

Thermal Conductivity of Ionic Liquids and IoNanofluids. Can Molecular Theory Help?

Xavier Paredes, Maria José Lourenço, Carlos Nieto de Castro and William Wakeham

Correspondence: cacaastro@ciencias.ulisboa.pt

It includes the references for density, speed of sound and thermal conductivity used for all the tests performed. Mass fractions of MWCNTs for the IoNanofluids studies are also shown.

Table SM1 - Literature references for experimental data for density, speed of sound and thermal conductivity used for all the tests performed

Ionic Liquid	Density	Speed of Sound	Thermal Conductivity	IoNanofluids studied, w/%
[C ₂ mim][[(CN) ₂ N]	França et al. (2014) ¹	NA	França et al. (2014) ¹	1, 3
[C ₄ mim][[(CN) ₂ N]	França et al. (2014) ¹	Seoane et al. (2012) ²	França et al. (2014) ¹	1, 3
[C ₄ mpyrr][[(CN) ₂ N]	França et al. (2014) ¹	Cumicheo et al. (2015) ³	França et al. (2014) ¹	1, 3
[C ₄ mim][[(CF ₃ SO ₂) ₂ N]	Castro et al. (2010) ⁴	Zorebski et al. (2018) ⁵	França et al. (2013) ⁶	0.5, 1, 3
[C ₂ mim][EtOSO ₃]	Castro et al. (2010) ⁴	Zorebski et al. (2013) ⁷	França et al. (2013) ⁶	0.5, 1, 3
[C ₂ mim][[(CF ₃ SO ₂) ₂ N]	Jacquemin et al. (2007) ⁸	Zorebski et al. (2013) ⁷	Ribeiro et al. (2013) ⁹	1
[C ₈ mim][[(CF ₃ SO ₂) ₂ N]	Kato and Gmelhing (2005) ¹⁰	Zorebski et al. (2013) ⁷	Ribeiro et al. (2013) ⁹	1
[C ₄ mim][BF ₄]	Gardas et al. (2007) ¹¹	Ebrahiminejadhasanabadi et al. (2018) ¹²	Ribeiro et al. (2013) ⁹	1
[C ₆ mim][[(CF ₃ SO ₂) ₂ N]	Paredes et al. (2020) ¹³	Paredes et al. (2020) ¹³	Paredes et al. (2020) ¹³	1, Ribeiro et al. (2013) ⁹
[C ₆ mim][BF ₄]	Harris and Kanakubo (2016) ¹⁴	Garcia-Miaja et al. (2008) ¹⁵	Castro et al. (2010) ¹⁶	1
[C ₄ mim][CF ₃ SO ₃]	Safarov et al. (2019) ¹⁷	Seoane et al. (2012) ²	Castro et al. (2010) ¹⁶	1
[C ₄ mpyrr][[(CF ₃ SO ₂) ₂ N]	Harris et al. (2011) ¹⁸	Seoane et al. (2012) ²	Castro et al. (2010) ¹⁶	1
[C ₄ mim][PF ₆]	Tomida et al. (2007) ¹⁹	Krishna et al. (2016) ²⁰	Castro et al. (2010) ¹⁶	1
[C ₆ mim][PF ₆]	Gardas et al. (2007) ¹¹	Singh et al. (2014) ²¹	Castro et al. (2010) ¹⁶	1

[C ₂ mim][CH ₃ SO ₃]	Bioucas et al. (2018) ²²	Bioucas et al. (2018) ²²	Bioucas et al. (2018) ²²	NA
[C ₄ mim][[(C ₂ F ₅) ₃ PF ₃]	Castro et al. (2021) ²³	Castro et al. (2021) ²³	Castro et al. (2021) ²³	1
[C ₂ mim][OCH ₃ CO]	Queirós et al. (2020) ²⁴	Queirós et al. (2020) ²⁴	Queirós et al. (2020) ²⁴	NA
[C ₂ mim][SCN]	Neves et al. (2013) ²⁵	Zorebski et al. (2018) ⁵	França et al. (2018) ²⁶	0.5, 1
[C ₄ mim][SCN]	Domanska et al. (2012) ²⁷	Shekaari et al. (2019) ²⁸	França et al. (2018) ²⁶	0.5, 1
[C ₂ mim][C(CN) ₃]	Krolikowski et al. (2013) ²⁹	Zorebski et al. (2018) ⁵	França et al. (2018) ²⁶	0.5, 1
[C ₄ mim][C(CN) ₃]	Krolikowski (2016) ³⁰	NA	França et al. (2018) ²⁶	0.5, 1

