



UNIVERSITY OF LEEDS

This is a repository copy of *Measurement of the Thermal Conductivity of 1-Butyl-3-methylimidazolium I-Tryptophan + Water + Ethanol Mixtures at T = (283.15 to 333.15) K.*

White Rose Research Online URL for this paper:

<https://eprints.whiterose.ac.uk/id/eprint/144105/>

Version: Accepted Version

Article:

Cui, X, Zhu, H, He, C-H et al. (1 more author) (2019) Measurement of the Thermal Conductivity of 1-Butyl-3-methylimidazolium I-Tryptophan + Water + Ethanol Mixtures at T = (283.15 to 333.15) K. *Journal of Chemical & Engineering Data*, 64 (4). pp. 1586-1593. ISSN 0021-9568

<https://doi.org/10.1021/acs.jced.8b01147>

(c) 2019, American Chemical Society. This is an author produced version of a paper published in the *Journal of Chemical & Engineering Data*. Uploaded in accordance with the publisher's self-archiving policy.

Reuse

Items deposited in White Rose Research Online are protected by copyright, with all rights reserved unless indicated otherwise. They may be downloaded and/or printed for private study, or other acts as permitted by national copyright laws. The publisher or other rights holders may allow further reproduction and re-use of the full text version. This is indicated by the licence information on the White Rose Research Online record for the item.

Takedown

If you consider content in White Rose Research Online to be in breach of UK law, please notify us by emailing eprints@whiterose.ac.uk including the URL of the record and the reason for the withdrawal request.



eprints@whiterose.ac.uk
<https://eprints.whiterose.ac.uk/>

Measurement of Thermal Conductivity of 1-Butyl-3-Methylimidazolium L-tryptophan + Water + Ethanol Mixtures at $T = (283.15 \text{ to } 333.15) \text{ K}$

Xing Cui,¹ Hai Zhu,¹ Chao-Hong He*,¹ Ke-Jun Wu²

¹Zhejiang Provincial Key Laboratory of Advanced Chemical Engineering Manufacture Technology, College of Chemical and Biological Engineering, Zhejiang University, Hangzhou, 310027, China.

Corresponding author: chhezju@zju.edu.cn

²School of Chemical and Process Engineering, University of Leeds, Leeds LS2 9JT, UK

Abstract: Thermal conductivities of 1-butyl-3-methylimidazolium L-tryptophan ([BMIM][L-trp]), water, ethanol, [BMIM][L-trp] + water, [BMIM][L-trp] + ethanol, water + ethanol and [BMIM][L-trp] + water + ethanol were investigated from 283.15 K to 333.15 K covering the whole scale of concentrations at atmospheric pressure with transient hot wire method. The thermal conductivities of pure [BMIM][L-trp] decrease linearly from 0.180 to 0.177 $\text{W}\cdot\text{m}^{-1}\cdot\text{K}^{-1}$ with increasing temperature. The uncertainty of the measurement was less than 2% at 0.95 confident level. The experimental data of binary and ternary mixtures were correlated by second-order Scheffé polynomial as a function of composition and temperature. The average relative deviation of the calculated values with experiment data was 0.58%.

1. Introduction

Ionic liquids (ILs) have attracted widespread attention in recent years as environmental friendly solvents and were utilized in extraction, gas absorption, chemical catalysis and

other fields, because of their negligible vapor pressure, higher thermal stability, good solubility and adjustable structure.¹⁻³ Thermal conductivity is the measurement of the heat transfer ability of the materials and the study of thermal conductivities is significant for scale-up and industrialization of the chemical engineering process, so as for the application of ILs.⁴⁻⁷ Hot wire method is an important technique of thermal conductivity measurement, which was considered as the most stable and accurate method for fluid measurement.⁸⁻¹⁰ For example, Tomida et al.¹¹ studied the thermal conductivities of several kinds of imidazolium-based ionic liquids with different alkyl chain lengths by hot wire method and the pressure dependences of the thermal conductivity of ILs. Castro et al.¹² measured the thermal conductivities of several kinds of alkyl-methylimidazolium ionic liquids and corresponding IoNanofluids which is composed by ionic liquids with a few multiwall carbon nanotubes (MWCNTs) dispersed. The thermal conductivity enhancement by the addition of MWCNTs and the temperature dependence of the IoNanofluids system were also investigated.

Ionic liquids, especially chiral ionic liquids, are mainly combined with other solvents when applied in chemical process to reduce the viscosity. In consideration of the surroundings in the industrial scale process, Ge et al.¹³ investigated the thermal conductivities of [BMIM][OTf] + water, [EMIM][EtSO₄] + water binary mixtures and correlated the data by the Jamieson correlation equation. Chen et al.¹⁴ studied the thermal conductivities of [MMIM][DMP] + water and [MMIM][DMP] + methanol binary mixtures and fitted the data with higher accuracy. Besides that, several other ionic liquid binary mixture systems were measured mainly by hot wire method recent years.¹⁵⁻¹⁹

Amino acid ionic liquid is an important kind of ionic liquids. As chiral molecular, it has the general characteristics of chiral molecules and well chiral selectivity. Recently, amino acid ionic liquids have been widely applied in extraction separation and asymmetric synthesis process, with scale-up potential.²⁰⁻²⁴ There are some published works about the density and viscosity measurement of amino acid ionic liquids,²⁵⁻²⁸ but the thermal conductivities measurements of those have been rarely reported. Only Gardas et al.²⁹ studied the thermal conductivities of several kinds of ammonium- and phosphonium- based amino acid ionic liquids and correlated the experiment data by group contribution method.

In extraction process, in addition to binary mixtures system, sometimes the separation process is carried out through ternary mixtures system by the addition of co-solvent like alcohols or weak acids, to improve the solubility of the extracted substances.^{30, 31}

In this work, the thermal conductivities of [BMIM][L-trp], water, ethanol, their binary mixtures and ternary mixtures from 283.15 K to 333.15 K within the whole scale of concentrations have been determined at room pressure and the experimental data were correlated by second-order Scheffé polynomial.³²⁻³⁴

2. Experimental section

2.1 Materials

The supplier and purity grades (expressed as mass fraction) of chemical reagents used in this work are shown in Table 1.

Ultrapure water purchased from Wahaha Group Co., Ltd. was further purified by lab ultrapure water purification system (resistivity > 18.2 MΩ·cm at room temperature).

