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Article

Heat Capacity, Density, Vapor Pressure, and Enthalpy of Vaporization of Propyl Cinnamate

导师签字

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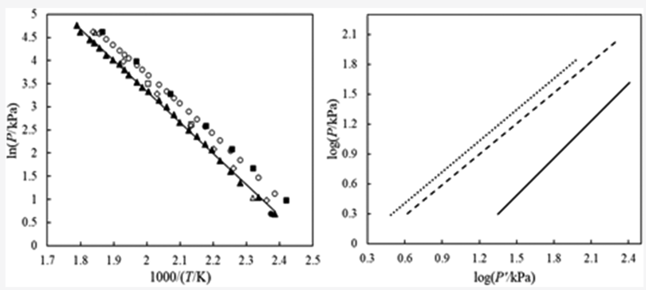
ABSTRACT: The density and liquid heat capacity of propyl cinnamate were measured in the temperature range from 290.15 to 503.15 K by a pycnometer and automatic adiabatic calorimeter and correlated with temperature by the linear equation and quadratic polynomial, respectively. Vapor pressure data of propyl cinnamate were determined by the ebulliometric method at 419.15−559.15 K, and they are in accordance with the Antoine equation. The vaporization enthalpy $\Delta_{vap}H$ (T_b) of propyl cinnamate at normal boiling point was attained based on the Clausius−Clapeyron equation. The standard enthalpy of vaporization $\Delta_{vap}H$ (298.15 K) was calculated by the Othmer method and verified by the Watson relation.



■ INTRODUCTION

Physicochemical properties of compounds play crucial roles for their applications.[1] Among them, density is an important characteristic of substances which can monitor product quality[2] and is also essential in the calculation of chemical processes.[3,4] Vapor pressure, a fundamental physicochemical property of substances, is also indispensable in plenty of significant applications, such as the distillation process and two-phase reactions.[5−7] Furthermore, the vaporization enthalpy, being able to obtain from vapor pressure data, is one of the important thermodynamic data required for the calculation, analysis, and design of chemical processes.[8] Heat capacity values are characteristic data related to the structure of substances, and can be widely applied to chemical engineering, energy, and material engineering.[9] For instance, standard Gibbs energy change of a reaction can be calculated by heat capacity, enthalpy, and entropy.[10−12] Therefore, it is necessary to make efforts to carry out extensive research concerning these fundamental physicochemical properties.

Propyl cinnamate (propyl 3-phenyl-2-acrylate, CAS 7778-83-8) has a fruit aroma and can be available as a spice for the preparation of beverages, candy, food, and cosmetics. Cinnamic acid and its esters are often used as synthetic raw materials for plant growth regulators and expected to be alternatives for synthetic pesticides because of their repellent or insecticidal activity. In addition, they were also reported as antimicrobial agents.[13,14] Unfortunately, only limited data for the vapor pressure[15,16] and density[15,17] of propyl cinnamate are available. In addition, other thermodynamic properties such as heat capacity and enthalpy of vaporization of propyl cinnamate were not mentioned in the literature studies.

Consequently, this study mainly laid emphasis on investigating the density, vapor pressure, and heat capacity of propyl cinnamate at different temperatures. The experimental values obtained were regressed or correlated as functions of temperature. The enthalpy of vaporization of propyl cinnamate at normal boiling point was calculated according to the Clausius−Clapeyron equation. In addition, the standard enthalpy of evaporation, namely, $\Delta_{vap}H$ (298.15 K), of propyl cinnamate was estimated by the Othmer method with α-methyl cinnamaldehyde, methyl benzoate, and ethyl cinnamate as reference substances. Ultimately, the Watson relation was utilized to further verify the accuracy of the $\Delta_{vap}H$ (298.15 K) values estimated.

■ EXPERIMENTAL SECTION

The experimental installations and procedures performed in attaining data were introduced in some literature studies. In this section, details are provided as a simple description.

Materials. Propyl cinnamate was purchased from Shanghai Macklin Biochemical Co., Ltd. and the sample specification is listed in Table 1. After purification by vacuum distillation, the purity was measured by gas chromatography (GC) which is equipped with a flame ionization detector (FID) using the area correction normalization method, and the purity of the sample

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Notes

The authors declare no competing financial interest.

REFERENCES

(1) Yin, J. G.; Ke, J. J.; Zhao, G. J.; Ma, S. X. Experimental Vapor Pressures and Gaseous PvT Properties of Trans-1-Chloro-3,3,3-Trifluoropropene (R1233zd(E)). *Int. J. Refrig.* **2021**, *121*, 253–257.

