benzene..... | 266 | 760 | 0.8602 | 1.4897 | | (196) | |
| | 1- <i>tert</i> -Butyl-2- <i>tert</i> -amylbenzene..... | 243 | | 0.8645 | 1.4885 | | (218a; contains 87 per cent <i>tert</i> -octylbenzene) | |
| | 1,3-Dimethyl-5-(triethylmethyl)benzene..... | 259 | 760 | (0.858)‡ | (1.487)‡ | | (24) | |
| | 1-Methyl-4-isopropyl-2-isoamylbenzene..... | 245 | | 0.887? (0.866)‡ | (1.496)‡ | | (66) | |
| | 1-Methyl-2,4?-di- <i>tert</i> -butylbenzene..... | 247 | 760 | 0.9044? (0.866)‡ | 1.5158? (1.496)‡ | | (215) | |
| | 1-Methyl-3,5?-di- <i>tert</i> -butylbenzene..... | 244 | 760 | (0.858)‡ | (1.487)‡ | 32 | (26, 58, 59, 213, 257) | |
| | 1,2,4-Tri- <i>n</i> -propylbenzene..... | 135 (261)‡ | 20 760 | (0.865)‡ | 1.4950 | | (18, 324?) | |
| | 1,3,5-Tri- <i>n</i> -propylbenzene..... | 133 (257)‡ | 20 760 | (0.858)‡ | (1.487)‡ | (-29)‡ | (18, 132?) | |
| | 1,2,4-Triisopropylbenzene..... | 244 | | 0.8620 | 1.4924 | | (34, 48, 160, 185, 237, 248, 327) | |
| | 1,3,5-Triisopropylbenzene..... | 238 | 760 | 0.8547 | 1.4882 | -15 | (34, 88, 135, 136, 248) | |
| | 1,3,5-Trimethyl-2,4,6-triethylbenzene..... | 247? (283)‡ | | (0.906)‡ | (1.519)‡ | | (281) | |
| | C ₁₆ H ₂₆ (5749 possible; 19 known) | <i>n</i> -Decylbenzene?..... | 293? (302)‡ | 760 | 0.8805? (0.858)‡ | 1.4970? (1.486)‡ | | (81) |
| | | 2-Phenyldecane..... | 132 (293)‡ | 3 760 | 0.8620 | 1.4864 | | (144, 359, 360, 361) |

| | | | | | | | |
|--|--------|-----|----------|----------|----------|------------------------------|---------------|
| 1-Phenyl-6-methylnonane | } | } | 289? | 0.8809? | 1.4988? | | |
| 1-Phenyl-6-ethyloctane | | | (299)† | (0.858)† | (1.480)† | | (81, mixture) |
| 1-Phenyl-3,7-dimethyloctane | | | 275 | 0.8722? | 1.4919 | | (197) |
| 4-Phenyl-4- <i>n</i> -propylheptane | 141 | 15 | 0.8694 | 1.4902 | | (138) | |
| | (283)† | 760 | | | | | |
| 4-Phenyl-2,4,6-trimethylheptane | 144 | 18 | 0.8753? | 1.4930 | | (138) | |
| | (277)† | 760 | (0.863)† | | | | |
| 1-Methyl-4- <i>n</i> -nonylbenzene | 161 | 12 | (0.858)† | (1.487)† | < -20 | (140) | |
| | (298)† | 760 | | | (-20)† | | |
| 1-Ethyl-4-(1'-methylheptyl)benzene | 126 | 7 | 0.8609 | 1.4874 | | (384) | |
| | (286)† | 760 | | | | | |
| 1,3-Di- <i>sec</i> ?-amylbenzene | 265 | | 0.8522 | 1.4830 | < -75 | (108?, 316, 360) | |
| 1,4-Di-(1'-methylbutyl)benzene | 265 | | 0.8619 | 1.4880 | | (263, 368, 384) | |
| 1,3-Di- <i>tert</i> ?-amylbenzene | 265 | | 0.8727? | 1.4948? | < -20 | (10, 75) | |
| | | | (0.858)† | (1.487)† | | | |
| 1,4-Di- <i>tert</i> -amylbenzene | 265 | 760 | 0.8526 | 1.4862 | | (263, 322, 323) | |
| 1,3-Dimethyl-5?- <i>n</i> -octylbenzene | (271)† | | (0.858)† | (1.487)† | -66 | (274) | |
| 1,3,5-Trimethyl-2- <i>n</i> -heptylbenzene | 272 | 760 | 0.8732 | 1.4958 | | (199) | |
| 1-Methyl-2,4,6-triisopropylbenzene | 253? | | 0.8695 | 1.4994 | < -20 | (83, 91) | |
| | (261)† | | | | | | |
| Diethyldiisopropylbenzene (probably a mixture) | 257 | | 0.8686 | 1.4986 | < -50 | (90) | |
| Pentaethylbenzene | 277 | 760 | 0.8965 | 1.5166 | < -20 | (85, 99, 170, 333, 335, 353) | |
| 1,3-Dimethyltetraethylbenzene | 260? | | 0.8771? | 1.4958? | | (117, 345) | |
| | (289)† | | (0.903)† | (1.518)† | | | |

