ALKYL BENZENES

In this chapter we discuss the correlations obtained using $M'$, $A'$, $\chi_l^V$ and $Pn\chi_l$ parameters of alkyl benzenes with their 14 physicochemical properties which are the same which have been studied for alkanes and monoaliphatic alcohols in the last two chapters. The molar refraction of the alkyl benzenes has been studied at 293.15°K instead of at 293.15°K studied for alkanes and alcohols. The second virial coefficient at 393.10°K has been studied in the case of alkylbenzenes while in case of alkanes and monoaliphatic alcohols the second virial coefficient was studied at 298.15°K and 393.20°K respectively.

The propertywise discussion of the significant correlations obtained are given below and the results obtained have also been evaluated with reference to the earlier works, uncertainties in the data used and the suitability of the topological parameters used:

1. ENTHALPY OF VAPORIZATION AT 298.15°K, $\Delta H_v^{298}$ (kJ mol$^{-1}$), $N = 47$; RANGE : 33.85-109.2

   (a) $M'$ & $A'$ PARAMETERS

   $\Delta H_v^{298} = 0.942 M' + 12.026$ ... (254)
   $r = 0.9958$, $s = 1.64$; $F = 5269$

   $\Delta H_v^{298} = 23.433 A' - 3.771$ ... (255)
   $r = 0.9954$, $s = 1.71$; $F = 4817$
\[ \Delta_{v}^{293} = 4.649 M^* - 92.309 A' + 74.313 \]
\[ r = 0.9965, s = 1.50 \ ; \ F = 3126 \]

(b) $^n\chi_t$ PARAMETERS

\[ \Delta_{v}^{298} = 6.857 \chi_v^v + 5.837 \]
\[ r = 0.9967, s = 1.44 \ ; \ F = 6774 \]

\[ \Delta_{v}^{298} = 6.745 \chi_v^v - 4.403 \chi_C^v + 8.020 \]
\[ r = 0.9981, s = 1.11 \ ; \ F = 5720 \]

\[ \Delta_{v}^{298} = 7.282 \chi_v^v - 4.172 \chi_C^v + 18.426 / \chi_v^v - 0.800 \]
\[ r = 0.9986, s = 0.95 \ ; \ F = 5241 \]

(c) $^{m}\chi_t$ PARAMETERS

\[ \Delta_{v}^{298} = 23.466 P_1^1 \chi - 3.953 \]
\[ r = 0.9962, s = 1.54 \ ; \ F = 5926 \]

\[ \Delta_{v}^{298} = 23.981 P_1^1 \chi + 13.317 P_4^4 \chi_{PC}^t - 7.446 \]
\[ r = 0.9979, s = 1.16 \ ; \ F = 5260 \]

\[ \Delta_{v}^{298} = -39.316 P_0^0 \chi + 111.826 P_1^1 \chi + 16.974 P_4^4 \chi_{PC}^t - 26.029 \]
\[ r = 0.9961, s = 0.79 \ ; \ F = 7640 \]

The uncertainties in the data of 47 alkyl benzenes used in the present investigations have been reported between 0.04 to 4. J mol$^{-1}$. Eq.(262) which is three variable correlation using $^{m}\chi_t$ is the best three parameter equation
with $s = 0.79 \text{ kJ mol}^{-1}$ and is of the same order as have been obtained in case of alkanes using a three parameter correlation, Eq.(9) ($s = 0.59 \text{ kJ mol}^{-1}$) and for monoaliphatic alcohols for a three parameter correlation Eq.(135); $s = 0.69 \text{ kJ mol}^{-1}$. The observed and calculated values of $\Delta H^\circ_v$ for alkyl benzenes based on Eq.(262) are given in table 9. For the 47 alkylbenzenes used in the regression analysis in table 9 the maximum positive and negative deviations are +2.77 kJ mol$^{-1}$ and -1.01 kJ mol$^{-1}$ for benzene and 1-methyl-3-isopropylbenzene respectively. Besides these two compounds there are only five more compounds which have deviations of $>\pm 1 \text{ kJ mol}^{-1}$.

(2) BOILING POINT, $T_b$ (°C), $N = 47$; RANGE: 81.100-378.

(a) $M'$ & $A'$ PARAMETERS

\[
T_b = 3.596 M' + 28.882 \quad \ldots \quad (263)
\]

\[
r = 0.9809, \; s = 10.06 \; ; \; F = 2028
\]

\[
T_b = 89.475 A' - 31.372 \quad \ldots \quad (264)
\]

\[
r = 0.9884, \; s = 10.36 \; ; \; F = 1907
\]

\[
T_b = 30.049 M' - 658.734 A' + 473.444 \quad \ldots \quad (265)
\]

\[
r = 0.9914, \; s = 9.05 \; ; \; F = 1259
\]

(b) $\chi_c^V$ PARAMETERS

\[
T_b = 26.241 \chi_c^V + 4.826 \quad \ldots \quad (266)
\]

\[
r = 0.9922, \; s = 8.53; \; F = 2835
\]
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<th>COMPOUND</th>
<th>( \Delta H^\circ / \text{kJ mol}^{-1} )</th>
<th>( T / ^\circ \text{C} )</th>
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\[ T_b = 21.393 \chi^y - 168.108/\chi^y + 84.230 \quad \ldots \quad (267) \]
\[ r = 0.9953, \; s = 6.68; \; F = 2327 \]

\[ T_b = 31.833 \chi^y - 203.318 \chi^y - 150.277/\chi^y + 65.241 \]
\[ r = 0.9965, \; s = 5.82; \; F = 2049 \]