1-Butyl-3-methylimidazolium L-tryptophan, as shown in Figure 1, was purchased from

Shanghai Chengjie Chemical Co., Ltd. Mass content of water for the sample analyzed by Karl Fisher titration (Metrohm 870 KF Titrino Plus) was lower than 500 ppm. The bromine contents were below the detection limit (< 200 ppm) determined by titration with AgNO_3 . The structure of the ionic liquid was confirmed by ^1H NMR (AVANCE III 500 MHz Digital NMR Spectrometer). The weights of material were recorded by an analytical balance (Mettler Toledo XS205 Dual Range) to a precision of ± 0.1 mg.

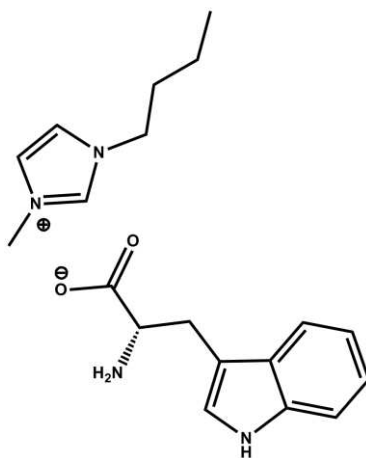


Figure 1. The structure of 1-butyl-3-methylimidazolium L-tryptophan

2.2 Methods

The thermal conductivity measuring instrument (Xi'an Xiatech Electronic Technology Co., Ltd., TC 3000L) was used to collect the thermal data of pure components and mixtures by transient hot wire method. Detailed descriptions of the apparatus and measuring theory can be found in previous references including our works.³⁵⁻³⁷ In brief, the equipment contains two anodized 25 μm diameter tantalum as hot wires in the cells of the instrument. The length of tantalum wires were 29 mm and 58 mm, respectively. An automatic Wheatstone-type electronic bridge was used to measure the time evolution of temperature of the wires during the application of a constant heat flux to the transient hot wire instrument. The isothermal environment for the thermal cell was provided by a

thermostatic bath (Hui Chuang, YHX 2014, uncertainty of $\pm 0.1^{\circ}\text{C}$) and the temperature of the sample was measured by the platinum resistance thermometer of the apparatus automatically. The total uncertainty of the temperature for thermal conductivity measurement is less than $\pm 20\text{ mK}$. The injection volume of sample of each different components mixture is 40 cm^3 approximately. The data acquisition time is 1 second. The heating voltage is adjusted for each sample within the range from 1.2 V (for pure ethanol) to 2.2 V (for pure water), to keep the transient temperature rise at approximately 3 K. All measurements were repeated at least five times for each data point. The thermal conductivity of deionized water, pure ethanol and pure toluene were chosen to check the accuracy and stability of the instrument at the selected temperature range. The detected results had good reproducibility within $\pm 0.73\%$ and were in well agreement with the reference standard data,³⁸ from which the maximum deviation and average relative deviation were 1.02% and 0.62% for water, 1.95% and 1.42% for ethanol, 2.24% and 1.60% for toluene, respectively. Accounting for all the random errors of measurement, the overall uncertainty of the present thermal conductivity data was estimated to be less than 2.0% with a coverage factor of $k = 2$, at a 0.95 confidence interval.

3. Results and Discussion

3.1 Pure components

The experimental and reference thermal conductivities of pure components including [BMIM][L-trp], water and ethanol are listed in Table 2 for comparison and correlation. The reproducibility of pure components is smaller than 0.5% and the uncertainty is less than 2% and $\pm 0.0015\text{ W}\cdot\text{m}^{-1}\cdot\text{K}^{-1}$. The thermal conductivities of [BMIM][L-trp] are between 0.180

and $0.177 \text{ W}\cdot\text{m}^{-1}\cdot\text{K}^{-1}$ from 283.15 K to 343.15 K, similar with those of ammonium- and phosphonium- based amino acid ionic liquids reported by Gardas et al.²⁶ The thermal conductivities decrease linearly with the increase of temperature, which is in agreement with the tendency of most ionic liquids from published references.^{39, 40} So we correlate the thermal conductivity of [BMIM][L-trp] as a linear function of temperature here.

$$\lambda_i = a_0 + a_1 T \quad (1)$$

The thermal conductivities of water and ethanol at different temperature have been studied by many researchers and can be correlated as a function of temperature using a second-order polynomial.^{34, 41}

$$\lambda_i = a_0 + a_1 T + a_2 T^2 \quad (2)$$

Where λ_i ($\text{W}\cdot\text{m}^{-1}\cdot\text{K}^{-1}$) is the thermal conductivity of pure component i , T (K) is the temperature, subscript i represents each pure component as 1 for [BMIM][L-trp], 2 for water and 3 for ethanol. a_0 , a_1 and a_2 are the correlation coefficients. As for ionic liquid system, equation 2 is also suitable when $a_2 = 0$. The parameters a_0 , a_1 , a_2 for equation 2, the values of average absolute relative deviation (AARD) and standard deviation (SD) are listed in Table 3.

3.2 Binary systems

The thermal conductivities data of binary mixtures [BMIM][L-trp] + water, [BMIM][L-trp] + ethanol, water + ethanol measured from 283.15 K to 333.15 K at approximately 10 K interval are listed in Table 4, Table 5 and Table 6 respectively. The thermal conductivities of [BMIM][L-trp] + water increase with the increase of the temperature in the tested concentration range, and those increase with the increase of water content. Similarly with

the [BMIM][L-trp] + water mixture system, the thermal conductivities of water + ethanol mixture increase with the increase of the mass fraction of water and temperature when the mass fraction of water is more than 0.3 and those decrease with the temperature increasing while the mass fraction of water is less than 0.3, which is consistent with the published works.^{42, 43} The thermal conductivities of [BMIM][L-trp] + ethanol are less than $0.2 \text{ W}\cdot\text{m}^{-1}\cdot\text{K}^{-1}$ in the whole concentration range and decrease with the increase of temperature and the mass fraction of [BMIM][L-trp].

The empirical correlation equation second-order Scheffé polynomial, which can well correlate most binary mixtures from pure component and directly calculate the values for ternary data with parameters correlated from binary mixtures with simple forms, was applied in this work.