TABLE 1—Continued

| FORMULA | HYDROCARBON | BOILING POINT | | d_4^{20} | n_D^{20} | MELTING POINT | REFERENCES |
|---|--|---------------|----------|------------|------------|---------------|---|
| | | °C. | mm. | | | °C. | |
| C ₁₇ H ₂₆ (14,837 possible; 10 known) | <i>n</i> -Hendecylbenzene | 296? | 760 | (0.8575)‡ | 1.4868 | (-11)‡ | (242) |
| | 2-Phenylhendecane | 171 | 12 | 0.8600 | 1.4824 | -35 | (274, 278, 359, 360, 361) |
| | 2-Phenyl-2-methyldecane | 160 | 20 | 0.8676 | 1.4859 | | (396) |
| | 2-Phenyl-2-methyl-4-ethyl- octane | 149 | 20 | 0.8620 | 1.4875 | | (396) |
| | 4-Phenyl-2-methyl-4-propyl- heptane | 144 | 11 | 0.8722 | 1.4932 | | (138) |
| | 1-Methyl-4- <i>n</i> -decylbenzene | 169 | 11 | 0.8549 | 1.4854 | -11.5 | (305) |
| | | (316)‡ | | | | | |
| | 1-Ethyl-2,4,5?-triiisopropyl- benzene | 260? | 760 | (0.871)‡ | (1.500)‡ | 106.9 | (91) |
| | | (271)‡ | | | | | |
| | 1-Ethyl-2,4,6?-triiisopropyl- benzene | 256? | | 0.8670 | 1.4981 | -35 | (91?, 116) |
| | (271)‡ | | | | | | |
| 1,3,-Dimethyl-2,4,6?-triiiso- propylbenzene | 276 | | 0.893 | 1.5105 | -25 | (91) | |
| Methylpentaethylbenzene | 294 | 760 | (0.900)‡ | (1.516)‡ | 43 | (89) | |
| C ₁₈ H ₂₀ (38,636 possible; 18 known) | <i>n</i> -Dodecylbenzene | 185 | 15 | 0.8564 | 1.4838 | -3 | (124, 158, 175, 176, 177, 266, 274, 277, 302, 303, 304) |
| | 2-Phenyldodecane | 184 | 20 | 0.8547 | 1.4822 | | (124, 144, 303, 368) |
| | 3-Phenyldodecane | 171 | 13 | 0.8569 | 1.4837 | | (124, 303) |
| | 4-Phenyldodecane | 164 | 17 | 0.8581 | 1.4852 | -24 | (124, 274, 279, 303) |
| | 5-Phenyldodecane | 158 | 7.5 | 0.8589 | 1.4865 | | (124, 303) |
| | 6-Phenyldodecane | 190 | 35 | 0.8570 | 1.4868 | | (124, 303) |
| | 1-Phenyl-3-methylhendecane | 144 | 2 | 0.8618 | 1.4870 | | (219) |
| | 5-Phenyl-2,5,8-trimethyl- nonane | 155 | 15 | 0.8728 | 1.4913 | | (138) |

