Journal of
**Physical and
Chemical
Reference Data**
Volume 2, 1973
Supplement No. 1

Physical and Thermodynamic Properties of Aliphatic Alcohols

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Published by the **American Chemical Society**
and the **American Institute of Physics** for
the **National Bureau of Standards**

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Physical and Chemical Reference Data

David R. Lide, Jr., Editor

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J. Phys. Chem. Ref. Data
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Published by the **American Chemical Society**
and the **American Institute of Physics** for
the **National Bureau of Standards**

Library of Congress Catalog Card Number 73-84178

International Standard Book Numbers
0-88318-202-5 (Hard cover) 0-88318-205-X (Paper cover)

American Institute of Physics, Inc.
335 East 45 Street
New York, New York 10017

Printed in the United States of America

Foreword

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The regular issues of the *Journal of Physical and Chemical Reference Data* are published quarterly and contain compilations and critical data reviews of moderate length. Longer monographs, volumes of collected tables, and other material unsuited to a periodical format are published separately as *Supplements* to the *Journal*. This monograph, "Physical and Thermodynamic Properties of Aliphatic Alcohols", by R. C. Wilhoit and B. J. Zwolinski, is presented as Supplement No. 1 to Volume 2 of the *Journal of Physical and Chemical Reference Data.*

David R. Lide, Jr., Editor
Journal of Physical and Chemical Reference Data

Physical and thermodynamic properties of aliphatic alcohols

R. C. Wilhoit and B. J. Zwolinski

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Critically evaluated data are presented on the thermodynamic properties and certain physical properties of the monohydroxy aliphatic alcohols. Properties studied include refractive index, density, vapor pressure, phase transitions, heat capacity, properties of the saturated real gas and the ideal gas, properties of standard states at 25 °C, and critical properties to the extent that these have been measured. Data are given for 722 alcohols in the carbon range of C_1 to C_{50}.

Key words: Critical properties; critically evaluated data; density; heat capacity; ideal gas properties; monohydroxy aliphatic alcohols; refractive index; saturated real gas properties; standard entropy of formation; standard heat of formation; thermodynamic data; transition properties; vapor pressure.

Preface

In 1947, the National Bureau of Standards published Circular 461 entitled "Selected Values of Properties of Hydrocarbons" which was prepared as part of the work of the American Petroleum Institute Research Project 44 at the National Bureau of Standards under the direction of Frederick D. Rossini. This publication, currently known as the 'API 44 green volume,' was the first of its kind that attempted to survey all the existing scientific literature on certain properties of a large group of chemically similar substances, namely, the hydrocarbons, and to present an internally consistent set of tables of selected numerical data on the physical and thermodynamic properties of these individual hydrocarbons.

In the preface of this volume the NBS director, Edward U. Condon, stresses the importance of such critical or standard reference data studies and publications as follows:

> "One of the bulwarks of any technical or scientific research program is the collection and critical appraisal of the pertinent information already available. One type of such information that is required by all laboratories in industry and science comprises selected values of the fundamental physical constants and of the properties of the chemical substances. Many advantages result from having such fundamental work performed systematically and consistently in a cooperative program by a full-time staff of experts, rather than incidentally and sporadically by workers in different laboratories. In addition to the obvious advantage of producing a complete, accurate, and self-consistent set of values of constants and properties, such a cooperative program results in a considerable saving in over-all cost and manpower."

Next of fundamental and technical importance to the class of chemical substances known as the hydrocarbons are their oxygen derivatives or, more specifically, the monohydroxy alcohols or alkanols. An exhaustive study on the physical and chemical properties of these alcohols was initiated at the Thermodynamics Research Center of the Department of Chemistry of Texas A&M University under the auspices of the NBS Office Standard Reference Data in 1965, culminating in the preparation of this volume.

This monograph represents the most exhaustive review and critical analysis of certain physical and thermodynamic properties of aliphatic alcohols that has been published in the world literature of chemistry during the last 100 years. The usual properties of the liquid, vapor, and ideal gaseous states are covered as well as pertinent solid state data necessary to equilibrium calculations ordinarily encountered in chemical and chemical engineering applications. The available quantitative literature data on each property for each aliphatic alcohol are fully documented and critically analyzed providing a "data bank" for the 722 monohydroxy alcohols in the carbon range of C_1 to C_{50}. The literature coverage is complete through 1967 and the early months of 1968. To meet the needs of the ordinary "handbook user," internally consistent tables of critical, standard, or selected "best" values are tabulated for each chemical compound. These experimentally determined numerical values of physical and thermodynamic properties are comprehensively indexed for ease of accession to both tables and text.

