



**Y A W S**

# THE YAWS HANDBOOK OF VAPOR PRESSURE

ANTOINE COEFFICIENTS

CARL L. YAWS



SECOND EDITION

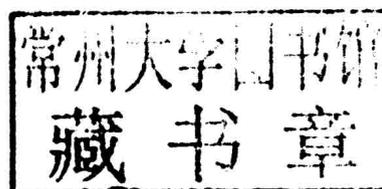


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# The Yaws Handbook of Vapor Pressure



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**Carl L. Yaws, Montgomery, Texas**

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# Vapor Pressure – Organic Compounds

Carl L. Yaws, Marco A. Satyro

## TABULATION RESULTS

The tabulation is arranged by carbon number (C, C2, C3,....., C100) to provide ease of use in quickly locating the data by using the chemical formula. The compound name, chemical abstracts registry number (CAS No), and Antoine coefficients are provided in the adjacent columns. The range of application is denoted by minimum and maximum temperatures (TMIN and TMAX). Temperatures outside the range of application should not be used. The next column provides the code for the tabulation, which is based on both experimental data and estimated values.

In preparing the tabulation, a literature search was conducted to identify data source publications (1–52). Both experimental values for the property under consideration and parameter values for estimation of the property are included in the source publications. The publications were screened and copies of appropriate data were made. These data were then keyed into the computer to provide a database of values for compounds for which experimental data are available. The database also served as a basis to check the accuracy of the estimation methods. Upon completion of data collection, estimation of values for the remaining compounds was performed.

The estimates are primarily based on literature methods and empirical procedures developed by the author. If initial analysis using the estimates is favorable, follow-up experimental determination is recommended. This is especially true for highly polar and high molecular weight compounds.

A code of 1 in the tabulation is based on experimental data. A code of 2 indicates an estimate. The estimates with a code of 3 should be considered rough approximations. The estimates with a code of 2 are more accurate. For those substances which undergo decomposition (such as nitro compounds with explosive decomposition and very large compounds with thermal decomposition) prior to attaining the boiling point temperature, the boiling point temperature is a hypothetical value.

A comparison of calculated and data values is shown in Figure 1 for a representative compound. The graph discloses favorable agreement of equation and data.

## EXAMPLE

Calculate the vapor pressure of acetone (C<sub>3</sub>H<sub>6</sub>O) at 47.35°C.

Substitution of the Antoine coefficients from the table and temperature into the equation for vapor pressure yields:

$$\log_{10} P = 7.31742 - 1315.6735 / (47.35 + 240.479) = 2.7464$$

$$P = 10^{2.7464} = 557.70 \text{ mmHg}$$

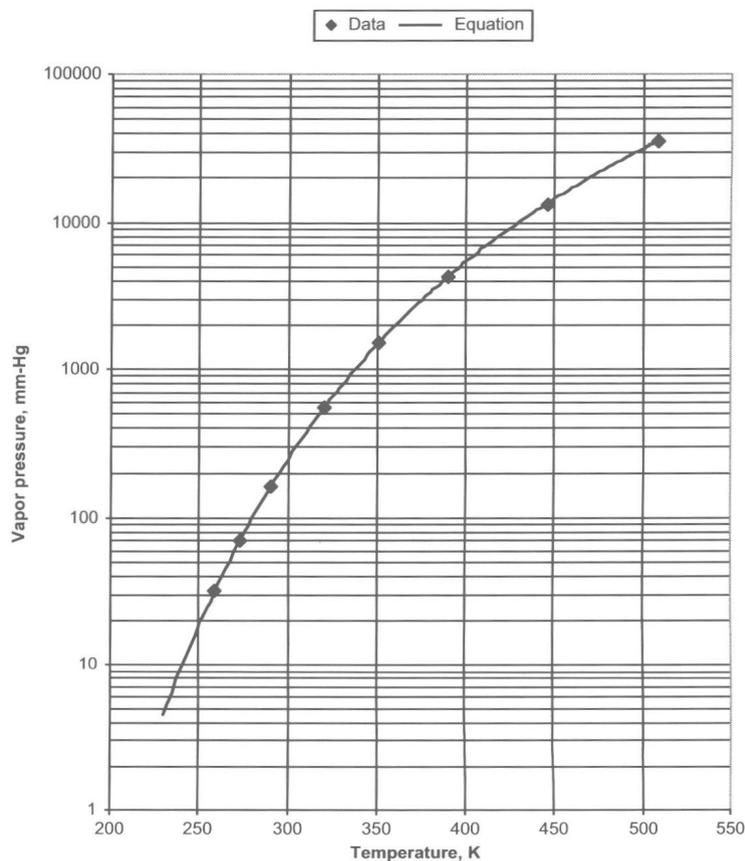


FIGURE 1 Vapor Pressure of Acetone