¹ J.M.P. França, F. Reis, S.I.C. Vieira, M.J.V. Lourenço, F.J.V. Santos, C.A. Nieto de Castro, A.H. Pádua. Thermophysical Properties of Ionic Liquid Dicyanamide (DCA) Nanosystems. J. Chem. Thermodyn., **2014**, 79, 248–257. DOI: <http://dx.doi.org/10.1016/j.jct.2014.05.008>

² R.G. Seoane, S. Corderi, E. Gomez, N. Calvar, E.J. Gonzalez, E.A. Macedo, A. Dominguez. Temperature Dependence and Structural Influence on the Thermophysical Properties of Eleven Commercial Ionic Liquids. Ind. Eng. Chem. Res., **2012**, 51, 2492-2504. DOI: <https://doi.org/10.1021/ie2029255>

³ M.C. Cumicheo, L.C.S. Nobre, A.F. Santos, I.M.S. Lampreia, M.S.C.S. Santos, F.J.V. Santos, H. Segura, C.A. Nieto de Castro. Thermophysical Properties of 1-Butyl-1-methyl-pyrrolidinium Dicyanamide + H₂O Mixtures. J. Chem. Eng. Data, **2015**, 60, 3766-3775. DOI: <http://dx.doi.org/10.1021/acs.jced.5b00944>

⁴ C.A. Nieto de Castro, E. Langa, A.L. Morais, M.L. Matos Lopes, M.J.V. Lourenço, F.J.V. Santos, M.S.C.C.S. Santos, J.N. Canongia Lopes, H.I.M. Veiga, M. Macatrão, J.M.S.S. Esperança, L.P.N. Rebelo, C.S. Marques, C.A.M. Afonso. Studies on the density, heat capacity, surface tension and infinite dilution diffusion with the ionic liquids [C₄mim][NTf₂], [C₄mim][dca], [C₂mim][EtOSO₃] and [aliquat][dca]. Fluid Phase Equilib., **2010**, 294, 157-179. DOI: <https://doi.org/10.1016/j.fluid.2010.03.010>

⁵ E. Zorebski, M. Musial, K. Baluszynska, M. Zorebski, M. Dzida. Isobaric and Isochoric Heat Capacities as Well as Isentropic and Isothermal Compressibilities of Di- and Trisubstituted Imidazolium-Based Ionic Liquids as a Function of Temperature. Ind. Eng. Chem. Res., **2018**, 57, 5161-5172. DOI: <https://doi.org/10.1021/acs.iecr.8b00506>

⁶ J.M.P. França, S.I.C. Vieira, M.J.V. Lourenço, S.M.S. Murshed, C.A. Nieto de Castro. Thermal Conductivity of [C₄mim][[(CF₃SO₂)₂N] and [C₂mim][EtSO₄] and their Ionanofluids with Carbon Nanotubes: Experiment and Theory. J. Chem Eng. Data, **2013**, 58, 467-476. DOI: <http://dx.doi.org/10.1021/je301183r>

⁷ E. Zorebski, M. Geppert-Rybczynska, M. Zorebski. Acoustics as a Tool for Better Characterization of Ionic Liquids: A Comparative Study of 1-Alkyl-3-methylimidazolium Bis[(trifluoromethyl)sulfonyl]imide Room-Temperature Ionic Liquids. J. Phys. Chem. B, **2013**, 117, 3867-3876. DOI: <https://doi.org/10.1021/jp400662w>