| | | | | | | | |
|--|--|--------------|-----|-------------------------|-------------------|--------|---|
| C ₁₅ H ₃₂ (100,622 possible; 10 known) | 1-Phenyl-5-methyl-3-isoamyl-hexane (5-benzyl-2,8-dimethylnonane) | 150 | 11 | (0.857) ‡ | (1.485) ‡ | | (46) |
| | 1-Methyl-4- <i>n</i> -hendecylbenzene | 172 | 12 | (0.857) ‡ | (1.485) ‡ | (-2) ‡ | (140) |
| | 1,4-Di(1'-ethylbutyl)benzene | 106 | 0.3 | 0.916? (0.857) ‡ | 1.5020? (1.485) ‡ | | (344) |
| | 1,3-Dimethyl-5?--(2'-methyl-nonyl)benzene | 155-174 | 10 | (0.857) ‡ | (1.485) ‡ | | (144) |
| | 1,2,4?-Tri- <i>tert</i> -butylbenzene | 285-305 | 760 | (0.863) ‡ | (1.493) ‡ | | (160, 162, 202, 213, 218a) |
| | 1,3,5?-Tri- <i>tert</i> -butylbenzene | 293 | | (0.857) ‡ | (1.485) ‡ | 128 | (313, 341) |
| | 1,2,4,5-Tetraisopropylbenzene | 260? (283) ‡ | 760 | 0.850 †? (0.870) ‡ | (1.50) ‡ | 118.4 | (34, 48, 58, 91, 102, 132, 160, 185, 202, 248, 327) |
| | 1,2,4-Triethyl-3,6?-diisopropylbenzene | 285 | | 0.887 | (1.510) ‡ | | (90) |
| | 1,3,5-Triethyl-2,4-diisopropylbenzene | 279 | | 0.883 | (1.508) ‡ | | (90) |
| | Hexaethylbenzene | 300 | | 0.907 † 0.99 (solid) | 1.521 † | 128.3 | (5, 34, 48, 85, 90, 99, 110, 117, 132, 134, 170, 202, 217, 245, 301, 333, 353, 395) |
| | <i>n</i> -Tridecylbenzene | 189 | 10 | (0.856) ‡ | (1.484) ‡ | (5) ‡ | (394) |
| | 2-Phenyltridecane | 120 | 1 | (0.855) ‡ | 1.4824 | | (330) |
| | 7-Phenyltridecane | 184 | 20 | 0.8541 | 1.4811 | -28.2 | (275, 300) |
| | 5-Phenyl-2,8-dimethyl-5-ethyl-nonane | 172 | 14 | 0.8945? (0.863) ‡ | 1.5053? (1.493) ‡ | | (138) |
| | 1-Methyl-4- <i>n</i> -dodecylbenzene | 155 | 1.5 | 0.8560 | 1.4845 | 5.0 | (305) |
| | 1-Methyl-4-(1'-methylhendecyl)benzene | 167 | 8 | 0.8594 | 1.4841 | | (384) |
| | 1- <i>n</i> -Hexyl-4- <i>n</i> -heptylbenzene | 187 | 10 | (0.856) ‡ | (1.484) ‡ | -32 | (289) |
| | 1-Methyl-2,4,5?-tri- <i>tert</i> -butylbenzene | 160-170 | 4 | (0.869) ‡ | 1.584? (1.498) ‡ | | (215) |