The equation of second-order Scheffé polynomial for binary mixture is

$$\lambda_{ij} = \lambda_i w_i^2 + \lambda_j w_j^2 + 2\beta_{ij} \lambda_i \lambda_j \quad (3)$$

where subscripts i and j represent two different components as 1 for [BMIM][L-trp], 2 for water, 3 for ethanol, respectively. The λ_{ij} ($\text{W}\cdot\text{m}^{-1}\cdot\text{K}^{-1}$) is the thermal conductivity of binary mixture of component i and j . λ_i ($\text{W}\cdot\text{m}^{-1}\cdot\text{K}^{-1}$) is the thermal conductivity of pure component i , and w_i is the mass fraction of component i in the mixture. β_{ij} is the nonlinear mixing effect between component i and j . The parameter β_{ij} is expected to be a function of temperature and can be assumed as a linear dependence on temperature,⁴⁴

$$\beta_{ij} = A_{ij} + B_{ij}T \quad (4)$$

where A_{ij} and B_{ij} is correlation coefficients.

The thermal conductivities of binary mixtures [BMIM][L-trp] + water, [BMIM][L-trp] +

ethanol, water + ethanol were correlated by equations 3 and 4. The coefficients A_{ij} , B_{ij} for three binary mixtures systems together with fitting AARD and SD are listed in Table 7.

3.3 Ternary systems

For ternary mixtures of [BMIM][L-trp] + water + ethanol, the thermal conductivities data of 36 different compositions measured from 283.15 K to 333.15 K at approximately 10 K interval at atmosphere were list in Table 8. Overall, because the thermal conductivities of water are much higher than that of organic compounds in the experiment temperature range, the thermal conductivities of the ternary mixtures were mainly decided by the mass fraction of water content, and increase with the increase of the mass fraction of water. When the mass fraction of water is constant, the thermal conductivities of mixtures slightly decreased with the increase of mass fraction of ethanol. Besides, the thermal conductivities of ternary mixtures increase with the increase of temperature when the mass fraction of water is higher than 0.2 and decrease with the increase of temperature when the mass fraction of water is lower than 0.2.

The previously mentioned second-order Scheffé polynomial was used to calculate the ternary mixture data and can be expanded as

$$\lambda_{\text{ternary}} = \lambda_1 w_1^2 + \lambda_2 w_2^2 + \lambda_3 w_3^2 + 2\lambda_1 \lambda_2 \beta_{12} + 2\lambda_1 \lambda_3 \beta_{13} + 2\lambda_2 \lambda_3 \beta_{23} \quad (5)$$

where λ_{ternary} ($\text{W} \cdot \text{m}^{-1} \cdot \text{K}^{-1}$) is the thermal conductivity of the ternary mixtures, λ ($\text{W} \cdot \text{m}^{-1} \cdot \text{K}^{-1}$) and w is the thermal conductivity and mass fraction of pure component. Subscript 1, 2, 3 represent [BMIM][L-trp], water, and ethanol, respectively. β is the nonlinear mixing effect between two components that calculated from their binary mixtures.

The thermal conductivities of [BMIM][L-trp] + water + ethanol ternary mixtures can be

calculated by equations 4 and 5 with the parameters listed in Table 7. Figure 2 shows the relative deviations between experimental data and calculated values with the change of temperature. The AARD and SD are 0.58% and $0.0018 \text{ W}\cdot\text{m}^{-1}\cdot\text{K}^{-1}$, respectively. The result indicates that the second-order Scheffé polynomial can be used to estimate the thermal conductivity of [BMIM][L-trp] + water + ethanol ternary mixtures with high accuracy from experimental data of their binary mixtures.

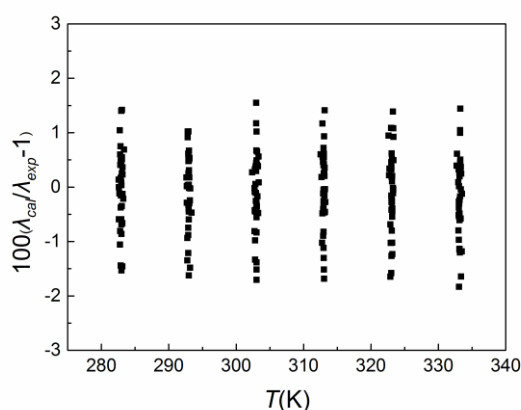


Figure 2. Relative deviations $100(\lambda_{cal}/\lambda_{exp}-1)$ between experimental data λ_{exp} and the values λ_{cal} calculated by equations 4 and 5 for [BMIM][L-trp] + water + ethanol from 283.15 K to 333.15 K at pressure $p = 0.1 \text{ MPa}$. The average absolute relative deviation (AARD) is 0.58% and maximum absolute deviation is 1.83%. ■, this work.

Conclusion

The thermal conductivities of [BMIM][L-trp], water, ethanol, their binary mixtures and ternary mixtures were measured by the instrument with transient hot wire method over the whole concentration range from 283.15 K to 333.15 K. The pure component data were correlated by empirical equation as a function of temperature and the binary mixtures data were correlated as the function of temperature and compositions by second-order Scheffé polynomial. The thermal conductivities data of ternary mixtures were directly calculated by the coefficient correlated from data of their binary mixtures through second-order Scheffé polynomial, and were in good agreement with the experiment results.

Acknowledgement

The authors are grateful for the financial support from National Natural Science Foundation of China (Grant No. 21576231) to this work.

Reference

1. Huang, K.; Wu, Y. T.; Hu, X. B. Effect of alkalinity on absorption capacity and selectivity of SO₂ and H₂S over CO₂: Substituted benzoate-based ionic liquids as the study platform. *Chem Eng J* **2016**, *297*, 265-276.
2. Claus, J.; Sommer, F. O.; Kragl, U. Ionic liquids in biotechnology and beyond. *Solid State Ionics* **2018**, *314*, 119-128.
3. Yao, N.; Wang, H. B.; Hu, Y. L. Recent progress on electrochemical application of room-temperature ionic liquids. *Mini-Rev Org Chem* **2017**, *14*, 237-254.
4. Wang, X. Q.; Mujumdar, A. S. Heat transfer characteristics of nanofluids: A review. *Int J Therm Sci* **2007**, *46*, 1-19.
5. Ogiwara, K.; Arai, Y.; Saito, S. Thermal-conductivities of liquid alcohols and their binary-mixtures. *J Chem Eng Jpn* **1982**, *15*, 335-342.
6. Chen, Q. L.; Wu, K. J.; He, C. H. Thermal conductivity of ionic liquids at atmospheric pressure: Database, analysis, and prediction using a topological index method. *Ind Eng Chem Res* **2014**, *53*, 7224-7232.
7. Zhao, Y. S.; Zhen, Y. P.; Jelle, B. P.; Bostrom, T. Measurements of ionic liquids thermal conductivity and thermal diffusivity. *J Therm Anal Calorim* **2017**, *128*, 279-288.
8. Horrocks, J. K.; McLaughlin, E. Non-steady-state measurements of the thermal conductivities of liquid polyphenyls. *Proceedings of the Royal Society of London* **1963**,

273, 259-274.