(c) \( P^\alpha \chi_t \) PARAMETERS

\[ T_b = 89.593 P^1 \chi - 32.091 \quad \ldots \quad (269) \]
\[ r = 0.9894, \; s = 9.93; \; F = 2083 \]

\[ T_b = 54.390 P^1 \chi - 310.387 / P^1 \chi + 185.913 \quad \ldots \quad (270) \]
\[ r = 0.9959, \; s = 6.24; \; F = 2675 \]

\[ T_b = -139.449 P^0 \chi + 362.281 P^1 \chi - 338.479/P^1 \chi + 143.149 \]
\[ r = 0.9970, \; s = 5.44; \; F = 2345 \]

There are no correlations between \( T_b \) of alkylbenzenes and topological or other parameter available in literature. Eq.(272) is the best 3 parameter correlation using \( P^\alpha \chi_t \) with \( s = 5.44 ^\circ C \) which is well within the uncertainties (\pm 0.02-20 ^\circ C) in the data. The following 7 variable correlation in terms of \( P^\alpha \chi_t \) parameters:

\[ T_b = 55.221 P^1 \chi - 9.407 P^2 \chi - 112.015 P^3 \chi - 68.044 P^4 \chi + 211.659 P^4 \chi p + 4836.433 /P^0 \chi - 3158.153/P^1 \chi + 477.894 \]
\[ r = 0.9997, \; s = 1.67; \; F = 10902 \]
reduces the value of $s$ to 1.66°C which is equivalent to an average absolute error of about 0.7%.

The observed and calculated values of $T_b$ of alkyl benzenes based on Eq. (272) have been given in Table 9. The $M^+$ and $M^-$ deviations are $+2.79°C$ and $-3.70°C$ for ethylbenzene and 1-methyl-3-isopropyl benzene respectively and there are only nine compounds including the two mentioned above with deviations of $\pm 2°C$ between the observed and calculated values of the normal boiling points.

(3) ENTHALPY OF VAPORIZATION AT BOILING POINT, $\Delta H_v^T$ (kJ mol$^{-1}$),

$N = 47$; RANGE: 30.76 to 61.1

(a) $M'$ & $A'$ PARAMETERS

$$\Delta H_v^T = 0.360 M' + 24.458$$

$r = 0.9807$, $s = 1.35$; $F = 1135$

$$\Delta H_v^T = 8.967 A' + 18.422$$

$r = 0.9799$, $s = 1.38$; $F = 1088$

$$\Delta H_v^T = 3.537 M' - 79.093 A' + 77.935$$

$r = 0.9840$, $s = 1.24$; $F = 672$

(b) $m^T$ PARAMETERS

$$\Delta H_v^T = 7.545 3m^T + 26.290$$

$r = 0.9892$, $s = 1.01$; $F = 2045$
\[ \Delta H^T_{\text{b}} = 5.654 \, 3\chi^V_P + 2.690 \, 4\chi^V_P + 26.691 \quad \ldots \quad (277) \]

\[ r = 0.9906, \quad s = 0.96; \quad F = 1153 \]

\[ \Delta H^T_{\text{b}} = 6.053 \, 3\chi^V_P + 2.054 \, 4\chi^V_P - 0.555 \, 4\chi^V_{PC} + 26.983 \]

\[
\begin{align*}
&\text{(FORCED)} \\
&\ldots \quad (278)
\end{align*}
\]

\[ r = 0.9908, \quad s = 0.95; \quad F = 771 \]

(c) \( F^m\chi_t \) PARAMETERS

\[ \Delta H^T_{\text{b}} = 8.986 \, F^1\chi + 18.332 \quad \ldots \quad (279) \]

\[ r = 0.9817, \quad s = 1.32; \quad F = 1194 \]

\[ \Delta H^T_{\text{b}} = 9.371 \, F^1\chi + 9.966 \, F^4\chi_{PC} + 15.717 \quad \ldots \quad (280) \]

\[ r = 0.9830, \quad s = 1.08; \quad F = 900 \]

\[ \Delta H^T_{\text{b}} = -32.649 \, F^0\chi + 82.320 \, F^1\chi + 13.003 \, F^4\chi_{PC} + 0.290 \]

\[ \ldots \quad (281) \]

\[ r = 0.9932, \quad s = 0.82; \quad F = 1041 \]

Eq. (281) a three variable correlation using \( F^m\chi_t \) parameters is the best correlation with \( s = 0.82 \) kJ mol\(^{-1}\). The uncertainties in the data\(^76\) have been reported to be between 0.04 to 4. kJ mol\(^{-1}\). The regression error of 0.82 kJ mol\(^{-1}\) is well within these uncertainties and the observed and calculated values of \( \Delta H^T_{\text{b}} \) of alkyl benzenes have been given in table-9. The maximum deviations of +2.64 kJ mol\(^{-1}\) and -1.28 kJmol\(^{-1}\) have been registered by 1, 2, 3, 4-tetramethylbenzene and 2-ethyl-1,4-dimethylbenzene respectively.
and there are only seven compounds with deviations of \( \pm 1 \) kJ mol\(^{-1} \) between the observed and the calculated values of the enthalpy of vaporization at normal boiling point, including the two compounds mentioned above.