TABLE 1—Continued

| FORMULA | HYDROCARBON | BOILING POINT | | d_4^{20} | n_D^{20} | MELTING POINT | REFERENCES |
|---|---|----------------|-----|---------------------|---------------------|---------------|---|
| | | °C. | mm. | | | | |
| C ₁₉ H ₃₂ (continued) | 1-Methyl-2,3,5,6-tetraiso-propylbenzene..... | 271? (303)‡ | 760 | 0.9111? (0.892)‡ | 1.5123 | 10 | (91) |
| | 1,3-Diethyl-2,4,6?-triisopropylbenzene..... | 280? (297)‡ | | 0.8837 | 1.5051 | -65 | (91) |
| C ₂₀ H ₃₄ (263,381 possible; 5 known) | <i>n</i> -Tetradecylbenzene..... | 196 | 9 | 0.8565 | 1.4836 | 8.6 | (124, 175, 176, 177, 302, 304) |
| | 2-Phenyltetradecane..... | 188 | 7 | 0.8555 | 1.4820 | -7 | (276) |
| | 5-Phenyl-2,8-dimethyl-5- <i>n</i> -propylnonane..... | 181 | 15 | 0.8677 | 1.4855 | | (138) |
| | 1-Ethyl-4-(1'-methylhendecyl)benzene..... | 173 | 7 | 0.8586 | 1.4852 | | (384) |
| | ?-Diheptylbenzene..... | 165 | 9 | 0.854 | 1.4839 | | (360) |
| C ₂₁ H ₃₆ (690,709 possible; 4 known) | 5-Phenyl-2,8-dimethyl-5- <i>iso</i> -butylnonane..... | 173 | 11 | 0.8982? (0.861)‡ | 1.5042? (1.491)‡ | | (138) |
| | 1-Methyl-4- <i>n</i> -tetradecylbenzene..... | 170 | 0.8 | 0.8560 | 1.4839 | 16.8 | (305) |
| | 1,2,4?-Triamylbenzene..... | 312-318 | 760 | 0.867 | 1.497 | | (160, 316) |
| | 1,3,5?-Triamylbenzene..... | 282-288 | 760 | (0.856)‡ | (1.483)‡ | | (160) |
| C ₂₂ H ₃₈ (1,817,544 possible; 8 known) | <i>n</i> -Hexadecylbenzene..... | 237 | 16 | 0.8560 | 1.4814 | 27 | (1, 96, 124, 208, 209, 210, 217, 249, 276, 302, 304, 389) |
| | 2-Phenylhexadecane..... | 191 | 6 | 0.8643 | 1.4834 | | (359, 360, 361) |