9. Babu, S. K.; Praveen, K. S.; Raja, B.; Damodharan, P. Measurement of thermal conductivity of fluid using single and dual wire transient techniques. *Measurement* **2013**, *46*, 2746-2752.

10. Stanimirovic, A. M.; Zivkovic, E. M.; Miloavic, N. D.; Kijevcanin, M. L. Application and testing of a new simple experimental set-up for thermal conductivity measurements of liquids. *Therm Sci* **2017**, *21*, 1195-1202.

11. Tomida, D.; Kenmochi, S.; Tsukada, T.; Qiao, K.; Yokoyama, C. Thermal conductivities of [BMIM][PF₆], [HMIM][PF₆], and [OMIM][PF₆] from 294 to 335 K at pressures up to 20 MPa. *Int J Thermophys* **2007**, *28*, 1147-1160.

12. de Castro, C. A. N.; Lourenco, M. J. V.; Ribeiro, A. P. C.; Langa, E.; Vieira, S. I. C.; Goodrich, P.; Hardacre, C. Thermal properties of ionic liquids and ionanofluids of imidazolium and pyrrolidinium liquids. *J Chem Eng Data* **2010**, *55*, 653-661.

13. Ge, R.; Hardacre, C.; Nancarrow, P.; Rooney, D. W. Thermal conductivities of ionic liquids over the temperature range from 293 K to 353 K. *J Chem Eng Data* **2007**, *52*, 1819-1823.

14. Chen, W.; Qiu, L.; Liang, S. Q.; Zheng, X. H.; Tang, D. W. Measurement of thermal conductivities of [MMIM]DMP/CH₃OH and [MMIM]DMP/H₂O by freestanding sensor-based 3 omega technique. *Thermochim Acta* **2013**, *560*, 1-6.

15. Tomida, D.; Odashima, T.; Qiao, K.; Yokoyama, C. Densities at pressures up to 20 MPa and thermal conductivities at 0.1 MPa of 1-butyl-3-methylimidazolium tetrafluoroborate plus methanol mixtures. *High Temp-High Press* **2018**, *47*, 299-310.

16. Zivkovic, E. M.; Zivkovic, N. V.; Majstorovic, D. M.; Stanimirovic, A. M.; Kijevcanin, M. L. Volumetric and transport properties of binary liquid mixtures with 1-ethyl-3-methylimidazolium ethyl sulfate as candidate solvents for regenerative flue gas desulfurization processes. *J Chem Thermodyn* **2018**, *119*, 135-154.
17. Oster, K.; Goodrich, P.; Jacquemin, J.; Hardacre, C.; Ribeiro, A. P. C.; Elsinawi, A. A new insight into pure and water-saturated quaternary phosphonium-based carboxylate ionic liquids: Density, heat capacity, ionic conductivity, thermogravimetric analysis, thermal conductivity and viscosity. *J Chem Thermodyn* **2018**, *121*, 97-111.
18. Carrete, J.; Mendez-Morales, T.; Garcia, M.; Vila, J.; Cabeza, O.; Gallego, L. J.; Varela, L. M. Thermal conductivity of ionic liquids: A pseudolattice approach. *J Phys Chem C* **2012**, *116*, 1265-1273.
19. Chen, Q. L.; Wu, K. J.; He, C. H. Thermal conductivities of [EMIM][EtSO₄], [EMIM][EtSO₄] + C₂H₅OH, [EMIM][EtSO₄] + H₂O, and [EMIM][EtSO₄] + C₂H₅OH + H₂O at T = (283.15 to 343.15) K. *J Chem Eng Data* **2013**, *58*, 2058-2064.
20. Kirchhecker, S.; Esposito, D. Amino acid based ionic liquids: A green and sustainable perspective. *Curr Opin Green Sust* **2016**, *2*, 28-33.
21. Suzuki, Y. Asymmetric michael addition mediated by chiral ionic liquids. *Mini-Rev Org Chem* **2018**, *15*, 236-245.
22. Wu, D. T.; Cai, P. F.; Zhao, X. Y.; Kong, Y.; Pan, Y. J. Recent progress of task-specific ionic liquids in chiral resolution and extraction of biological samples and metal ions. *J Sep Sci* **2018**, *41*, 373-384.
23. Ding, Q.; Cui, X.; Xu, G. H.; He, C. H.; Wu, K. J. Quantum chemistry calculation aided

design of chiral ionic liquid-based extraction system for amlodipine separation. *Aiche J* **2018**, *64*, 4080-4088.

24. Cui, X.; Yu, F.; Zhu, H.; Wu, K. J.; He, C. H. Progress of enantioseparation using chiral ionic liquids. *Journal of Chemical Engineering of Chinese Universities* **2016**, *30*, 1229-1240.

25. Romero, C. M.; Rojas, J. L. Apparent molar volumes and viscosities of dl-alpha-alanine in water-ethanol mixtures. *Phys Chem Liq* **2000**, *38*, 237-243.

26. Gao, H. Y.; Yu, Z. C.; Wang, H. J. Densities and volumetric properties of binary mixtures of amino acid ionic liquid [BMIM][Glu] or [BMIM][Gly] with benzylalcohol at T = (298.15 to 313.15) K. *J Chem Thermodyn* **2010**, *42*, 640-645.

27. Yu, Z. C.; Gao, H. Y.; Wang, H. J.; Chen, L. W. Thermodynamic properties of binary mixtures of the amino acid ionic liquids [BMIM][Glu] or [BMIM][Gly] with methanol at T=298.15 to 313.15 K. *J Solution Chem* **2012**, *41*, 173-186.

28. Feder-Kubis, J. Physical properties of chiral ionic liquids based on (-)-menthol. *Phosphorus Sulfur* **2013**, *188*, 515-520.

29. Gardas, R. L.; Ge, R.; Goodrich, P.; Hardacre, C.; Hussain, A.; Rooney, D. W. Thermophysical properties of amino acid-based ionic liquids. *J Chem Eng Data* **2010**, *55*, 1505-1515.

30. Yan, J. H.; Sheng, Y.; Huang, K. L. Separation of ibuprofen enantiomers by chiral extraction with hydrophobic tartaric esters. *Journal of Chemical Industry and Engineering (China)* **2007**, *58*, 679-684.

