# Vapor Pressure of Ethyltriethoxysilane

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The vapor pressure of ethyltriethoxysilane was measured from (335.0 to 432.0) K with a pressure range from (2.325 to 100.325) kPa using an inclined ebulliometer. The correlation between vapor pressure and temperature were conducted with the relative difference ranging from 0.01 to 0.18. The molar enthalpy of vaporization ($\Delta_{vap}H_m$) of ethyltriethoxysilane in the experimental temperature range was calculated from the Clausius−Clapeyron equation.

## Introduction

Ethyltriethoxysilane (CAS RN: 78-07-9) is an important chemical in the silicone industry, and it has been widely used in many fields such as functional materials, silane coupling agents, and modifying agents for zeolite nanoparticle-supported catalysts with good stability and high selectivity. Besides, ethyltriethoxysilane also plays an important role in the fabrication of organosilicon polymers due to its three hydrolyzable ethoxy groups. Subsequent reactions are seriously influenced by the purity of the chemical products; the properties of the products thus obtained are also greatly governed by the quality of reactants or reagents. To obtain chemicals with high purity, the relationship between vapor pressures and temperatures should be known; meanwhile, the molar enthalpy of vaporization should also be investigated because it is one of the important thermodynamic parameters for vapor−liquid equilibrium processes and is useful for the design and operation of multicomponent systems.

The normal boiling point of pure ethyltriethoxysilane has ever been reported by many researchers,[1−8] but the reported values were plausible and different each other. Freidlina et al.[9] reported saturated vapor pressure of pure ethyltriethoxysilane under certain controlled pressure, but there was only one experimental point. The data of pure ethyltriethoxysilane in the pressure range of (0.133 to 101.325) kPa have been reported by Jenkins and Chambers,[10] but there were only six experimental points higher than room temperature, and they were applied to a correlation. Obviously, these data are insufficient owing to the variation of pressure with temperature. To improve the data reliability and overcome the data deficiency in organosilicon chemistry and provide the detailed fundamental data for engineering fields, the 36 temperatures at various pressures ranging from (2.325 to 100.325) kPa were measured by means of an inclined ebulliometer.

Although the range of experimental values should be as wide as possible, unfortunately, the saturated temperature of ethyltriethoxysilane is significantly influenced by its saturated vapor pressure, and it would be easily transformed from liquid to vapor phase under 2.325 kPa. Therefore, the lower limit for pressure data acquisition is set to 2.325 kPa. The local atmospheric pressure was 100.325 kPa when the experiment was conducted. Thus the saturated temperatures at various pressures ranging from (2.325 to 100.325) kPa corresponding to temperatures ranging from (335.0 to 432.0) K were measured. The relationship between the saturated vapor pressures and temperatures was fitted by the Antoine equation. The equation was regressed by nonlinear least-squares regression method, and thus the Antoine constants were obtained. The molar enthalpy of vaporization and the normal boiling point were also calculated.

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## Experimental Section

***Chemicals.*** Ethyltriethoxysilane was purified at 432.0 K and 100.325 kPa. Its mass fraction purity, determined by a gas chromatograph equipped with a HP-5 column and a flame ionization detector (FID), was higher than 0.995.

***Apparatus.*** The apparatus used in this work has been described previously.[11] It includes a high-accuracy pressure controller and measurement system, an inclined ebulliometer, and a vacuum pump (RZ6 model, Germany Vacuubrand GMBH+ CO KG). The pressures of the system were controlled by a DPI 515 precision pressure controller. The uncertainty of the pressure controller was ± 0.02 kPa at pressures up to 200 kPa with a control stability of 0.002 kPa. The temperature was measured by a calibrated mercury thermometer with an uncertainty of ± 0.1 K.

The sample with an approximate volume of 100 $cm^3$ was charged into the inclined ebulliometer. All measurements were conducted in a sequence of increasing pressures, and the pressure was controlled at the desired value at each experimental point. The sample was heated and stirred with a magnetic stirrer to provide isothermal conditions and to prevent superheating. When thermal equilibrium was reached, the temperature and pressure were recorded. The experimental temperature values were measured three times at the same pressure.

## Results and Discussion

***Regressed Parameters of Antoine Equation.*** The boiling temperatures of ethyltriethoxysilane in the pressure range (2.325 to 100.325) kPa are listed in Table 1. The experimental data were fitted by Antoine equation.