(2) Chuong, H. D.; Sang, T. T.; Tam, H. D. Monte Carlo Simulation Combined with Experimental Measurements Based on Gamma Transmission Technique for Determining the Density of Liquid. *Radiat. Phys. Chem.* **2021**, *179*, No. 109216.

(3) Ramírez-Ramos, G. E.; Zgar, Y.; Salavera, D.; Coulier, Y.; Ballerat-Busserolles, K.; Coronas, A. Vapor-Liquid Equilibrium, Liquid Density and Excess Enthalpy of the Carbon Dioxide+acetone Mixture: Experimental Measurements and Correlations. *Fluid Phase Equilib.* **2021**, *532*, No. 112915.

(4) Xu, J. M.; Li, S. T.; Zeng, Z. X.; Xue, W. L. Heat Capacity, Density, Vapor Pressure, and Enthalpy of Vaporization of Isoamyldl-Lactate. *J. Chem. Eng. Data* **2019**, *64*, 3793–3798.

(5) Yuan, X. J.; Xue, W. L.; Zeng, Z. X.; Pu, T. Vapor Pressure and Enthalpy of Vaporization of 2-Amino-3-Methylpyridine. *J. Chem. Eng. Data* **2007**, *52*, 2431–2435.

(6) Cui, X. L.; Chen, G. M.; Han, X. H. Experimental Vapor Pressure Data and a Vapor Pressure Equation for N,N-Dimethylformamide. *J. Chem. Eng. Data* **2006**, *51*, 1860–1861.

(7) Fan, C. L.; Wang, L. S. Vapor Pressure of Dimethyl Phosphite and Dimethyl Methylphosphonate. *J. Chem. Eng. Data* **2010**, *55*, 479–481.

(8) Zeng, Z. X.; Chen, J.; Xue, W. L.; Zhang, P.; Xie, Y. Vapour Pressure and Vapourisation Enthalpy of Pyridine N-Oxide. *Can. J. Chem. Eng.* **2012**, *90*, 570–575.

(9) Xu, X. G.; Zeng, Z. X.; Xue, W. L.; Zhang, H. Y. Heat Capacity and Enthalpy of Formation of Trimethyl Phosphite, 2-Chloromethylbenzonitrile, and 2-Dimethylphosphonomethylbenzonitrile. *J. Chem. Eng. Data* **2007**, *52*, 1189–1194.

(10) Zeng, Z. X.; Li, X. N.; Xue, W. L.; Zhang, C. S.; Bian, S. C. Heat Capacity, Enthalpy of Formation, and Entropy of Methyl Carbamate. *Ind. Eng. Chem. Res.* **2010**, *49*, 5543–5548.

(11) Liu, X. Y.; Su, C.; Qi, X. T.; He, M. G. Isobaric Heat Capacities of Ethyl Heptanoate and Ethyl Cinnamate at Pressures up to 16.3 MPa. *J. Chem. Thermodyn.* **2016**, *93*, 70–74.

(12) Paukov, I. E.; Kovalevskaya, Y. A.; Arzamastcev, A. E.; Pankrushina, N. A.; Boldyreva, E. V. Heat Capacity of Methacetin in a Temperature Range of 6 to 300 K. *J. Therm. Anal. Calorim.* **2012**, *108*, 243–247.

(13) Narasimhan, B.; Belsare, D.; Pharande, D.; Mourya, V.; Dhake, A. Esters, Amides and Substituted Derivatives of Cinnamic Acid: Synthesis, Antimicrobial Activity and QSAR Investigations. *Eur. J. Med. Chem.* **2004**, *39*, 827–834.

(14) Fujiwara, G. M.; Annies, V.; de Oliveira, C. F.; Lara, R. A.; Gabriel, M. M.; Betim, F. C. M.; Nadal, J. M.; Farago, P. V.; Dias, J. F. G.; Miguel, O. G.; Miguel, M. D.; Marques, F. A.; Zanin, S. M. W. Evaluation of Larvicidal Activity and Ecotoxicity of Linalool, Methyl Cinnamate and Methyl Cinnamate/Linalool in Combination against Aedes Aegypti. *Ecotoxicol. Environ. Saf.* **2017**, *139*, 238–244.

(15) Derbentseva, N. A. Relation between Odor and Chemical Structure. *Izv. Akad. Nauk B. SSR* **1948**, *2*, 114–124.

(16) Pollard, C. B.; Mattson, G. C. The Addition of Saturated Heterocyclic Amines to Cinnamate Esters. *J. Am. Chem. Soc.* **1956**, *78*, 4089–4090.