-
- ⁸ J. Jacquemin, P. Husson, V. Mayer, I. Cibulka. High-Pressure Volumetric Properties of Imidazolium-Based Ionic Liquids: Effect of the Anion. *J. Chem. Eng. Data*, **2007**, 52, 2204-2211. DOI: <https://doi.org/10.1021/je700224j>
- ⁹ A.P.C. Ribeiro, S.I.C. Vieira, P. Goodrich, C. Hardacre, M.J.V. Lourenço, C.A. Nieto de Castro. Thermal conductivity of [Cnmim][(CF₃SO₂)₂N] and [C₄mim][BF₄] IoNanofluids with carbon nanotubes – Measurement, theory and structural characterization. *J. Nanofluid.*, **2013**, 2, 55-62. DOI: <http://dx.doi.org/10.1166/jon.2013.1035>
- ¹⁰ R. Kato, J. Gmehling. Systems with ionic liquids: Measurement of VLE and γ^∞ data and prediction of their thermodynamic behavior using original UNIFAC, mod. UNIFAC(Do) and COSMO-RS(OI). *J. Chem. Thermodyn.*, **2005**, 37, 603-619. DOI: <https://doi.org/10.1016/j.jct.2005.04.010>
- ¹¹ R.L. Gardas, M.G. Freire, P.J. Carvalho, I.M. Marrucho, I.M.A. Fonseca, A.G.M. Ferreira, J.A.P. Coutinho. High-Pressure Densities and Derived Thermodynamic Properties of Imidazolium-Based Ionic Liquids. *J. Chem. Eng. Data*, **2007**, 52, 80-88. DOI: <https://doi.org/10.1021/je060247x>
- ¹² M. Ebrahimejadhasanabadi, W.M. Nelson, P. Naidoo, A.H. Mohammadi, D. Ramjugernath. Experimental measurement of carbon dioxide solubility in 1-methylpyrrolidin-2-one (NMP) + 1-butyl-3-methyl-1H-imidazol-3-ium tetrafluoroborate ([bmim][BF₄]) mixtures using a new static-synthetic cell. *Fluid Phase Equilibr.*, **2018**, 477, 62-77. DOI: <https://doi.org/10.1016/j.fluid.2018.08.017>
- ¹³ X. Paredes, C.S.G.P. Queirós, F.J.V. Santos, A.F. Santos, M.S.C. S. Santos, M. J. V. Lourenço, C.A. Nieto de Castro. Thermophysical Properties of 1-Hexyl-3-Methylimidazolium Bis(Trifluoromethylsulfonyl)Imide, [C₆mim][(CF₃SO₂)₂N] – New Data, Reference Data and Reference Correlations. *J. Phys. Chem. Ref. Data*, **2020**, 49, 043101. DOI: <https://doi.org/10.1063/5.0023160>
- ¹⁴ K.R. Harris, M. Kanakubo. Revised and Extended Values for Self-Diffusion Coefficients of 1-Alkyl-3-methylimidazolium Tetrafluoroborates and Hexafluorophosphates: Relations between the Transport Properties. *J. Phys. Chem. B*, **2016**, 120, 12937-12949. DOI: <https://doi.org/10.1021/acs.jpcc.6b10341>
- ¹⁵ G. Garcia-Miaja, J. Troncoso, L. Romani. Excess properties for binary systems ionic liquid + ethanol: Experimental results and theoretical description using the ERAS model. *Fluid Phase Equilibr.*, **2008**, 274(1-2), 59-67. DOI: <https://doi.org/10.1016/j.fluid.2008.09.004>
- ¹⁶ C.A. Nieto de Castro, M.J.V. Lourenço, A.P.C. Ribeiro, E. Langa and S.I.C. Vieira. Thermal Properties of Ionic Liquids and IoNanofluids of Imidazolium and Pyrrolidinium Liquids. *J. Chem. Eng. Data*, **2010**, 55, 653–661. DOI: <http://dx.doi.org/10.1021/je900648p>
- ¹⁷ J. Safarov, A. Guluzade, E. Hassel. Thermophysical Properties of 1-Butyl-3-methylimidazolium Trifluoromethanesulfonate in a Wide Range of Temperatures and Pressures. *J. Chem. Eng. Data*, **2019** 64, 2247-2258. DOI: <https://doi.org/10.1021/acs.jced.8b00837>
- ¹⁸ K.R. Harris, L.A. Woolf, M. Kanakubo, T. R  ther. Transport Properties of N-Butyl-N-methylpyrrolidinium Bis(trifluoromethylsulfonyl)amide. *J. Chem. Eng. Data*, **2011**, 56, 4672-4685. DOI: <https://doi.org/10.1021/je2006049>

