

IUPAC Ionic Liquids Database – ILThermo

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It has long been understood that experimental thermophysical and thermochemical properties data are vital to scientific research and industrial design. Their importance has been expeditiously recognized by scientists and engineers working in the field of ionic liquids, one of the most active research topics in chemistry during recent years. To utilize these compounds requires an extensive investigation of the chemical and physical properties of both the pure fluids and their mixtures. Furthermore, a living, up-to-date database that stores and organizes property data for ionic liquids and their mixtures has the ability to become an invaluable tool to speed up research in academia and the development of their use in industry. In 2003, an IUPAC task group was formed with an objective to “create an open-access, free, on-line, comprehensive database for storage and retrieval of metadata and numerical data for ionic liquids, including their syntheses, structure, properties, and uses; lack of this information is impeding progress in a burgeoning field of significant current interest”. Here, we present the first public release of the IUPAC Ionic Liquids Database (ILThermo). The present version (as of February 1, 2006) contains information on 206 ions and 315 ionic liquids. The collected data cover the relevant literature from 1982 to 2006 for pure ionic liquids as well as for binary and ternary systems containing ionic liquids. The experimental data stored in the database include that for phase transitions, transport, volumetric, and thermal properties as well as electrical conductivity, surface tension, refractive index, speed of sound, vapor pressure, and activity coefficients. The database presently contains 17958 experimental data points. Various options of data retrieval from the ILThermo will be discussed. Continuous database growth proceeds as a part of the NIST/TRC data collection effort, and the web-accessible ILThermo updates will be provided on a regular basis.