(4) MOLAR HEAT CAPACITY OF VAPORIZATION, \( \Delta C_{P_V} \) (J mol\(^{-1} \) K\(^{-1} \)),

\[ N = 47; \text{ RANGE: 55.21-136.26} \]

(a) \( M' \) & \( A' \) PARAMETERS

\[ \Delta C_{P_V} = 1.089 M' + 28.021 \]
\[ r = 0.9545, s = 6.39 ; F = 461 \] (282)

\[ \Delta C_{P_V} = 27.095 A' + 6.779 \]
\[ r = 0.9538 , s = 6.44 ; F = 453 \] (283)

\[ \Delta C_{P_V} = 9.951 M' - 220.688 A' + 176.951 \]
\[ r = 0.9573, s = 6.26 ; F = 241 \] (284)

(b) \( \chi_V \) PARAMETERS

\[ \Delta C_{P_V} = 7.930 \chi_V + 20.858 \]
\[ r = 0.9555, s = 6.32 ; F = 473 \] (285)

\[ \Delta C_{P_V} = 6.573 \chi_V - 47.064/\chi_V + 43.088 \]
\[ r = 0.9581, s = 6.20; F = 246 \] (286)

\[ \Delta C_{P_V} = 9.337 \chi_V + 5.244 \chi_{P_C} - 42.628/\chi_V + 47.173 \]
\[ \text{(FORCED)} \]
\[ r = 0.9604 , s = 6.10 ; F = 170. \] (287)
(c) $P^mX_t$ PARAMETERS

\[-\Delta C_{P_V} = 12.154 P^0 \chi + 15.055 \quad \text{... (288)}\]

$r = 0.9542 , s = 6.41 ; F = 457$

\[-\Delta C_{P_V} = 9.548 P^0 \chi + 69.590 P^4 \chi - 0.623 \quad \text{... (289)}\]

$r = 0.9635 , s = 5.80 ; F = 285$

\[-\Delta C_{P_V} = 6.208 P^0 \chi + 134.570 P^4 \chi - 68.567 P^3 \chi - 2.684 \quad \text{... (290)}\]

$r = 0.9681 , s = 5.49 ; F = 214$

No correlations for estimation of $\Delta C_{P_V}$ are available in literature for comparison of our work. Eq. (290) which is the best three variable correlation using $P^mX_t$ parameters gives $s = 5.49 \text{ J mol}^{-1} \text{ K}^{-1}$. This is comparable with the uncertainties ($\pm 4-40 \text{ J mol}^{-1} \text{ K}^{-1}$) in the data. These uncertainties in the data have been calculated from the uncertainties in the data of $\Delta H^b_V$, $\Delta H_{298}^b$ and $T_b$ and the method of calculation has been detailed in chapter-IV (4). The observed and calculated values of $\Delta C_{P_V}$ for alkylbenzenes based on Eq. (290) are given in table-12. It can be seen that out of the 47 alkylbenzenes studied in table-12 there are only 5 compounds which register deviations $\geq 2 \text{ J mol}^{-1} \text{ K}^{-1}$ between the observed and calculated values of molar heat capacity of vaporization. The $M^+$ and $M^-$ are $9.89 \text{ J mol}^{-1} \text{ K}^{-1}$ and $-11.62 \text{ J mol}^{-1} \text{ K}^{-1}$ for tert-butyl benzene and 1,3,5-trimethylbenzene respectively.
(5) MOLAR VOLUME AT 293.15°K, $V_m^{293}$ (cm$^3$ mol$^{-1}$), N = 120; RANGE : 88.86-682.56

(a) $M'$ & $A'$ PARAMETERS

\[ V_m^{293} = 3.311 M' + 13.336 \]
\[ r = 0.9999, \ s = 2.25; \ F = 485195 \]

\[ V_m^{293} = 82.538 A' - 42.110 \]
\[ r = 0.9999, \ s = 1.91; \ F = 670971 \]

\[ V_m^{293} = -4.068 M' + 183.938 A' -110.177 \]
\[ r = 0.9998, \ s = 2.57; \ F = 185294 \]

(b) $\chi^v_t$ PARAMETERS

\[ V_m^{293} = 32.640 \chi^v + 29.637 \]
\[ r = 0.9998, \ s = 2.99; \ F = 274140 \]

\[ V_m^{293} = 27.214 \chi^v + 8.073 \chi^{v^2} + 27.130 \]
\[ r = 0.9999, \ s = 1.42; \ F = 606378 \]

\[ V_m^{293} = 25.292 \chi^v + 10.698 \chi^{v^2} - 3.312 \chi^{v^4} + 29.464 \]
\[ r = 0.9999, \ s = 1.12; \ F = 646761 \]

(c) $\chi^r_t$ PARAMETERS

\[ V_m^{293} = 36.976 \chi^r - 25.986 \]
\[ r = 0.9999, \ s = 2.15; \ F = 528048 \]
\[ V_{m}^{293} = 36.738 \rho N \chi - 18.660 \rho^{2} \chi_{t} - 20.742 \quad \ldots \ (298) \]

\[ r = 0.9999, s = 1.43 \ ; \ F = 597913 \]

\[ V_{m}^{293} = 32.129 \rho N \chi + 23.445 \rho^{2} \chi_{t} - 44.472 \rho^{4} \chi_{PC} - 27.404 \quad \ldots \ (299) \]

\[ r = 0.9999, s = 1.05 \ ; \ F = 735445 \]

No correlations for the estimation of \( V_{m}^{293} \) or \( D_{293} \) (liquid density) exist in literature for the comparison of this work. Eq. (299) is the best three variable correlation using \( \rho N \chi_{t} \) parameters. It estimates \( V_{m}^{293} \) within an average absolute error of \( \leq 0.3 \% \) \( (s = 1.05 \text{ cm}^{3} \text{ mol}^{-1}) \). The observed and calculated values of \( V_{m}^{293} \) of alkyl benzenes based on Eq. (299) have been given in table-10. Out of the 120 alkyl benzenes studied in table-10, there are only 8 compounds with deviations of \( \pm 2 \text{ cm}^{3} \text{ mol}^{-1} \) between the observed and the calculated values of the molar volume; the maximum deviations \( M^{+} \) \& \( M^{-} \) are \( 4.04 \text{ cm}^{3} \text{ mol}^{-1} \) and \( -2.79 \text{ cm}^{3} \text{ mol}^{-1} \) for 1,4-diisopropyl benzene and pentamethyl benzene respectively.