31. Zhang, W. Y.; Cui, X.; He, C. H. Enantioseparation of ofloxacin enantimers via diethyl

L-tartrate extraction. *Journal of Chemical Engineering of Chinese Universities* **2017**, *31*, 769-775.

32. Scheffe, H. Experiments with mixtures. *J Roy Stat Soc B* **1958**, *20*, 344-360.

33. Draper, N. R.; Pukelsheim, F. Mixture models based on homogeneous polynomials. *J Stat Plan Infer* **1998**, *71*, 303-311.

34. Focke, W. W. Correlating thermal-conductivity data for ternary liquid mixtures. *Int J Thermophys* **2008**, *29*, 1342-1360.

35. Wu, J. T.; Zheng, H. F.; Qian, X. H.; Li, X. J.; Assael, M. J. Thermal conductivity of liquid 1, 2-dimethoxyethane from 243K to 353K at pressures up to 30MPa. *Int J Thermophys* **2009**, *30*, 385-396.

36. Wu, J. T.; Li, X. J.; Zheng, H. F.; Assael, M. J. Thermal conductivity of liquid dimethyl ether from (233 to 373) K at pressures up to 30 MPa. *J Chem Eng Data* **2009**, *54*, 1720-1723.

37. Pan, J.; Li, X. J.; Wu, J. T. Thermal conductivity of liquid 1,1,1,3,3,3-hexafluoropropane (HFC-236fa) from 253 K to 373 K and pressure up to 30 MPa. *Fluid Phase Equilib* **2011**, *304*, 64-67.

38. Lemmon, E. W.; Huber, M. L.; McLinden, M. O. Nist reference fluid thermodynamic and transport properties-REFPROP. *NIST Standard Reference Database* **2002**, *23*.

39. Liu, H. J.; Maginn, E.; Visser, A. E.; Bridges, N. J.; Fox, E. B. Thermal and transport properties of six ionic liquids: An experimental and molecular dynamics study. *Ind Eng Chem Res* **2012**, *51*, 7242-7254.

40. Albert, J.; Muller, K. Thermal conductivity of ionic liquids: An estimation approach.

Chem Eng Sci **2014**, *119*, 109-113.

41. Ramires, M. L. V.; Decastro, C. A. N.; Nagasaka, Y.; Nagashima, A.; Assael, M. J.; Wakeham, W. A. Standard reference data for the thermal-conductivity of water. *J Phys Chem Ref Data* **1995**, *24*, 1377-1381.

42. Zhou, J. C.; Che, Y. Y.; Wu, K. J.; Shen, J.; He, C. H. Thermal conductivity of DMSO + C₂H₅OH, DMSO + H₂O, and DMSO + C₂H₅OH + H₂O mixtures at T = (278.15 to 338.15) K. *J Chem Eng Data* **2013**, *58*, 663-670.

43. Assael, M. J.; Charitidou, E.; Wakeham, W. A. Absolute measurements of the thermal-conductivity of mixtures of alcohols with water. *Int J Thermophys* **1989**, *10*, 793-803.

44. Aguila-Hernandez, J.; Gomez-Quintana, R.; Murrieta-Guevara, F.; Romero-Martinez, A.; Trejo, A. Liquid density of aqueous blended alkanolamines and n-methylpyrrolidone as a function of concentration and temperature. *J Chem Eng Data* **2001**, *46*, 861-867.

List of Tables

Table 1. Chemical Sample Description

| chemical names | CAS | supplier | mass fraction | purification method | purity analysis method |
|---|---------|--------------------------------------|---------------|---------------------|------------------------|
| 1-butyl-3-methylimidazolium L-tryptophan | 64-17-5 | Chengjie Chemical Co., Ltd., China | 0.99 | none | HPLC ^a |
| ethanol | | Aladdin Chemical Co., Ltd. | 0.998 | none | GC ^b |
| methylbenzene | | Sinopharm Chemical Reagent Co., Ltd. | 0.995 | none | GC ^b |
| silver nitrate | | Sinopharm Chemical Reagent Co., Ltd. | 0.998 | none | GC ^b |

^aHigh performance liquid chromatography. ^bGas chromatography

Table 2. Experimental and Reference Thermal Conductivities Data of Pure Components from 283.15 K to 343.15 K at Pressure $p = 0.1$ MPa^a

| [BMIM][L-trp] | | water | | | ethanol | | |
|---------------|--|--------|--|-------------------|---------|--|-------------------|
| $T(K)$ | $\lambda(W \cdot m^{-1} \cdot K^{-1})$ | $T(K)$ | $\lambda(W \cdot m^{-1} \cdot K^{-1})$ | | $T(K)$ | $\lambda(W \cdot m^{-1} \cdot K^{-1})$ | |
| | exp. | | exp. | ref. ^b | | exp. | ref. ^b |
| 283.92 | 0.180 | 283.10 | 0.585 | 0.5800 | 283.54 | 0.168 | 0.1687 |
| 293.50 | 0.180 | 293.05 | 0.602 | 0.5983 | 293.31 | 0.166 | 0.1663 |
| 303.46 | 0.179 | 303.17 | 0.618 | 0.6155 | 303.28 | 0.163 | 0.1640 |
| 313.48 | 0.179 | 313.34 | 0.633 | 0.6309 | 313.25 | 0.160 | 0.1617 |
| 323.45 | 0.178 | 323.19 | 0.646 | 0.6436 | 323.07 | 0.158 | 0.1595 |
| 333.58 | 0.178 | 332.85 | 0.656 | 0.6541 | 332.97 | 0.154 | 0.1573 |
| 343.39 | 0.177 | 343.02 | 0.664 | 0.6630 | 342.82 | 0.152 | 0.1551 |

^aThe expanded uncertainties U (0.95 level of confidence, $k = 2$) are $U(\lambda) = 0.02\lambda$, $U(T) = 20$ mK and $U(p) = 0.002$ MPa.

^bReference 38.

