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## Standard Practice for Calculating Heat of Vaporization or Sublimation from Vapor Pressure Data<sup>1</sup>

This standard is issued under the fixed designation E2071; the number immediately following the designation indicates the year of original adoption or, in the case of revision, the year of last revision. A number in parentheses indicates the year of last reapproval. A superscript epsilon ( $\epsilon$ ) indicates an editorial change since the last revision or reapproval.

### 1. Scope

1.1 This practice describes the calculation of the heat of vaporization of a liquid or the heat of sublimation of a solid from measured vapor pressure data. It is applicable to pure liquids, azeotropes, pure solids, and homogenous solid solutions over the temperature range for which the vapor pressure equation fitted to the measured data is applicable.

NOTE 1—This practice is generally not applicable to liquid mixtures. For a pure liquid or azeotrope, composition does not change upon vaporization so that the integral heat of vaporization is identical to the differential heat of vaporization. Non-azeotropic liquid mixtures change composition upon vaporizing. Heat of vaporization data computed from this practice for a liquid mixture are valid only as an approximation to the mixture differential heat of vaporization; it is not a valid approximation to the mixture integral heat of vaporization.

1.2 The values stated in SI units are to be regarded as standard. No other units of measurement are included in this standard.

1.3 There is no ISO standard equivalent to this practice.

1.4 *This standard does not purport to address all of the safety concerns, if any, associated with its use. It is the responsibility of the user of this standard to establish appropriate safety and health practices and determine the applicability of regulatory limitations prior to use.*

### 2. Referenced Documents

2.1 *ASTM Standards:*<sup>2</sup>

[D2879 Test Method for Vapor Pressure-Temperature Relationship and Initial Decomposition Temperature of Liquids by Isoteniscope](#)

[E1142 Terminology Relating to Thermophysical Properties](#)

[E1194 Test Method for Vapor Pressure \(Withdrawn 2013\)](#)<sup>3</sup>

[E1719 Test Method for Vapor Pressure of Liquids by Ebulliometry](#)

[E1782 Test Method for Determining Vapor Pressure by Thermal Analysis](#)

### 3. Terminology

3.1 *Symbols:*

3.1.1  $A, B, C$ —Antoine vapor pressure equation constants ( $\log_{10}$ , kPa, K), Antoine vapor pressure equation:

$$\log_{10}P = A - B/(T+C)$$

3.1.2  $P$ —vapor pressure, kPa.

3.1.3  $P_c$ —critical pressure, kPa.

3.1.4  $P_r$ —reduced pressure =  $P/P_c$ .

3.1.5  $T$ —absolute temperature, K.

3.1.6  $T_c$ —critical temperature, K.

3.1.7  $T_r$ —reduced temperature =  $T/T_c$ .

<sup>1</sup> This practice is under the jurisdiction of Committee E37 on Thermal Measurements and is the direct responsibility of Subcommittee E37.10 on Fundamental, Statistical and Mechanical Properties.

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<sup>2</sup> For referenced ASTM standards, visit the ASTM website, [www.astm.org](http://www.astm.org), or contact ASTM Customer Service at [service@astm.org](mailto:service@astm.org). For *Annual Book of ASTM Standards* volume information, refer to the standard's Document Summary page on the ASTM website.

<sup>3</sup> The last approved version of this historical standard is referenced on [www.astm.org](http://www.astm.org).

3.1.8  $V$ —molar volume,  $\text{cm}^3/\text{mol}$ .

3.1.9  $R$ —gas constant,  $8.31433 \text{ J/mol}\cdot\text{K}$ ;  $8314330 \text{ kPa}\cdot\text{cm}^3/\text{mol}\cdot\text{K}$ .

3.1.10  $\Delta H_v$ —heat of vaporization,  $\text{J/mol}$ .

3.1.11  $\Delta Z_v$ —difference in compressibility factor ( $Z = PV/RT$ ) upon vaporization. Clapeyron equation:

$$\Delta H_v = -R\Delta Z_v [d(\ln P)/d(1/T)]$$

3.1.11.1 *Discussion*—

The subscript “V” will be used throughout this practice to designate the vaporization of a liquid. If the vapor pressure data were measured for a solid, substitute the subscript “S” for the sublimation of a solid.

3.2 *Definitions:*

3.2.1 Specialized terms used in this practice are defined in Terminology **E1142**.

3.2.2 *sublimation*—transition from a solid phase to a gaseous phase.

3.2.3 *vaporization*—transition from a liquid phase to a gaseous phase.