(6) MOLAR REFRACTION AT 293.15 °K, \( R_{M}^{293} \) \( (\text{cm}^{3} \text{ mol}^{-1}) \),

\( N = 120; \ \text{RANGE: } 26.188-193.59 \)

(a) \( M' \) \& \( A' \) PARAMETERS

\[ R_{M}^{293} = 0.927 M' + 5.803 \quad \ldots \ (300) \]

\[ r = 0.9999, s = 0.23 \ ; \ F = 3.76 \times 10^{6} \]
<table>
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<tr>
<th>COMPOUND</th>
<th>293 V M / CM MOL</th>
<th>313 V M / CM MOL</th>
<th>293 R M / CM MOL</th>
<th>313 R M / CM MOL</th>
<th>ΔH / KJ MOL</th>
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<td>Mass Error</td>
<td>Distance</td>
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<td>±532.68</td>
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<td>±4</td>
<td>±549.63</td>
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<td>Hexacosyldodecylbenzene</td>
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<td>±4</td>
<td>±566.57</td>
<td>±161.10</td>
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<td>±4</td>
<td>±583.52</td>
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<td>±600.47</td>
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<td>±634.37</td>
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<td>±4</td>
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<td>±4</td>
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<td>±188.95</td>
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<td>±4</td>
<td>±685.22</td>
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</table>
\[ R_{293}^{M} = 23.114 A' - 9.721 \]  
\[ r = 0.9999, s = 0.32; F = 1.92 \times 10^6 \]  
\[ R_{293}^{M} = 1.181 M' - 6.313 A' + 9.298 \]  
\[ r = 1.0054, s = 1.068; F = -84196 \]  

(b) \( m_x^y \) PARAMETERS

\[ R_{293}^{M} = 0.139 \alpha^y + 10.378 \]  
\[ r = 0.9997, s = 0.96; F = 2.09602 \]  
\[ R_{293}^{M} = 2.893 \alpha^y + 5.193 \beta^y + 5.597 \]  
\[ r = 0.9999, s = 0.26; F = 1.46 \times 10^6 \]  
\[ R_{293}^{M} = 2.168 \alpha^y + 5.560 \beta^y + 0.925 \gamma^y + 6.507 \]  
\[ r = 0.9999, s = 0.11; F = 5.15 \times 10^6 \]  

(c) \( P_x^y \) PARAMETERS

\[ R_{293}^{M} = 10.355 P^0 x - 5.209 \]  
\[ r = 0.9999, s = 0.22; F = 3.95 \times 10^6 \]  
\[ R_{293}^{M} = 10.113 P^0 x + 1.323 P^2 x - 3.994 \]  
\[ r = 0.9999, s = 0.17; F = 3.23 \times 10^6 \]  
\[ R_{293}^{M} = 51.879 P^2 x - 96.841 P^3 x - 2.852 P^4 x \] \( \gamma^y \)  
\[ r = 0.9999, s = 0.15; F = 3.02 \times 10^6 \]
Kier and Hall\textsuperscript{1} have estimated the $R_M$ of 70 alkyl benzenes using $\bar{\mu}_t$ parameters and their one variable, two variable, three variable and four variable correlations have the values of $s$ equal to 0.97, 0.27, 0.17 and 0.16 cm$^3$mol$^{-1}$ respectively. During the present investigations a much bigger sample of 120 alkylbenzenes has been taken and Eq.(305) which is only a three parameter correlation in terms of $\bar{\mu}_t$ indices has $s = 0.11$ which is better than Kier and Hall's\textsuperscript{1} 4 variable correlation ($s = 0.16$, $N = 70$). Eq.(305) estimates $R_M^{293}$ of 120 alkyl benzenes within an average absolute error of 0.1\% only. The observed and calculated values of $R_M^{293}$ of alkyl benzenes are given in table-10. Out of the 120 alkyl benzenes studied there are only four compounds which have deviations of $> 0.3$ cm$^3$mol$^{-1}$ and the maximum deviations are +0.36 and -0.85 cm$^3$mol$^{-1}$; registered by 1, 3, 5-trimethylbenzene and (1,2-dimethyl-propyl)benzene respectively.

\textbf{(7) ENTHALPY OF FORMATION AT 298.15°K, $\Delta H_f^{298}$(kJmol$^{-1}$),}

$N = 33$ ; \textbf{RANGE : +49.03} -98.49

(a) $M'$ \& $A'$ \textbf{PARAMETERS}

$\Delta H_f^{298} = -6.065 \ M' + 177.664 ...

r = 0.9615, s = 8.94 ; F = 379

$\Delta H_f^{298} = -154.112 \ A' + 286.335 ...

r = 0.9544, s = 9.71 ; F = 317
\( \Delta H_{298}^f = -69.849 M^' + 1633.166 \times -993.135 \ldots (311) \\
 r = 0.9962, s = 2.87 ; F = 1972 \\

(b) \( m^\nu \) PARAMETERs

\( \Delta H_{298}^f = -37.643 \nu \psi + 177.875 \ldots (312) \\
r = 0.9941, s = 3.54 ; F = 2584 \\
\( \Delta H_{298}^f = -46.057 \nu \psi + 15.596 \nu \psi + 176.306 \ldots (313) \\
r = 0.9973, s = 2.43 ; F = 2756 \\
\( \Delta H_{298}^f = -54.710 \nu \psi + 26.890 \nu \psi + 10.672 \psi_{PC} + 184.781 \ldots (314) \\
r = 0.9983, s = 1.97 ; F = 2804 \\