Table 3. Correlation coefficient a_0 , a_1 , a_2 , Average Absolute Relative Deviation (AARD) and Standard Deviation (SD) of Pure Components

| | a_0 | a_1 | a_2 | AARD(%) | SD($W \cdot m^{-1} \cdot K^{-1}$) |
|---------------|-------------------------|-------------------------|-------------------------|---------|-------------------------------------|
| [BMIM][L-trp] | 1.938×10^{-1} | -4.889×10^{-5} | | 0.052 | 0.0001 |
| water | -6.634×10^{-1} | 6.942×10^{-3} | -8.951×10^{-6} | 0.035 | 0.0002 |
| ethanol | 2.091×10^{-1} | -2.404×10^{-5} | -4.228×10^{-7} | 0.116 | 0.0002 |

**Table 4. Experimental Thermal Conductivities Data of [BMIM][L-trp] (1) + Water (2)
from 283.15 K to 333.15 K at Pressure $p = 0.1$ MPa^a**

| w_1 | $T(K)$ | $\lambda(W \cdot m^{-1} \cdot K^{-1})$ | w_1 | $T(K)$ | $\lambda(W \cdot m^{-1} \cdot K^{-1})$ | w_1 | $T(K)$ | $\lambda(W \cdot m^{-1} \cdot K^{-1})$ |
|--------|--------|--|--------|--------|--|--------|--------|--|
| 0.1000 | 282.90 | 0.528 | 0.2000 | 283.16 | 0.476 | 0.3000 | 283.00 | 0.427 |
| | 293.16 | 0.543 | | 292.90 | 0.488 | | 293.22 | 0.437 |
| | 303.09 | 0.556 | | 303.35 | 0.501 | | 302.99 | 0.447 |
| | 312.97 | 0.568 | | 312.97 | 0.510 | | 313.37 | 0.456 |
| | 322.88 | 0.578 | | 322.95 | 0.520 | | 323.07 | 0.463 |
| | 333.27 | 0.587 | | 333.10 | 0.528 | | 333.09 | 0.469 |
| 0.3999 | 282.92 | 0.379 | 0.4999 | 283.29 | 0.335 | 0.5998 | 283.11 | 0.295 |
| | 293.22 | 0.388 | | 293.22 | 0.342 | | 293.08 | 0.299 |
| | 303.20 | 0.396 | | 303.08 | 0.347 | | 303.08 | 0.303 |
| | 313.33 | 0.403 | | 313.34 | 0.353 | | 313.15 | 0.307 |
| | 323.33 | 0.409 | | 322.94 | 0.357 | | 323.07 | 0.311 |
| | 333.20 | 0.414 | | 332.98 | 0.361 | | 333.18 | 0.314 |
| 0.6998 | 283.35 | 0.259 | 0.7997 | 283.41 | 0.228 | 0.8998 | 283.00 | 0.200 |
| | 293.17 | 0.262 | | 293.29 | 0.229 | | 293.09 | 0.201 |
| | 303.22 | 0.265 | | 303.33 | 0.230 | | 303.13 | 0.201 |
| | 312.97 | 0.266 | | 312.96 | 0.231 | | 313.28 | 0.202 |
| | 323.09 | 0.269 | | 323.05 | 0.232 | | 323.08 | 0.202 |
| | 333.08 | 0.271 | | 333.10 | 0.234 | | 333.11 | 0.202 |

^aThe expanded uncertainties U (0.95 level of confidence, $k = 2$) are $U(\lambda) = 0.02\lambda$, $U(T) = 20$ mK, $U(p) = 0.002$ MPa and $U(w) = 0.0001$.

**Table 5. Experimental Thermal Conductivities Data of [BMIM][L-trp] (1) + Ethanol (3)
from 283.15 K to 333.15 K at Pressure $p = 0.1$ MPa^a**

| w_1 | $T(K)$ | $\lambda(W \cdot m^{-1} \cdot K^{-1})$ | w_1 | $T(K)$ | $\lambda(W \cdot m^{-1} \cdot K^{-1})$ | w_1 | $T(K)$ | $\lambda(W \cdot m^{-1} \cdot K^{-1})$ |
|--------|--------|--|--------|--------|--|--------|--------|--|
| 0.0999 | 283.04 | 0.171 | 0.2000 | 283.13 | 0.172 | 0.3000 | 283.18 | 0.173 |
| | 292.94 | 0.169 | | 293.27 | 0.170 | | 293.01 | 0.171 |
| | 303.07 | 0.166 | | 303.21 | 0.168 | | 302.82 | 0.170 |
| | 313.10 | 0.163 | | 313.26 | 0.166 | | 312.97 | 0.167 |
| | 323.23 | 0.161 | | 323.22 | 0.163 | | 322.98 | 0.164 |
| | 333.16 | 0.158 | | 333.26 | 0.160 | | 333.35 | 0.163 |
| 0.3995 | 282.86 | 0.175 | 0.5000 | 282.99 | 0.175 | 0.5997 | 283.39 | 0.176 |
| | 293.32 | 0.173 | | 293.22 | 0.174 | | 293.36 | 0.175 |
| | 303.14 | 0.171 | | 302.88 | 0.172 | | 303.45 | 0.174 |
| | 313.27 | 0.169 | | 313.11 | 0.170 | | 312.99 | 0.172 |
| | 323.07 | 0.168 | | 323.14 | 0.169 | | 323.04 | 0.171 |
| | 333.27 | 0.165 | | 333.31 | 0.167 | | 332.89 | 0.170 |
| 0.6998 | 283.23 | 0.177 | 0.7996 | 282.95 | 0.177 | 0.8998 | 283.06 | 0.177 |
| | 293.03 | 0.176 | | 293.34 | 0.177 | | 292.84 | 0.177 |
| | 303.08 | 0.175 | | 303.15 | 0.176 | | 302.99 | 0.178 |
| | 313.34 | 0.174 | | 312.91 | 0.175 | | 312.92 | 0.176 |
| | 323.05 | 0.171 | | 323.12 | 0.174 | | 323.09 | 0.175 |
| | 333.09 | 0.171 | | 332.87 | 0.172 | | 332.94 | 0.174 |

^aThe expanded uncertainties U (0.95 level of confidence, $k = 2$) are $U(\lambda) = 0.02\lambda$, $U(T) = 20$ mK, $U(p) = 0.002$ MPa and $U(w) = 0.0001$.