-
- ¹⁹ D. Tomida, A. Kumagai, S. Kenmochi, K. Qiao, C. Yokoyama. Viscosity of 1-Hexyl-3-methylimidazolium Hexafluorophosphate and 1-Octyl-3-methylimidazolium Hexafluorophosphate at High Pressure. *J. Chem. Eng. Data*, **2007**, 52, 577-579. DOI: <https://doi.org/10.1021/je060464y>
- ²⁰ T.S. Krishna, K.T.S.S. Raju, M. Gowrisankar, A.K. Nain, B. Munibhadrayya. Volumetric, ultrasonic and spectroscopic studies of molecular interactions in binary mixtures of 1-butyl-3-methylimidazolium hexafluorophosphate with 2-propoxyethanol at temperatures from 298.15 to 323.15 K. *J. Mol. Liq.*, **2016**, 216, 484-495. DOI: <http://dx.doi.org/10.1016/j.molliq.2016.01.085>
- ²¹ M. Singh, S. Mandal, Y. Verma, A. Gupta, R. Singh, S. Chandra. Viscoelastic, Surface, and Volumetric Properties of Ionic Liquids [BMIM][O₂SO₄], [BMIM][PF₆], and [EMIM][MeSO₃]. *J. Chem. Eng. Data*, **2014**, 59, 2349-2359. DOI: <https://doi.org/10.1021/je5000617>
- ²² F.E.B. Bioucas, S.I.C. Vieira, M.J.V. Lourenço, F.J.V. Santos, M.L.M. Lopes, C. A. Nieto de Castro and K. Massonne. [C₂mim][CH₃SO₃] – A Suitable New Heat Transfer Fluid? Part 1. Thermophysical and Toxicological Properties. *Ind. Eng. Chem. Res.*, **2018**, 57, 8541-8551. DOI: <https://doi.org/10.1021/acs.iecr.8b00723>
- ²³ C.A. Nieto de Castro, A.P.C. Ribeiro, A.O. Figueiras, E.L. Langa, S.I.C. Vieira, M.J.V. Lourenço, A.F.S. Santos, F.J.V. Santos, I.M.S. Lampreia, P. Goodrich, C. Hardacre. Thermophysical Properties of 1-butyl-3-methylimidazolium tris(pentafluoroethyl)trifluorophosphate, [C₄mim][C₂F₅]₃PF₃ and of its IoNanofluid with multi-walled carbon nanotubes. *J. Chem. Eng. Data* (**2020**). Submitted.
- ²⁴ C.S.G.P. Queirós, X. Paredes, T.F.S. Avelino, D.E.N. Bastos, M. Ferreira, F.J.V. Santos, A.F. Santos, M.L.M. Lopes, M.J.V. Lourenço, H. Pereira and C.A. Nieto de Castro. The Influence of Water on the Thermophysical Properties of 1-Ethyl-3-methylimidazolium Acetate. *J. Mol. Liq.*, **2020**, 297, 111925. DOI: <https://doi.org/10.1016/j.molliq.2019.111925>
- ²⁵ C.M.S.S. Neves, K.A. Kurnia, J.A.P. Coutinho, I.M. Marrucho, J.N.C. Lopes, M.G. Freire, L.P.N. Rebelo. Systematic Study of the Thermophysical Properties of Imidazolium- Based Ionic Liquids with Cyano-Functionalized Anions. *J. Phys. Chem. B*, **2013**, 117, 10271-10283. DOI: <https://doi.org/10.1021/jp405913b>
- ²⁶ J.M.P. França, M.J.V. Lourenço, S.M.S. Murshed, A.A.H. Pádua, C.A. Nieto de Castro. Thermal Conductivity of Ionic Liquids and IoNanofluids and their Feasibility as Heat Transfer Fluids. *Ind. Eng. Chem. Res.*, **2018**, 57, 6516-6529. DOI: <https://doi.org/10.1021/acs.iecr.7b04770>
- ²⁷ U. Domanska, M. Krolkowska. Density and Viscosity of Binary Mixtures of Thiocyanate Ionic Liquids +Water as a Function of Temperature. *J. Solution Chem.*, **2012**, 41, 1422-1445. DOI: <https://doi.org/10.1007/s10953-012-9875-7>
- ²⁸ H. Shekaari, M.T. Zafarani-Moattar, B. Golmohammadi. Solvation properties of 1-alkyl-3-methylimidazolium thiocyanate ionic liquids in the presence of lithium halide salts in N-methyl-2-pyrrolidone. *J. Mol. Liq.*, **2019**, 280, 191-204. DOI: <https://doi.org/10.1016/j.molliq.2019.02.017>
- ²⁹ M. Krolkowski, K. Walczak, U. Domanska. Solvent extraction of aromatic sulfur compounds from n-heptane using the 1-ethyl-3-methylimidazolium tricyanomethanide ionic liquid. *J. Chem. Thermodyn.*, **2013**, 65, 168-173. DOI: <https://doi.org/10.1016/j.jct.2013.05.048>

³⁰ M. Krolikowski. Liquid-liquid extraction of p-xylene from their mixtures with alkanes using 1-butyl-1-methylmorpholinium tricyanomethanide and 1-butyl-3-methylimidazolium tricyanomethanide ionic liquids. *Fluid Phase Equilibr.*, **2016**, 412, 107-114. DOI: <https://doi.org/10.1016/j.fluid.2015.12.032>