(17) Albert, O. Viscosity Measurements on Homologous Ester Series with Special Regard to the Relations of Thorpe and Roger. *Z. Phys. Chem., Abt. A* **1938**, *182*, 421–429.

(18) Tan, Z.; Zhang, J.; Meng, S.; Li, L. A Small Sample-Size Automated Adiabatic Calorimeter from 70 to 580 K. *Sci. China, Ser. B: Chem.* **1999**, *42*, 382–390.

(19) Chen, J.; Wang, H. Density, Viscosity, and Saturated Vapour Pressure of 3-Chloro-4-Fluoronitrobenzene and 3-Chloro-2-Fluoronitrobenzene. *J. Chem. Thermodyn.* **2021**, *154*, No. 106337.

(20) Lu, H. Z. *Handbook of Petrochemical Basic Data*; Chemical Industry Press: Beijing, 1982.

(21) Edition, S. L. R.; Williams, A.; Rosslein, M. *Quantifying Uncertainty in Analytical Measurement*, 3rd ed.; Eurachem, 2012.

(22) Silva, A. M.; Weber, L. A. Ebulliometric Measurement of the Vapor Pressure of 1-Chloro-1,1-Difluoroethane and 1,1-Difluoroethane. *J. Chem. Eng. Data* **1993**, *38*, 644–646.

(23) Archer, D. G. Thermodynamic Properties of Synthetic Sapphire (α-Al_2O_3), Standard Reference Material 720 and the Effect of Temperature-Scale Differences on Thermodynamic Properties. *J. Phys. Chem. Ref. Data* **1993**, *22*, 1441–1453.

(24) Jaeger, F. M. Uber Die Temperaturabhangigkeit Der Molekuran Freien Uberflackenenergie von Flussigkeiten Im Temperaturbereich von −80 Bis +1650 C. *Z. Anorg. Allg. Chem.* **1917**, *101*, 1–214.

(25) Perkin, W. H. LXIX. On Magnetic Rotatory Power, Especially of Aromatic Compounds. *J. Chem. Soc., Trans.* **1896**, *69*, 1025–1257.

(26) Perkin, W. H. XXIII.–On the Refractive Power of Certain Organic Compounds at Different Temperatures. *J. Chem. Soc., Trans.* **1892**, *61*, 287–310.

(27) Mozaffari, P.; Järvik, O.; Baird, Z. S. Vapor Pressures of Phenolic Compounds Found in Pyrolysis Oil. *J. Chem. Eng. Data* **2020**, *65*, 5559–5566.

(28) Xiao, R.; Zhu, Y.; Jin, W.; Dai, Z.; Li, S.; Zhang, F. Study on Wax Deposition Rate Optimization Algorithm Based on Levenberg-Marquardt Algorithm and Global Optimization. *Front. Heat Mass Transfer* **2019**, *12*, 1–6.

(29) Stull, D. R. Vapor Pressure of Pure Substances. Organic and Inorganic Compounds. *Ind. Eng. Chem.* **1947**, *39*, 517–540.

(30) Kozlovskiy, M.; Gobble, C.; Chickos, J. Vapor Pressures and Vaporization Enthalpies of a Series of Esters Used in Flavors by Correlation Gas Chromatography. *J. Chem. Thermodyn.* **2015**, *86*, 65–74.

(31) *ChemBlink Database of Chemicals from Around the World [WWW Document]*. https://www.chemblink.com/MSDS/MSDSFiles/7778-83-8_Alfa-Aesar.pdf.

(32) Chen, L. R.; Grant, D. J. W. Extension of Clausius-Clapeyron Equation to Predict Hydrate Stability at Different Temperatures. *Pharm. Dev. Technol.* **1998**, *3*, 487–494.

(33) Du, J.; Wang, L. Equilibrium Conditions for Semiclathrate Hydrates Formed with CO_2, N_2, or CH_4 in the Presence of Tri- N -Butylphosphine Oxide. *Ind. Eng. Chem. Res.* **2014**, *53*, 1234–1241.

(34) Othmer, D. F.; Brown, G. G. Correlating Vapor Pressure and Latent Heat Data: A New Plot. *Ind. Eng. Chem.* **1940**, *32*, 841–856.

(35) Steele, W. V.; Chirico, R. D.; Cowell, A. B.; Knipmeyer, S. E.; Nguyen, A. Thermodynamic Properties and Ideal-Gas Enthalpies of Formation for Trans-Methyl Cinnamate, α-Methyl Cinnamaldehyde, Methyl Methacrylate, 1-Nonyne, Trimethylacetic Acid, Trimethylacetic Anhydride, and Ethyl Trimethyl Acetate. *J. Chem. Eng. Data* **2002**, *47*, 700–714.