Table 6. Experimental Thermal Conductivities Data of Water (2) + Ethanol (3) from 283.15 K to 333.15 K at Pressure $p = 0.1$ MPa^a

| w_2 | $T(K)$ | $\lambda(W \cdot m^{-1} \cdot K^{-1})$ | w_2 | $T(K)$ | $\lambda(W \cdot m^{-1} \cdot K^{-1})$ | w_2 | $T(K)$ | $\lambda(W \cdot m^{-1} \cdot K^{-1})$ |
|--------|--------|--|--------|--------|--|--------|--------|--|
| 0.8999 | 282.71 | 0.516 | 0.8000 | 282.89 | 0.455 | 0.7001 | 282.92 | 0.403 |
| | 292.96 | 0.530 | | 292.86 | 0.467 | | 292.60 | 0.412 |
| | 302.89 | 0.546 | | 303.04 | 0.480 | | 303.05 | 0.420 |
| | 312.70 | 0.559 | | 312.98 | 0.491 | | 313.03 | 0.427 |
| | 322.88 | 0.568 | | 323.02 | 0.499 | | 323.12 | 0.434 |
| | 333.00 | 0.577 | | 333.09 | 0.505 | | 333.14 | 0.438 |
| 0.5999 | 283.04 | 0.356 | 0.4993 | 283.23 | 0.311 | 0.4000 | 283.02 | 0.273 |
| | 293.26 | 0.362 | | 293.19 | 0.314 | | 293.03 | 0.274 |
| | 303.05 | 0.367 | | 303.43 | 0.318 | | 303.15 | 0.275 |
| | 313.15 | 0.371 | | 313.23 | 0.319 | | 313.00 | 0.276 |
| | 322.94 | 0.375 | | 323.01 | 0.321 | | 323.33 | 0.277 |
| | 333.13 | 0.379 | | 333.26 | 0.323 | | 333.32 | 0.277 |
| 0.3000 | 283.10 | 0.240 | 0.1996 | 283.07 | 0.212 | 0.1000 | 282.85 | 0.189 |
| | 293.16 | 0.240 | | 293.13 | 0.211 | | 293.16 | 0.186 |
| | 303.19 | 0.240 | | 303.12 | 0.210 | | 303.11 | 0.184 |
| | 313.02 | 0.240 | | 313.19 | 0.208 | | 313.18 | 0.182 |
| | 323.05 | 0.239 | | 323.19 | 0.207 | | 323.15 | 0.180 |
| | 333.14 | 0.238 | | 333.26 | 0.206 | | 333.15 | 0.178 |

^aThe expanded uncertainties U (0.95 level of confidence, $k = 2$) are $U(\lambda) = 0.02\lambda$, $U(T) = 20$ mK, $U(p) = 0.002$ MPa and $U(w) = 0.0001$.

Table 7. Correlation Parameters, Average Absolute Relative Deviation (AARD) and Standard Deviation (SD) of Binary Mixtures for equations 3 and 4

| | | A_{ij} | B_{ij} | AARD(%) | SD(W·m ⁻¹ ·K ⁻¹) |
|-------------------------|----------------|------------------------|-------------------------|---------|--|
| [BMIM][L-trp] + water | $i = 1, j = 2$ | 1.914×10^{-1} | 3.407×10^{-4} | 0.778 | 0.0027 |
| [BMIM][L-trp] + ethanol | $i = 1, j = 3$ | 2.233×10^{-1} | -1.647×10^{-4} | 0.421 | 0.0009 |
| water + ethanol | $i = 2, j = 3$ | 2.429×10^{-1} | 8.334×10^{-6} | 0.459 | 0.0016 |

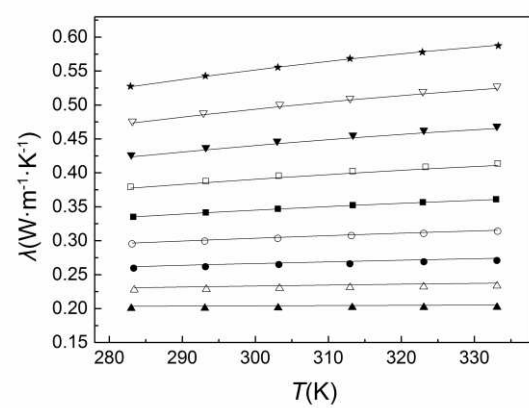
Table 8. Experimental Thermal Conductivities Data of [BMIM][L-trp] (1) + Water (2) + Ethanol (3) from 283.15 K to 333.15 K at Pressure $p = 0.1$ MPa^a

| w_1, w_2 | $T(K)$ | $\lambda(W \cdot m^{-1} \cdot K^{-1})$ | w_1, w_2 | $T(K)$ | $\lambda(W \cdot m^{-1} \cdot K^{-1})$ | w_1, w_2 | $T(K)$ | $\lambda(W \cdot m^{-1} \cdot K^{-1})$ |
|------------|--------|--|------------|--------|--|------------|--------|--|
| 0.7998 | 282.99 | 0.201 | 0.6992 | 282.88 | 0.225 | 0.6999 | 283.12 | 0.197 |
| 0.1002 | 292.91 | 0.201 | 0.2005 | 293.16 | 0.226 | 0.0999 | 292.77 | 0.198 |
| | 303.02 | 0.202 | | 303.03 | 0.227 | | 303.02 | 0.197 |
| | 313.24 | 0.202 | | 313.03 | 0.228 | | 312.98 | 0.197 |
| | 323.10 | 0.202 | | 323.03 | 0.229 | | 323.04 | 0.197 |
| | 333.09 | 0.202 | | 333.37 | 0.230 | | 333.46 | 0.197 |
| 0.5997 | 282.97 | 0.255 | 0.5994 | 283.13 | 0.226 | 0.5999 | 282.77 | 0.197 |
| 0.3002 | 292.98 | 0.257 | 0.2004 | 293.20 | 0.227 | 0.0999 | 292.90 | 0.197 |
| | 303.02 | 0.259 | | 302.93 | 0.228 | | 303.03 | 0.196 |
| | 313.05 | 0.261 | | 313.10 | 0.228 | | 312.91 | 0.196 |
| | 322.88 | 0.263 | | 323.32 | 0.229 | | 323.18 | 0.194 |
| | 333.06 | 0.264 | | 333.24 | 0.229 | | 333.00 | 0.195 |
| 0.4993 | 282.78 | 0.291 | 0.4991 | 282.96 | 0.254 | 0.5000 | 282.99 | 0.222 |
| 0.4009 | 292.76 | 0.294 | 0.3004 | 292.97 | 0.256 | 0.2000 | 292.89 | 0.221 |
| | 302.81 | 0.298 | | 303.03 | 0.258 | | 302.80 | 0.222 |
| | 312.75 | 0.301 | | 313.08 | 0.260 | | 312.96 | 0.223 |
| | 322.93 | 0.304 | | 322.87 | 0.261 | | 323.15 | 0.223 |
| | 333.15 | 0.306 | | 333.13 | 0.261 | | 333.20 | 0.223 |
| 0.4997 | 282.60 | 0.196 | 0.4001 | 282.86 | 0.329 | 0.3998 | 283.12 | 0.287 |
| 0.1002 | 292.95 | 0.195 | 0.4999 | 293.39 | 0.335 | 0.4004 | 292.89 | 0.290 |
| | 302.76 | 0.195 | | 303.26 | 0.340 | | 302.74 | 0.293 |
| | 312.96 | 0.194 | | 313.18 | 0.344 | | 312.97 | 0.296 |
| | 323.17 | 0.193 | | 323.04 | 0.349 | | 323.10 | 0.299 |
| | 333.31 | 0.192 | | 333.03 | 0.352 | | 333.04 | 0.301 |
| 0.3999 | 282.82 | 0.253 | 0.4000 | 283.02 | 0.220 | 0.3999 | 282.97 | 0.195 |
| 0.2999 | 293.06 | 0.255 | 0.2003 | 292.97 | 0.220 | 0.1002 | 292.69 | 0.194 |
| | 303.03 | 0.256 | | 302.82 | 0.221 | | 302.86 | 0.193 |

| | | | | | | | | |
|--------|--------|-------|--------|--------|-------|--------|--------|-------|
| | 312.67 | 0.257 | | 312.81 | 0.220 | | 313.10 | 0.192 |
| | 322.68 | 0.259 | | 323.15 | 0.220 | | 323.03 | 0.191 |
| | 333.39 | 0.260 | | 333.16 | 0.220 | | 333.34 | 0.190 |
| 0.3000 | 282.58 | 0.372 | 0.2997 | 282.99 | 0.325 | 0.2985 | 282.95 | 0.284 |
| 0.6001 | 292.91 | 0.381 | 0.5004 | 292.67 | 0.330 | 0.3985 | 292.82 | 0.287 |
| | 302.36 | 0.387 | | 303.09 | 0.335 | | 303.36 | 0.290 |
| | 312.53 | 0.395 | | 312.98 | 0.339 | | 313.18 | 0.292 |
| | 322.62 | 0.402 | | 323.12 | 0.343 | | 323.28 | 0.294 |
| | 332.71 | 0.405 | | 333.04 | 0.346 | | 333.04 | 0.296 |
| 0.2984 | 283.26 | 0.250 | 0.3000 | 282.88 | 0.219 | 0.3000 | 282.79 | 0.194 |
| 0.3035 | 293.15 | 0.251 | 0.2000 | 293.06 | 0.219 | 0.1000 | 292.96 | 0.193 |
| | 302.96 | 0.252 | | 302.77 | 0.218 | | 303.02 | 0.192 |
| | 312.90 | 0.253 | | 312.91 | 0.218 | | 312.89 | 0.190 |
| | 323.17 | 0.254 | | 323.25 | 0.217 | | 323.05 | 0.189 |
| | 333.14 | 0.254 | | 333.51 | 0.217 | | 333.23 | 0.187 |
| 0.1992 | 282.94 | 0.418 | 0.1998 | 283.07 | 0.369 | 0.1999 | 282.90 | 0.321 |
| 0.6986 | 292.93 | 0.427 | 0.6006 | 293.00 | 0.376 | 0.5004 | 293.06 | 0.325 |
| | 303.31 | 0.437 | | 302.98 | 0.382 | | 302.93 | 0.329 |
| | 313.08 | 0.444 | | 312.97 | 0.389 | | 312.97 | 0.333 |
| | 323.35 | 0.454 | | 323.08 | 0.393 | | 323.04 | 0.336 |
| | 333.26 | 0.458 | | 332.81 | 0.398 | | 333.07 | 0.338 |
| 0.1995 | 283.06 | 0.283 | 0.1999 | 283.13 | 0.246 | 0.1998 | 282.86 | 0.217 |
| 0.4011 | 293.09 | 0.285 | 0.3000 | 293.00 | 0.247 | 0.2006 | 292.92 | 0.217 |
| | 303.11 | 0.287 | | 302.97 | 0.248 | | 302.99 | 0.216 |
| | 313.03 | 0.289 | | 312.99 | 0.249 | | 312.84 | 0.216 |
| | 323.03 | 0.291 | | 323.13 | 0.249 | | 323.34 | 0.215 |
| | 333.14 | 0.292 | | 333.08 | 0.249 | | 333.33 | 0.214 |
| 0.2000 | 282.73 | 0.193 | 0.1000 | 282.69 | 0.465 | 0.1000 | 282.61 | 0.411 |
| 0.0998 | 292.82 | 0.191 | 0.8000 | 292.98 | 0.480 | 0.6999 | 293.07 | 0.420 |

| | | | | | | | | |
|--------|--------|-------|--------|--------|-------|--------|--------|-------|
| | 303.02 | 0.190 | | 302.88 | 0.491 | | 302.71 | 0.428 |
| | 313.04 | 0.188 | | 313.03 | 0.502 | | 312.97 | 0.435 |
| | 323.33 | 0.187 | | 323.14 | 0.508 | | 323.07 | 0.443 |
| | 333.24 | 0.185 | | 333.08 | 0.516 | | 332.95 | 0.448 |
| 0.1000 | 283.03 | 0.362 | 0.0999 | 283.15 | 0.317 | 0.0999 | 283.35 | 0.278 |
| 0.5999 | 292.63 | 0.368 | 0.5001 | 292.98 | 0.320 | 0.4002 | 292.88 | 0.280 |
| | 302.79 | 0.374 | | 303.16 | 0.324 | | 303.23 | 0.282 |
| | 312.96 | 0.380 | | 313.11 | 0.327 | | 313.14 | 0.283 |
| | 322.75 | 0.384 | | 323.04 | 0.330 | | 323.01 | 0.285 |
| | 333.01 | 0.388 | | 333.15 | 0.332 | | 333.13 | 0.286 |
| 0.1000 | 282.86 | 0.244 | 0.0998 | 282.96 | 0.216 | 0.0999 | 283.07 | 0.192 |
| 0.3000 | 293.01 | 0.244 | 0.2003 | 292.81 | 0.214 | 0.1007 | 292.93 | 0.189 |
| | 303.11 | 0.245 | | 302.96 | 0.214 | | 302.97 | 0.188 |
| | 313.01 | 0.245 | | 312.79 | 0.213 | | 313.12 | 0.186 |
| | 323.13 | 0.245 | | 322.98 | 0.212 | | 323.26 | 0.184 |
| | 333.30 | 0.244 | | 333.22 | 0.210 | | 333.25 | 0.182 |

^aThe expanded uncertainties U (0.95 level of confidence, $k = 2$) are $U(\lambda) = 0.02\lambda$, $U(T) = 20$ mK, $U(p) = 0.002$ MPa and $U(w) = 0.0001$.



for Table of Contents use only