| | | | | | | | |
|---|---|-------|------|-------------------|-------------------|----------|---|
| C ₂₃ H ₄₀ (4,793,449 possible; 4 known) | 2-Phenyl-2-methylpentadecane..... | 195 | 7 | 0.8611 | 1.4825 | -29 | (276) |
| | 4-Phenyl-2-methyl-4-isobutylhendecane..... | 180 | 6 | 0.8700 | 1.4982 | -50 | (278) |
| | 1-Phenyl-2- <i>n</i> -heptylnonane (8-benzylpentadecane)..... | 204 | 14 | (0.855) ‡ | (1.482) ‡ | | (46) |
| | 7-Di- <i>sec</i> -octylbenzene..... | 341 | 760 | (0.855) ‡ | (1.482) ‡ | | (144, 160) |
| | 1,4? -Di-(3'-methylheptyl)benzene..... | >190 | 10 | (0.855) ‡ | (1.482) ‡ | | (144) |
| | 1-Methyl-4-isopropyl-2- <i>n</i> -dodecylbenzene..... | 164 | 1 | 0.8595 | 1.4878 | | (249) |
| | <i>n</i> -Heptadecylbenzene..... | | | (0.855) ‡ | (1.481) ‡ | 38? (32) | (394) |
| | 1-Methyl-2- <i>n</i> -hexadecylbenzene..... | 239 | 15 | 0.8604 | (1.490) ‡ | 9 | (209) |
| | 1-Methyl-3- <i>n</i> -hexadecylbenzene..... | 237 | 15 | 0.8557 | (1.483) ‡ | 12 | (209) |
| | 1-Methyl-4- <i>n</i> -hexadecylbenzene..... | 240 | 15 | 0.8548 | (1.480) ‡ | 27.5 | (209) |
| C ₂₄ H ₄₂ (12,675,741 possible; 10 known) | <i>n</i> -Octadecylbenzene..... | 249 | 15 | 0.8565 | 1.4816 | 36 | (1, 125a, 145, 204, 208, 210, 216, 217, 238, 240, 312, 354, 375, 383, 389) (297a) |
| | 9-Phenyloctadecane..... | 150 | 0.08 | 0.8744? (0.857) ‡ | 1.4862 | | |
| | 2-Phenyl-2-methylheptadecane..... | 190 | 9 | 0.8870? (0.860) ‡ | 1.5096? (1.490) ‡ | -40 | (278) |
| | 5-Phenyl-5- <i>n</i> -butyltetradecane.. | 185 | 6 | 0.8559 | 1.4814 | -48 | (279) |
| | 1-Phenyl-2,2-dimethylhexadecane..... | | | (0.855) ‡ | (1.481) ‡ | -19 | (273) |
| | 2-Phenyl-2,4-dimethylhexadecane..... | 182 | 3 | (0.856) ‡ | 1.4825 | | (330) |
| | 1-Phenyl-12- <i>n</i> -propylpentadecane..... | 153.5 | 0.1 | (0.854) ‡ | 1.4781 | | (342b) |

TABLE 1—*Concluded*

| FORMULA | HYDROCARBON | BOILING POINT | | d_4^{20} | n_D^{20} | MELTING POINT | REFERENCES |
|---|--|---------------|------|------------|------------|---------------|-----------------------------|
| | | °C. | mm. | | | | |
| C ₂₄ H ₄₂ (continued) | ?-Dinonylbenzene..... | 152-163 | 5 | (0.855)‡ | (1.481)‡ | | (160) |
| | 1,3-Dimethyl-4- <i>n</i> -hexadecylbenzene..... | 250 | 15 | 0.858b† | (1.487)‡ | 33.5 | (209, 210) |
| | Hexa- <i>n</i> -propylbenzene..... | 332 | 760 | 0.871b† | (1.500)‡ | 103 | (132) |
| C ₂₅ H ₄₄ (6 known) | 4-Phenyl-13- <i>n</i> -propylhexadecane..... | 147.5 | 0.08 | (0.855)‡ | 1.4813 | | (342b) |
| | 1-Phenyl-3- <i>n</i> -octylhendecane (9-(2'-phenylethyl)heptadecane)..... | 189 | 1 | 0.8560 | 1.4806 | -26.7 | (298, 299, 300) |
| | 1-Methyl-4-(1'-methylheptadecyl)benzene (2- <i>p</i> -tolyl-octadecane)..... | 237 | 8 | 0.8563 | 1.4798 | | (384) |
| | 1-Methyl-4-(1'-octyldecyl)benzene (9- <i>p</i> -tolyl-octadecane)..... | 185 | 1 | 0.8551 | 1.4811 | < -40 | (74, 298, 299, 300) |
| | 1,2,4-Trimethyl-5- <i>n</i> -hexadecylbenzene..... | 224 | 2 | 0.8782 | 1.4977 | -50 | (276) |
| | 1,3,5-Trimethyl-2- <i>n</i> -hexadecylbenzene..... | 258 | 15 | 0.858† | (1.487)‡ | 40 | (209, 210) |
| | | | | | | | |
| C ₂₆ H ₄₆ (10 known) | 1-Phenyleicosane..... | 212 | 1 | 0.8544† | 1.4801† | 43 | (299, 300, 317a, 342a, 387) |
| | 2-Phenyleicosane..... | 204.5 | 1 | 0.8550† | 1.4795 | 29.0 | (299, 300, 388) |
| | 3-Phenyleicosane..... | 202 | 1 | 0.8549† | 1.4796 | 29.3 | (298, 299, 300, 388) |
| | 4-Phenyleicosane..... | 199 | 1 | 0.8548† | 1.4794 | 31.4 | (299, 300, 388) |
| | 5-Phenyleicosane..... | 197 | 1 | 0.8548† | 1.4796 | 30.2 | (276, 298, 299, 300, 388) |
| | 7-Phenyleicosane..... | 196 | 1 | 0.8537 | 1.4794 | 16.4 | (298, 299, 300, 388) |
| | 9-Phenyleicosane..... | 196 | 1 | 0.8532 | 1.4790 | 17.9 | (298, 299, 300, 388) |
| | 1-Methyl-4-(1'- <i>n</i> -heptyldodecyl)benzene (8- <i>p</i> -tolyl-nonadecane)..... | 195 | 1 | 0.8530 | 1.4808 | 8.7 | (300) |