#### 4. Summary of Practice

4.1 Vapor pressure data are measured by other referenced ASTM Standards standards and then correlated with the Antoine equation. The heat of vaporization or sublimation is computed at the desired temperature from the vapor-pressure temperature derivative from the fitted Antoine equation by use of the Clapeyron equation (1).<sup>4</sup> In the Clapeyron equation,  $\Delta Z_v$  is determined by either the Clausius-Clapeyron (2) approximation approximation:

$$(\Delta Z_v = 1)$$

or the Haggmacher (3) approximation approximation:

$$\left(\Delta Z_v = \left\{1 - \left[\frac{P_r(T_r)}{P_r(T)}\right]^{\frac{1}{2}}\right\}\right)$$

4.2 An example calculation is given in Annex A1.

#### 5. Significance and Use

5.1 If the heat of vaporization or sublimation is absorbed or liberated in a process at constant pressure, it is called enthalpy of vaporization or sublimation. Enthalpy of vaporization or sublimation is a fundamental thermodynamic property of a liquid or solid. It is an important quantity in the design of heat exchangers and other chemical process units. Enthalpy of vaporization is also used to calculate solubility parameters (4).

5.2 This practice may be used in research, regulatory compliance, and quality assurance applications.

#### 6. Experimental Vapor Pressure Data

6.1 Vapor pressure data are measured by Test Methods **D2879**, **E1194**, **E1719**, or **E1782**. Note the safety precautions contained in the test method used.

6.1.1 Vapor pressure data from other reliable sources, for example, peer-review technical journals, may be used. The source of the vapor pressure data must be noted.

6.2 The measured vapor pressure data are fitted to an Antoine vapor pressure equation. See 10.3 in Test Method **E1719** for details on least-squares regression of vapor pressure data.

#### 7. Calculation

7.1 At each temperature of interest, calculate the vapor pressure from the Antoine equation and calculate the vapor-pressure temperature derivative from the fitted Antoine equation constants from:

$$[d(\ln P)/d(1/T)] = -2.3025851[BT^2/(T+C)^2]$$

7.2 Calculate an approximation to  $\Delta Z_v$  at each temperature.

7.2.1 The Clausius-Clapeyron approximation to  $\Delta Z_v$  is:

$$\Delta Z_v \approx 1.0$$

7.2.2 The Haggmacher approximation to  $\Delta Z_v$  is:

<sup>4</sup> The boldface numbers given in parentheses refer to a list of references at the end of the text.

$$\Delta Z_v = \{1 - [P_r / (T_r)^3]\}^{\frac{1}{2}}$$

NOTE 2—The Clausius-Clapeyron approximation is generally used for solids and for liquids at low  $T_r$ . The Haggenmacher approximation is generally used for liquids up to  $T_r \approx 0.75$ .

7.2.3 If equation of state ( $Z$ ) data are available for both the condensed and gaseous phases,  $\Delta Z_v$  may be calculated directly from the equation of state data.

7.3 Calculate the heat of vaporization or heat of sublimation at each temperature from the Clapeyron equation:

$$\Delta H_v = -R\Delta Z_v [d(\ln P)/d(1/T)]$$

## 8. Report

8.1 Report the following information:

8.1.1 The test method and source of the vapor pressure data used in the heat of vaporization or heat of sublimation calculation. A vapor pressure data table shall also be reported.

8.1.2 The Antoine equation constants fitted to the vapor pressure data.

8.1.3 The approximation to  $\Delta Z_v$  used in the calculation.

8.1.4 The values and source of the critical temperature and critical pressure data if the Haggenmacher approximation was used for  $\Delta Z$ .

8.1.5 A table that contains temperature, vapor pressure, the vapor pressure temperature derivative [ $d(\ln P)/d(1/T)$ ], difference in compressibility factor ( $\Delta Z_v$ ), and  $\Delta H_v$ , the heat of vaporization or heat of sublimation.

8.1.6 The specific dated version of this practice used.

8.2 See the sample calculations and report in [Annex A1](#).

## 9. Keywords

9.1 Antoine equation; Clausius-Clapeyron equation; enthalpy of sublimation; enthalpy of vaporization; Haggenmacher equation; heat of sublimation; heat of vaporization; vapor pressure

## ANNEX

### (Mandatory Information)

#### A1. SAMPLE CALCULATIONS AND REPORT

##### A1.1 Source of Sample Vapor Pressure Data

A1.1.1 This sample calculation is performed on the sample vapor pressure data given for a toluene specimen in Annex A3 of Test Method [E1719](#). Heat of vaporization is calculated in 10 K increments between 290 and 400 K. Calculations for both the Clausius-Clapeyron and Haggenmacher approximations to  $\Delta Z_v$  are listed.

##### A1.2 Sample Experimental Data

A1.2.1 These controlled pressure-boiling temperature data pairs were measured by Test Method [E1719](#) on a 75 cm<sup>3</sup> specimen charged to a vapor-lift pump ebulliometer:

$P$ (kPa)	$T$ (K)
10.0	318.4
20.0	335.4
30.0	345.8
50.0	360.7
70.0	371.2
85.0	377.9
100.0	383.3

A1.2.2 A non-linear least-squares fit of the Antoine equation,  $\log_{10} P = A - B/(T + C)$ , produced these constants: