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Thermodynamic Properties of Organic Compounds and their Mixtures

Subvolume I

Densities of Phenols, Aldehydes, Ketones, Carboxylic Acids,
Amines, Nitriles, and Nitrohydrocarbons

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Edited by M. Frenkel and K.N. Marsh



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Preface

Critically evaluated experimental data covering the densities of organic compounds are essential for both scientific and industrial applications. Knowledge of densities is important in many areas, including custody transfer of materials, product specification, development of various predictive methods, and for characterizing compounds and estimating their purity.

Various compilations of densities for organic compounds have been published. The early Landolt-Börnstein compilation [1923-ano] contained recommended values at specific temperatures. International Critical Tables [1928-ano-1] provided recommended densities at 0 °C and values of constants for either a second- or third-order polynomial equation to represent densities as a function of temperature. This compilation also gave the range of validity of the equation and the limits of uncertainty, references used in the evaluation and those not considered. This compilation is one of the most comprehensive ever published. Timmermans [1950-tim, 1965-tim], Dreisbach [1955-dre, 1959-dre, 1961-dre] and Landolt-Börnstein [1971-ano] published additional compilations, primarily of experimental data. These compilations contained experimental data along with reference sources but no estimates of uncertainty for the data nor recommended values.

The Thermodynamics Research Center has published recommended values for the densities of organic compounds since 1942 in its two loose-leaf publications: TRC Thermodynamic Tables - Hydrocarbons and Non-Hydrocarbons. These compilations are updated with four supplements per year. References to the literature values used in the selection and those not used in the selection appear in the references for each table. The accuracy of the values is apparent from the number of significant figures provided. More recently, the Design Institute of Physical Property Data, Project 801 has assembled a set of recommended equations for the densities of over 1500 compounds [1989-dau/dan, 1991-dau/dan, 1992-dau/dan, 1993-dau/dan, 1994-dau/dan, 1995-dau/dan, 1996-dau/dan, 1997-dau/dan, 1998-ano, 1999-ano]. Densities are represented by an equation fit to selected values from the freezing temperature to the critical temperature. References to sources of data used in the evaluation and those not used are given along with a quality assessment. In many cases, the equation does not fit density values at intermediate temperatures, especially at 293.15 K and 298.15 K, within the experimental uncertainty. Thus, the equation may not be useful for purity comparisons, custody transfer, or product specification when the highest accuracy is required. Smith and Srivastava [1986-smi/sri, 1986-smi/sri-1] have published a compilation (in two volumes) which contains recommended values in tabular form as well as equations with statistical information regarding the fit. However, this compilation contains no indication of data quality or uncertainties.

The present volume contains densities for phenols, aldehydes, ketones, carboxylic acids, amines, nitriles, and nitrohydrocarbons both fully saturated and with various extents of unsaturation which have been collected from the literature published from 1845 to early 2001. The various compilations listed above also have been consulted for sources of original data. This volume continues our effort in evaluation of the densities of organic compounds [see volume IV/8B (1996-wil/mar) for the densities of alkanes, volume IV/8C (1996-wil/mar-1) for the densities of alkenes, alkynes and alkadienes, volume IV/8D (1997-wil/hon) for the densities of monocyclic non-aromatic hydrocarbons, volume IV/8E (1998-wil/hon) for the densities of aromatic hydrocarbons, volume IV/8F (1999-wil/hon) for the densities of polycyclic hydrocarbons, volume IV/8G (2000-fre/hon) for the densities of non-cyclic alcohols, and volume IV/8H (2001-fre/hon) for the densities of esters and ethers]. All experimental density values have been evaluated critically and assigned numerical uncertainties individually. These assessments have been used to derive an equation to fit the data and to obtain recommended values with uncertainties. Detailed evaluation procedures appear in Chapter 1. Algorithms for the automatic selection of data used in the fit and for the selection of the type of equation and order of polynomial have been developed. The algorithms depend upon the assigned uncertainties, the distribution of density values over the experimental temperature range, and the magnitude and distribution of differences between observed and

smoothed values. These algorithms can fit any kind of data to a function of independent variables. We have collected data for 746 compounds, consisting of data sets drawn from more than 1,200 sources.

The volume contains eight chapters; a list of references; and two indexes (Chemical Abstracts Service Registry Number Index and Chemical Name Index). Chapter 1 contains: a short introduction; a description of the tables; a detailed description of the methods used in the evaluation, selection and smoothing process; and a glossary of symbols and a description of the order of compounds. Chapter 2 covers the phenols, Chapter 3, the aldehydes, Chapter 4, the ketones, Chapter 5, the carboxylic acids, Chapter 6, the amines, Chapter 7, the nitriles, and Chapter 8 contains the data for the nitrohydrocarbons. The tables contain the original literature data along with their estimated uncertainties and the evaluated data in both numerical form and as coefficients to equations with selected statistical information. When data cover a sufficient temperature range, graphical plots of the deviations of the experimental data from the recommended equation are given. The chemical name index contains the IUPAC names for the compounds, as well as alternate names that often appear in practice.

This volume should be useful to a wide community of researchers, data specialists, and engineers working in the field of physical and organic chemistry, chemical engineering, material science, environmental chemistry, chemical aspects of energy technology, and those engaged in the development of new predictive procedures. The book should also be of use to students and faculty in Chemistry and Chemical Engineering departments at universities as a reference book of evaluated thermophysical properties.

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Survey of volume IV/8

Thermodynamic Properties of Organic Compounds and their Mixtures

1. Enthalpies of Fusion and Transition of Organic Compounds	Subvolume A
2. Densities of Aliphatic Hydrocarbons: Alkanes	Subvolume B
3. Densities of Aliphatic Hydrocarbons: Alkenes, Alkadienes, Alkynes, and Miscellaneous Compounds	Subvolume C
4. Densities of Monocyclic Hydrocarbons	Subvolume D
5. Densities of Aromatic Hydrocarbons	Subvolume E
6. Densities of Polycyclic Hydrocarbons	Subvolume F
7. Densities of Alcohols	Subvolume G
8. Densities of Esters and Ethers	Subvolume H
9. Densities of Phenols, Aldehydes, Ketones, Carboxylic Acids, Amines, Nitriles, and Nitrohydrocarbons	Subvolume I