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**Table 1. Comparison of the Calculated Saturated Temperature at Pressure $p^s$ and the Experimental Data for Ethyltriethoxysilane**

| | *T*/K | | | |
|---|---|---|---|---|
| $p^s$/kPa | exp. | calc. | (d ln($p^s$)/d(*T*)) | 100 RD[a] |
| 2.325 | 335.0 | 334.6 | 0.0558 | 0.12 |
| 3.325 | 340.8 | 341.2 | 0.0526 | 0.12 |
| 4.325 | 346.2 | 346.3 | 0.0503 | 0.03 |
| 5.325 | 350.4 | 350.5 | 0.0485 | 0.03 |
| 8.325 | 359.9 | 360.1 | 0.0448 | 0.06 |
| 11.325 | 367.1 | 367.2 | 0.0423 | 0.02 |
| 14.325 | 372.9 | 372.9 | 0.0405 | 0.01 |
| 17.325 | 377.7 | 377.6 | 0.0390 | 0.02 |
| 20.325 | 382.0 | 381.8 | 0.0378 | 0.05 |
| 23.325 | 385.8 | 385.5 | 0.0368 | 0.08 |
| 26.325 | 389.0 | 388.8 | 0.0359 | 0.05 |
| 29.325 | 392.0 | 391.9 | 0.0351 | 0.03 |
| 32.325 | 394.8 | 394.7 | 0.0344 | 0.03 |
| 35.325 | 397.4 | 397.3 | 0.0338 | 0.03 |
| 38.325 | 399.9 | 399.7 | 0.0332 | 0.05 |
| 41.325 | 402.2 | 402.0 | 0.0327 | 0.05 |
| 44.325 | 404.1 | 404.2 | 0.0322 | 0.01 |
| 47.325 | 405.5 | 406.2 | 0.0317 | 0.17 |
| 50.325 | 407.6 | 408.2 | 0.0313 | 0.14 |
| 53.325 | 410.1 | 410.0 | 0.0309 | 0.02 |
| 56.325 | 411.9 | 411.8 | 0.0306 | 0.03 |
| 59.325 | 413.7 | 413.5 | 0.0302 | 0.05 |
| 62.325 | 415.4 | 415.1 | 0.0299 | 0.06 |
| 65.325 | 416.8 | 416.7 | 0.0296 | 0.02 |
| 68.325 | 418.3 | 418.3 | 0.0293 | 0.01 |
| 71.325 | 419.4 | 419.7 | 0.0290 | 0.08 |
| 74.325 | 420.6 | 421.2 | 0.0287 | 0.13 |
| 77.325 | 421.8 | 422.5 | 0.0285 | 0.18 |
| 80.325 | 423.7 | 423.9 | 0.0282 | 0.04 |
| 83.325 | 425.4 | 425.2 | 0.0280 | 0.05 |
| 86.325 | 426.7 | 426.5 | 0.0277 | 0.06 |
| 89.325 | 427.9 | 427.7 | 0.0275 | 0.05 |
| 92.325 | 429.1 | 428.9 | 0.0273 | 0.05 |
| 95.325 | 430.2 | 430.1 | 0.0271 | 0.03 |
| 98.325 | 431.3 | 431.2 | 0.0269 | 0.02 |
| 100.325 | 432.0 | 432.0 | 0.0268 | 0.01 |

[a] Relative difference (RD) = $|T - T_{calc}|/T$.

$$\log(p^s/\text{kPa}) = A - \frac{B}{C + (T/\text{K})} \tag{1}$$

The *T* and $p^s$ values given in Table 1 using a nonlinear least-squares method from EVIEWS 5.0 software are shown in Figure 1. The parameters *A*, *B*, and *C* of eq 1 are listed in Table 2. The difference between the calculated vapor pressure values and the experimental data for ethyltriethoxysilane are also listed in Table 1 with a maximum relative difference of no more than 0.18. Therefore, the above Antoine constants are satisfactory for engineering design and application.

***Relationship between $\Delta_{vap}H_m$ and Temperature.*** The influence of pressure on temperature dependence of $\Delta_{vap}H_m$ usually can be neglected over the temperature range studied. The function relationship between $\Delta_{vap}H_m$ and temperature is given by eq 2.

$$\Delta_{vap}H_m = \left(\frac{d\ln(p^s)}{d(T)}\right)\cdot R(T)^2 \tag{2}$$

The differential equation of the relationship between ln($p^s$/kPa) and temperature data can be obtained from eq 1, and the data are listed in Table 1.

***Estimation of $\Delta_{vap}\bar{H}_m$ for Ethyltriethoxysilane.*** Accurate vapor pressure values can be used to estimate the molar enthalpy of vaporization from eq 1. The averaged molar vaporization enthalpy $\Delta_{vap}\bar{H}_m$ of ethyltriethoxysilane within the range of experimental temperatures and the normal boiling point at $p^s$ = 100.325 kPa could be further obtained.

$$\Delta_{vap}\bar{H}_m = 44.42\ \text{kJ}\cdot\text{mol}^{-1}$$

The calculated value of the normal boiling point for liquid ethyltriethoxysilane was 432.3 K, which was derived from the Antoine equation and presented in Table 3.