(c) \( F^m \) PARAMETERs

\( \Delta H_{298}^f = -184.761 F^2 \psi + 196.673 \ldots (315) \\
r = 0.9751, s = 7.21 ; F = 600 \\
\( \Delta H_{298}^f = -74.373 F \psi - 107.750 F^2 \psi + 257.198 \ldots (316) \\
r = 0.9988, s = 1.63 ; F = 6151 \\
\( \Delta H_{298}^f = -271.474 F \psi + 312.459 F^2 \psi - 824.840 F^3 \psi + 225.935 \ldots (317) \\
r = 0.9996, s = 0.92 ; F = 12895 \\

van Krevelen and Chermin\(^48\) estimated the \( \Delta H_f \) of alkyl benzenes by a group contribution method within \( \pm 2.51 \) kJmol\(^{-1}\).
of the experimental values. Eq. (317) which is the best
3 variable correlation using F"Xt parameter has the regression
error; s = 0.92 kJ mol\(^{-1}\) which is much better than van Krevelen
and Chermin's \(^{48}\) estimations. Eq. (317) estimates \(\Delta H_{\text{f}}^{298}\) of
alkylbenzene within an average error of about 1.2 %. Using
Eq. (317) the maximum deviations; \(M^+\) & \(M^-\) are +1.71 and
-2.68 kJ/mol respectively. As \(\Delta H_{\text{f}}, \Delta H_{\text{c}}\) and \(\Delta H_{\text{a}}\) are inter-
correlated no separate table for the observed and the
calculated values of \(\Delta H_{\text{f}}^{298}\) has been made. The observed and
calculated (Eq. (335)) values of \(\Delta H_{\text{a}}\) of alkyl benzenes
have been given in table-9.

(8) HEAT OF COMBUSTION AT 298.15\(^\circ\)K, \(\Delta H_{\text{c}}^{298}\) (kJ mol\(^{-1}\)),
N = 27 ; RANGE = 3169.46 -12990.86

(a) \(M^\prime\) & \(\alpha^\prime\) PARAMETERS

\[
\Delta H_{\text{c}}^{298} = 123.024 M^\prime + 385.437 \\
r = 0.9999, s = 6.14 ; F = 5.90 \times 10^6
\]

\[
\Delta H_{\text{c}}^{298} = 3068.882 \alpha^\prime -1708.616 \\
r = 0.9999, s = 11.65 ; F = 1.64 \times 10^6
\]

\[
\Delta H_{\text{c}}^{298} = 81.844 M^\prime + 1027.0 \alpha^\prime - 314.781 \\
r = 0.9999, s = 29.47 ; F = 127875
\]
(b) $\Delta H^{298}$ PARAMETERS

\[ \Delta H^{298}_c = 1207.965 \chi^y + 904.768 \]
\[ r = 0.9996, s = 81.59; F = 6657 \]  

\[ \Delta H^{298}_c = 321.473 \chi^y + 770.484 \chi^y + 477.146 \]
\[ r = 0.9999, s = 16.63; F = 401464 \]  

\[ \Delta H^{298}_c = 184.828 \chi^y + 813.752 \chi^y + 214.672 \chi^y + 632.685 \]
\[ r = 1.0000, s = 6.68; F = -1.66 \times 10^6 \]  

(c) $F^mX_t$ PARAMETERS

\[ \Delta H^{298}_c = 1374.617 F^0X - 1092.729 \]
\[ r = 0.9999, s = 1.83; F = 6.57 \times 10^7 \]  

\[ \Delta H^{298}_c = 1374.356 F^0X - 31.625 F^3X - 1088.577 \]
\[ r = 0.9999, s = 1.33; F = 6.31 \times 10^7 \]  

\[ \Delta H^{298}_c = 1374.290 F^0X - 86.209 F^3X + 44.535 F^4X - 1088.717 \]
\[ r = 0.9999, s = 0.75; F = 1.31 \times 10^8 \]  

Eq. (326) is a three variable correlation using $F^mX_t$ parameters. It has an average regression error of 0.75 kJmol$^{-1}$ only which is equivalent to an average absolute error of about 0.009%. Eq. (326) is therefore the best correlation so far for the estimation of $\Delta H^{298}_c$ of alkyl benzenes.
For Eq.(326) the maximum deviations, $M^+$ and $M^-$ in the observed and calculated values of $\Delta H_C^{298}$ are 1.95 and -1.43 kJ/mol respectively. As the $\Delta H_C$, $\Delta H_a$ and $\Delta H_f$ are inter-correlated no separate table has been given for the observed and calculated values of $\Delta H_C^{298}$. However, the observed and the calculated (Eq.(335)) values of $\Delta H_a$ are given in Table-9.

9. ENTHALPY OF ATOMIZATION, $\Delta H_a$ (kJ mol$^{-1}$), $N = 33$ ; RANGE : 5559.05 - 10291.89

(a) $M'$ & $A'$ PARAMETERS

\[
\Delta H_a = 236.642 M' + 250.018 
\]
\[r = 0.9999, \ s = 18.97; \ F = 128324\]  

\[
\Delta H_a = 6053.312 A' - 4080.661 
\]
\[r = 0.9993, \ s = 47.31; \ F = 20594\]  

\[
\Delta H_a = 342.828 M' - 2718.750 A' + 2198.913 ... (329)
\]
\[r = 0.9999, \ s = 11.83; \ F = 164885\]

(b) $m \chi^V$ PARAMETERS

\[
\Delta H_a = 1399.647 \chi^V + 675.543 
\]
\[r = 0.9852, \ s = 209.14; \ F = 1024\]  

\[
\Delta H_a = 737.344 \chi^V + 1227.585 \chi^V + 552.055 
\]
\[r = 0.9995, \ s = 39.68; \ F = 14645\]
\[ \Delta H_a = 556.747 - 1317.819 Y + 275.616 \chi^2 + 673.076 \]

\[ r = 0.999^9, \; s = 14.16 ; \; F = 76721 \]

Eq. (332) is the best three parameter correlation using \( P^\text{3t} \) parameters. The value of \( s = 2.93 \text{ kJ mol}^{-1} \) is equivalent to an average absolute error of 0.037 %.