| | | | | | | | |
|---|--|---------|-----|-------------------------|----------|------|--------------------------|
| | 1,4?-Di- <i>sec</i> -decylbenzene..... | 230 | 10 | (0.855)† | (1.481)‡ | | (144) |
| | ?-Tetraamylbenzene..... | 340-390 | 760 | 0.89‡ (0.864)‡ | (1.494)‡ | | (316) |
| C ₂₇ H ₄₈ | 11-Phenylheneicosane..... | 204 | 1 | 0.8533 | 1.4788 | 20.8 | (74, 298, 299, 300, 386) |
| C ₂₈ H ₅₀ (4 known) | 1-Phenyldocosane..... | 247 | 4 | 0.8547 | 1.4825 | 44 | (238, 239) |
| | 5-Phenyldocosane..... | 201 | 1 | 0.8587 | 1.4796 | 38 | (238, 240) |
| | 11-Benzylheneicosane..... | 211 | 1 | 0.8544 | 1.4838 | -2.1 | (46, 300) |
| | 1,3-Dimethyl-4,6?-di(2'-methylnonyl)benzene..... | >234 | 10 | (0.863)‡ | (1.493)‡ | | (144) |
| C ₃₀ H ₅₄ | ?-Di- <i>sec</i> -dodcylbenzene..... | >241 | 10 | (0.854)‡ | (1.48)‡ | | (144, 160) |
| | ?-Tri- <i>sec</i> -octylbenzene..... | >176 | 1 | (0.854)‡ | (1.48)‡ | | (144) |
| C ₃₁ H ₅₆ | 13-Phenylpentacosane..... | 235 | 1 | 0.8541† 0.95 (solid) | 1.4787 | 33 | (269, 298, 299, 300) |
| C ₃₂ H ₅₈ | 5-Phenylhexacosane..... | 255 | 4 | 0.8565 | 1.4806 | 33 | (238, 239) |
| C ₃₃ H ₇₀ | 1,4-Di- <i>n</i> -hexadecylbenzene..... | | | (0.853)‡ | (1.48)‡ | 53.6 | (375, 389) |
| C ₄₁ H ₇₆ | 18-Phenylpentatriacontane..... | | | 0.856† | (1.484)‡ | 62 | (346) |
| C ₄₂ H ₇₈ | 1,2-Dioctadecylbenzene..... | | | 0.856† | (1.484)‡ | 70 | (238) |
| C ₅₀ H ₉₄ | 1,2-Di-(1'-butyloctadecyl)-benzene..... | | | 0.850† | (1.48)‡ | 66 | (238) |
| C ₆₀ H ₁₁₄ | Trioctadecylbenzene..... | | | 0.855† | 1.4832‡ | 47 | (238) |

* Roman numerals indicate different crystalline forms.

† Extrapolated value.

‡ Observations in parentheses are calculated.

§ These hydrocarbons are unknown.

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