***Reliability Analysis of the Parameters.*** To check the reliability of regressed parameters obtained from the Antoine equation in this range, values of the boiling point for ethyltriethoxysilane were calculated ranging from $p$ = (2.826 to 101.325) kPa. The comparison between the above calculated values and literature data were conducted, and the results are listed in Table 3. It could be seen that calculated values agree well with those in literature. The parameters could satisfy the estimation requirements for the development and design of the chemical engineering process.

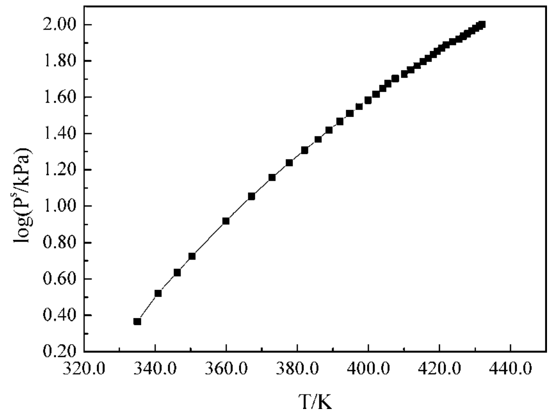


**Figure 1.** Nonlinear regression of Antoine equation for ethyltriethoxysilane. ◆, experimental data; the smoothed line is a nonlinear regression curve.

**Table 2. Regressed Antoine Constants for Ethyltriethoxysilane**

| *A* | *B* | *C*/K | $R^2$ |
|---|---|---|---|
| 5.68968 | 1169.42 | –114.91 | 0.99991 |

**Table 3. Comparison between Calculated Values and Literature Data[a]**

| | *T*/K | | | |
|---|---|---|---|---|
| $p^s$/kPa | literature data | calc.[b] | AD/K | 100 RD |
| 2.826 | 337.7[10] | 338.1 | 0.4 | 0.12 |
| 5.333 | 353.2 to 354.2[9] | 350.6 | 2.6 to 3.6 | 0.74 to 1.02 |
| 6.159 | 354.2[10] | 353.6 | 0.6 | 0.17 |
| 9.359 | 363.7[10] | 362.7 | 1.0 | 0.27 |
| 30.851 | 394.9[10] | 393.3 | 1.6 | 0.41 |
| 82.206 | 426.6[10] | 424.7 | 1.9 | 0.45 |
| 101.325 | 432.2 to 434.7[1] | 432.3 | 0.1 to 2.4 | 0.02 to 0.55 |
| 101.325 | 432.2 to 434.2[2] | 432.3 | 0.1 to 1.9 | 0.02 to 0.44 |
| 101.325 | 431.2 to 433.2[3] | 432.3 | 0.9 to 1.1 | 0.21 to 0.26 |
| 101.325 | 431.7[4] | 432.3 | 0.6 | 0.14 |
| 101.325 | 431.2 to 432.2[5,6,7] | 432.3 | 0.1 to 1.1 | 0.02 to 0.26 |
| 101.325 | 430.2 to 433.2[8] | 432.3 | 0.9 to2.1 | 0.21 to 0.49 |

[a] Absolute difference (AD) = $|T_{calc} - T_{lit}|$. Relative difference (RD) = $|T_{calc} - T_{lit}|/T_{lit}$. [b] Calculated by the Antoine equation with the constants listed in Table 2.

## Conclusion

The saturated temperature of ethyltriethoxysilane at various pressures ranging from (2.325 to 100.325) kPa was determined by means of an inclined ebulliometer. The results were fit to an Antoine equation. The correlations between the saturated vapor pressure and temperature were conducted with a relative difference less than 1.02. Besides, we found that it is interesting that the vapor pressure of ethyltriethoxysilane is very close to that of vinyltriethoxysilane (CAS RN: 78-08-0) as given by literature.[4,6,7,12−19]

The relationship between $\Delta_{vap}H_m$ and temperature for ethyltriethoxysilane was also estimated between (335.0 and 432.0) K. The obtained $\Delta_{vap}\bar{H}_m$ was 44.42 kJ·mol$^{-1}$, and the calculated normal boiling temperature was 432.3 K. The obtained Antoine parameters and the molar enthalpy of vaporization for ethyltriethoxysilane are useful fundamental data for the design and operation of rectifying tower.

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