The observed and calculated values of \( \Delta H_a \) of alkylbenzenes based on Eq. (335) are given in table 10. The maximum deviations \( \Delta M^+ \) and \( \Delta M^- \) are 10.71 kJmol\(^{-1}\) and -2.86 kJmol\(^{-1}\) for 1,2,3,4-tetramethyl benzene and 1,4-dimethyl benzene respectively. Besides these two compounds there are only two other alkyl benzenes which have the deviations of \(\pm 2\) kJ mol\(^{-1}\). If only 1,2,3,4-tetramethyl benzene is excluded from the regression analysis the results will further improve considerably.
(10) CRITICAL TEMPERATURE, $T_c$ (°K), $N = 21$;
RANGE : 562.1-767.

(a) $M'$ & $A'$ PARAMETERS

\[ T_c = 5.721 M' + 430.188 \]
\[ r = 0.9462, s = 13.24 ; F = 163 \]

\[ T_c = 147.416 A' + 323.388 \]
\[ r = 0.9417 , s = 13.77 ; F = 149 \]

\[ T_c = 44.769 M' - 1011.303 A' + 1170.386 \]
\[ r = 0.9605 , s = 11.71 ; F = 107 \]

(b) $\chi^X_4$ PARAMETERS

\[ T_c = 65.117 3\chi^y_4 + 539.579 \]
\[ r = 0.9624, s = 11.13 ; F = 238 \]

\[ T_c = 50.454 3\chi^y_f - 181.759/1\chi^y + 619.830 \]
\[ r = 0.9794, s = 8.49 ; F = 212 \]

\[ T_c = 20.966 1\chi^y + 4.151 2\chi^y + 44.188 3\chi^y_f + 492.486 \]
\[ \text{(FORCED)} \]
\[ r = 0.9795, s = 8.73 ; F = 134 \]

(c) $P^m\chi_t$ PARAMETERS

\[ T_c = 207.385 P^3\chi_f + 489.062 \]
\[ r = 0.9563, s = 11.97 ; F = 203 \]

\[ T_c = 69.950 P^1\chi + 118.744 P^3\chi_f + 402.556 \]
\[ r = 0.9780, s = 9.342 ; F = 173 \]
\[ T_c = 64.428 p^1 + 56.758 p^2 + 177.559 p^3 + 404.188 \]

\[ r = 0.9780, s = 9.03 ; F = 124 \]

Spencer and Daubert\textsuperscript{116} reported Nokay's\textsuperscript{116} method as modified by them\textsuperscript{116} to be the best method for the estimation of \( T_c \) of alkyl benzenes which estimated \( T_c \) within \(< 0.5 \%\) of average absolute error. Schmidt and Wenzel\textsuperscript{108} estimated the \( T_c \) of alkyl benzenes with an average error \( 0.8 \%\). Eq. (340) which is 2 variable correlation between \( T_c \) and \( a, \nu \) parameters has \( s = 8.49 \) \(^o\)K which is equivalent to about 1.3 \% average absolute error Eq. (340) therefore gives results better than Lydersen's\textsuperscript{102,118} method which estimates \( T_c \) within an error of 1-2 \% but Nokay's\textsuperscript{116,120} method with average error of \(< 0.5 \%\) & Schmidt and Wenzel method\textsuperscript{108} with average error = 0.8 \% are better than Eq. (340). However the method of Nokay requires the values of density and boiling point of the substances (property-activity correlation). The observed and calculated values of \( T_c \) based on Eq. (340) are given in table-11. The \( M^+ \) and \( M^- \) values are +17.48\(^o\)K and -22.35\(^o\)K for hexamethyl benzene and pentamethyl benzene respectively and if these two compounds are excluded from analysis these results will further improve. Besides these compounds there are only two more compounds which have deviation of \( \pm 8 \)\(^o\)K between the observed and the calculated values of the critical temperature.
<table>
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<th>Compound</th>
<th>$T_0$ / K</th>
<th>$P_0$ / atm</th>
<th>$V_0$ / cm$^3$ mol$^{-1}$</th>
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<td>n-dodecylbenzene</td>
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<td>n-tetradecylbenzene</td>
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<td>15.73</td>
<td>1033.05</td>
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<tr>
<td>n-pentadecylbenzene</td>
<td>823.23</td>
<td>15.06</td>
<td>1085.76</td>
</tr>
</tbody>
</table>
(11) CRITICAL PRESSURE, $P_c$ (atm), $N = 21$; RANGE: 23.5-48.6

(a) $M$ & $A^*$ PARAMETERS

\[ P_c = -0.785 M^\prime + 61.705 \]
\[ r = 0.9526, s = 1.70; F = 186 \]  \hspace{1cm} ... (345)

\[ P_c = -20.328 A^\prime + 76.579 \]
\[ r = 0.9527, s = 1.70; F = 187 \]  \hspace{1cm} ... (346)

\[ P_c = -0.181 M^\prime -15.644 A^\prime + 73.155 \]
\[ r = 0.9528, s = 1.74; F = 89 \]  \hspace{1cm} ... (347)

(b) $m^\pi y$ $X_t$ PARAMETERS

\[ P_c = 143.041 / lX^y + 7.852 \]
\[ r = 0.9873, s = 0.89; F = 735 \]  \hspace{1cm} ... (348)

\[ P_c = 99.229/ O^X^y + 32.848 / lX^y + 6.631 \]
\[ r = 0.9913, s = 0.76; F = 513 \]  \hspace{1cm} ... (349)

\[ P_c = -0.254 O^X^y + 80.887 O^X^y + 33.912 / lX^y + 9.440 \]
\[ \text{(FORCED)} \]
\[ r = 0.9915, s = 0.77; F = 328 \]  \hspace{1cm} ... (350)

(c) $p^n X_t$ PARAMETERS

\[ P_c = 165.272/fO^X - 5.731 \]
\[ r = 0.9879, s = 0.86; F = 773 \]  \hspace{1cm} ... (351)

\[ P_c = 3.036 fO^X - 218.620/fO^X - 31.439 \]
\[ r = 0.9972, s = 0.80; F = 290 \]  \hspace{1cm} ... (352)
Spencer and Daubert\textsuperscript{116} have pointed out that Forman and Thodos method\textsuperscript{119} was the best method for the estimation of $P_c$ within an average absolute error of 3-4\%. Schmidt and Wenzel\textsuperscript{108} have estimated the $P_c$ of 13 alkyl benzenes with an average error of 4.4\%. Eq.\textsuperscript{(350)} a 3 variable correlation using $\chi_l^V$ parameters gives, $s = 0.77$ atm which is equivalent to an average absolute error of about 2\%. This is less than the errors reported in the two previous estimations mentioned above. Eq.\textsuperscript{(350)} is, therefore, the best 3 variable correlation in terms of $\chi_l^V$ indices for the estimation of $P_c$ of alkyl benzenes and the observed and calculated values of $P_c$ of alkyl benzenes using Eq.\textsuperscript{(350)} are given in table\textsuperscript{-11}. Out of the 21 alkyl benzenes studied in table 11 there are only three compounds which have shown deviations of $\pm$ 1 atm between the observed and the calculated values of critical pressure and the $M^+$ & $M^-$ are + 1.46 atm and -1.45 atm for ethylbenzene and 1,4-dimethylbenzene respectively.

\textbf{(12) CRITICAL VOLUME, $V_c$ (cm$^3$mol$^{-1}$), N = 21 ; RANGE :260.-586.}

\textbf{(a) $M'$ & $A'$ PARAMETERS}

\[ V_c = 10.857 M' + 22.318 \quad ... (354) \]

\[ r = 0.9965, \ s = 6.20 ; \ F = 2669 \]
\( V_c = 281.296 \text{ A} - 183.736 \quad \ldots (355) \)
\( r = 0.9972; \ s = 5.53; \ F = 3364 \)
\( V_c = -6.761 \text{ M} + 456.270 \text{ A} - 311.635 \quad \ldots (356) \)
\( r = 0.9973; \ s = 5.56; \ F = 1666 \)

(b) \( \chi^V_t \) PARAMETERS
\( V_c = 124.514 \chi^V + 16.608 \quad \ldots (357) \)
\( r = 0.9912; \ s = 9.176; \ F = 1066 \)
\( V_c = 21.638 \chi^V + 81.626 \chi^V + 26.807 \quad \ldots (358) \)
\( r = 0.9977, \ s = 5.17; \ F = 1923 \)
\( V_c = 22.235 \chi^V + 69.158 \chi^V - 108.264 - 108.264 / \chi^V + 98.431 \quad \ldots (359) \)
\( r = 0.9980, \ s = 4.98; \ F = 1384 \)

(c) \( \chi^H_t \) PARAMETERS
\( V_c = 278.805 \chi^H - 180.322 \quad \ldots (360) \)
\( r = 0.9970; \ s = 5.71; \ F = 3151 \)
\( V_c = 293.434 \chi^H - 33.039 \chi_{PC} - 205.927 \quad \ldots (361) \)
\( r = 0.9978, \ s = 5.01; \ F = 2049 \)
\( V_c = 255.983 \chi^H - 24.549 \chi_{PC} - 153.108 / \chi^H + 54.652 \quad \text{(FORCED)} \quad \ldots (362) \)
\( r = 0.9980, \ s = 4.91; \ F = 1424 \)

In 1973 Spencer and Daubert\textsuperscript{116} reviewed the various methods available for the estimation of \( V_c \) and opined that
Reidel's method was the better method for the estimation of $V_c$ for all categories of compounds within an average absolute error of 2%. In 1976 Vetere estimated the $V_c$ of 18 alkylbenzenes with an average error of 0.96%. Eq. (362) is the best 3 variable correlation using $P^mX_t$ parameters giving $s = 4.91 \text{ cm}^3\text{ mol}^{-1}$. This is equivalent to an average absolute error of 1.1% and is better than the results of Reidel and is of the same order as that of Vetere. It may be pointed out that Vetere used a large number of group contributions to estimate $V_c$ of only 18 alkylbenzenes while Eq. (362) estimates the $V_c$ of 21 alkylbenzenes using only 3 parameters. Eq. (362) is, therefore, the best three variable correlation for the estimation of the $V_c$ of alkylbenzenes and the observed and calculated values of $V_c$ are given in table-11. It can be seen that the maximum positive and negative deviations are $+12.95 \text{ cm}^3\text{ mol}^{-1}$ and $-8.92 \text{ cm}^3\text{ mol}^{-1}$ for isopropylbenzene and isobutylbenzene respectively. Besides, these two compounds there are three more compounds out of 21 compounds studied in table-11 which have deviations $\pm 5 \text{ cm}^3\text{ mol}^{-1}$ between the observed and the calculated values of critical volume.
(13) DIAMAGNETIC SUSCEPTIBILITY, $\chi_M$, N = 12; RANGE: 54.84-173.90

(a) $M^i$ & $A^i$ PARAMETERS

$$\chi_M = 2.358 M^i + 0.813$$  \hspace{1cm} \ldots (363)  \\
$r = 0.9997$, $s = 0.87$; $F = 15651$

$$\chi_M = 59.887 A^i - 41.530$$  \hspace{1cm} \ldots (364)  \\
r = 0.9998$, $s = 0.64$; $F = 29275$

$$\chi_M = 0.035 M^i + 60.742 A^i - 42.156$$  \hspace{1cm} \ldots (365)  \\
r = 0.9998$, $s = 0.68$; $F = 12946$

(b) $m_X^j$ PARAMETERS

$$\chi_M = 25.664 \chi^j + 2.998$$  \hspace{1cm} \ldots (366)  \\
r = 0.9959$, $s = 3.17$; $F = 1214$

$$\chi_M = 18.013 \chi^j + 7.610 \chi^j + 10.162$$  \hspace{1cm} \ldots (367)  \\
r = 0.9995$, $s = 1.13$; $F = 4666$

$$\chi_M = 17.004 \chi^j + 7.229 \chi^j + 2.483 \chi^j + \ldots ... (368)$$

$$10.580$$  \\
r = 0.9999$, $s = 0.352$; $F = 32178$

(c) $F^T\chi_T$ PARAMETERS

$$\chi_M = 26.641 F^T\chi - 26.734$$  \hspace{1cm} \ldots (369)  \\
r = 0.9996$, $s = 0.92$; $F = 14059$

$$\chi_M = 52.797 F^T\chi - 60.421 F^T\chi - 12.900$$  \hspace{1cm} \ldots (370)  \\
r = 0.9999$, $s = 0.56$; $F = 19062$
\[ \chi_m = 46.879 P^0X - 45.309 P^1X - 8.126 P^4X - 16.402 \ldots \quad (371) \]

\[ r = 0.9999, \ s = 0.33; \ F = 37407 \]

In Eq. (371) a three variable correlation with \( P^mX \) indices the value of \( s \) is \( 0.33 \). The observed and calculated values based on Eq. (371) are given in Table 12. The \( M^+ \) and \( M^- \) are \( 0.41 \) and \( -0.56 \) for 1, 2-dimethylbenzene and 1,4-dimethylbenzene respectively and all other compounds have deviations \( \leq 0.4 \).

(14) Second Virial Coefficient at \( 393.10^9K \), \( B_{393}^{393} (cm^3 mol^{-1}) \), \( N = 5 \); RANGE : 729. - 1769.

(a) \( M' \) & \( A' \) Parameters

\[ -B_{393} = 106.791 M' - 1697.478 \quad \ldots \quad (372) \]

\[ r = 0.9985, \ s = 32.76; \ F = 879 \]

\[ -B_{393} = 2755.256 A' - 3750.516 \quad \ldots \quad (373) \]

\[ r = 0.9984, \ s = 31.36; \ F = 1919 \]

(b) \( \chi_v \) Parameters

Using \( 0X_v, 1X_v, (0X_v)^2, (1X_v)^2, (0X_v)^3 \) and \( (1X_v)^3 \) as independent variables and \( -B_{393} \) as a dependent one; by stepwise regression analysis the following one parameter correlation is automatically selected by the computer to be the best:

\[ -B_{393} = 64.801 (0X_v)^2 + 51.950 \quad \ldots \quad (374) \]

\[ r = 0.9999, \ s = 6.45; \ F = 21769 \]
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<th>COMPOUND</th>
<th>$-\Delta C_p$ / J mol $^{-1}$ K $^{-1}$</th>
<th>$\chi$ / mol $^{-1}$</th>
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(c) $F_4^\alpha$ PARAMETERS

Using $F_\alpha$, $F_\beta$, $(F_\alpha)^2$, $(F_\beta)^2$, $(F_\alpha)^3$ and $(F_\beta)^3$ as independent variables with $B_{393.10}^3$ as dependent one and by the stepwise regression analysis the following one parameter correlation has been selected by the computer to be the best:

$$-B_{393} = 276.234 (F_\alpha)^3 - 405.171$$

$$r = 0.9999, s = 4.90, F = 37813$$

The average error in the data$^{124}$ has been reported to be $\pm 8 \text{ cm}^3\text{ mol}^{-1}$ with maximum error upto $\pm 16 \text{ cm}^3\text{ mol}^{-1}$. Eq.$^{(375)}$ gives an average error of $4.90 \text{ cm}^3\text{ mol}^{-1}$ only which is within the limits of the uncertainties in the data$^{124}$. It is therefore, the best one parameter correlation and the average absolute error is 0.34 % only which is much less than Polak's$^{103}$ 3.2 % for alcohols and Kunz's$^{106}$ 10-15 % for alcohols and hydrocarbons. The observed and calculated values of $B_{393.10}^3$ for alkylbenzenes based on Eq.$^{(375)}$ are given in table-$12$. It can be seen that the maximum deviations $N^+ \times M^-$ are 5.18 cm$^3$ mol$^{-1}$ and -4.88 cm$^3$ mol$^{-1}$ for 1,3-dimethylbenzene and methylbenzene respectively and all other compounds have deviations $\leq 4 \text{ cm}^3\text{ mol}^{-1}$. For higher alkylbenzene, with heavy alkyl chain the vapour pressure is very small and therefore, we have not calculated the values of $B_{393.10}^3$ beyond n-heptyl benzene.