Ordinarily the critical evaluation and selection of standard or "best" numerical values for properties of chemical substances go hand-in-hand with correlations of properties with thermodynamic variables and specific molecular structural parameters. Since the purpose of this comprehensive publication was to tabulate only experimentally available quantitative numerical information on the monohydroxy alcohols, structural correlations were not used in the final selection of the measured values except where absolutely necessary. The problem of predicting properties of alcohols hitherto not synthesized in the laboratory and of known alcohols in a range of temperatures and pressures not accessible in the laboratory have been treated separately and will appear elsewhere.

The staff of the Project wishes to acknowledge the help, advice, and constructive criticism received from the personnel of the NBS Office of Standard Reference Data and from the reviewers of the earlier progress reports leading to the final preparation of this monograph. Special thanks are due to our professional colleagues in academic and industrial circles who have brought new or obscure information to our attention. We would greatly appreciate receiving comments regarding errors and omissions that have escaped our attention.

Bruno J. Zwolinski, Director
Thermodynamics Research Center

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I. Introduction

A. Technical and Scientific Background

The monohydroxy aliphatic alcohols represent an important class of compounds from both the industrial and scientific standpoints. Many members of this group are manufactured and sold in tonnage quantities throughout the world. Those having a small number of carbon atoms per molecule are used as industrial solvents, in pharmaceutical preparations, as intermediates in the manufacture of many other commodities, and as a beverage. Those members of six or more carbon atoms per molecule are known as "fatty alcohols." Many of these are important in the manufacture of surfactants, plasticizers, cosmetics, lubricants, evaporation surpressors, and numerous other products. Several alcohols, especially ethanol, play important roles in metabolic reactions in living organisms. The hydroxyl group is moderately reactive chemically; thus, the alcohols are involved either as reactants or products in a wide variety of chemical reactions which include esterification and hydrolysis, dehydration and hydration, dehydrogenation and hydrogenation, and oxidation and reduction.

Structurally, the alcohols are more closely related to alkanes than is any other class of organic oxygen compounds. Since alkanes are frequently used as a theoretical framework for predicting and correlating physical and thermodynamic properties of other classes of compounds, the alcohols themselves can serve as an important structural link between the properties of hydrocarbons and their oxygen derivatives. In spite of the close similarity in molecular structure, many of the properties of the alcohols are quite different from their parent alkanes. Melting points, viscosities, boiling points, and heats of vaporization of the alcohols are nearly always higher, reflecting the increased intermolecular attractions due to the high dipole moment and hydrogen bonding in the alcohols. The effects of these phenomena are clearly demonstrated by comparing the properties of an alcohol with those of the corresponding alkane. The quantitative effects of intermolecular interactions on the physical and thermodynamic properties of alcohols have posed a challenge to theoretical scientists for the past fifty years, and a great deal of attention has been given to this problem. In spite of the considerable effort which has been spent on studies of the molecular association in the solid, liquid, and gas states, our understanding of these phenomena is still unsatisfactory. A brief review of the current state of knowledge is given in appendix A.

Table 1 lists the number of structural isomers of monohydroxy alcohols containing up to 20 carbon atoms per molecule and, also, the number of which experimental data have been found. This table shows the practical impossibility of listing properties of all isomers up to 20 carbon atoms per molecule, even if they were available. It is our hope that the experimental data summarized in this report will serve as a basis for the development of methods for correlating and predicting physical and thermodynamic properties of alcohols. Figures 1 and 2 show additional information on the extent of experimental data for alcohols containing one to ten carbon

TABLE 1. Number of structural isomers and number included in the report

Number of Carbon Atoms per Molecule	Number of Structural Isomers of the Alkanols*				Number of "Common Alcohols" discussed in detail in the Report	Total number of Alcohols included in the Report
	Primary	Secondary	Tertiary	Total		
1	1	0	0	1	1	1
2	1	0	0	1	1	1
3	1	1	0	2	2	2
4	2	1	1	4	4	4
5	4	3	1	8	8	8
6	8	6	3	17	17	17
7	17	15	7	39	1	38
8	39	33	17	89	1	73
9	89	82	40	211	1	97
10	211	194	194	507	1	114
11	507	482	249	1,238	1	63
12	1,238	1,188	631	3,057	1	80
13	3,057	2,988	1,594	7,639	0	37
14	7,639	7,528	4,074	19,241	1	34
15	19,241	19,181	10,443	48,865	0	24
16	48,865	49,060	26,981	124,906	1	28
17	124,906	126,369	69,923	321,198	0	9
18	321,198	326,863	182,158	830,219	1	13
19	830,219	849,650	476,141	2,156,010	0	14
20	2,156,010	2,216,862	1,249,237	5,622,109	0	13
21–50					0	50

* Somayajulu, Kudchadker, and Zwolinski [1965].

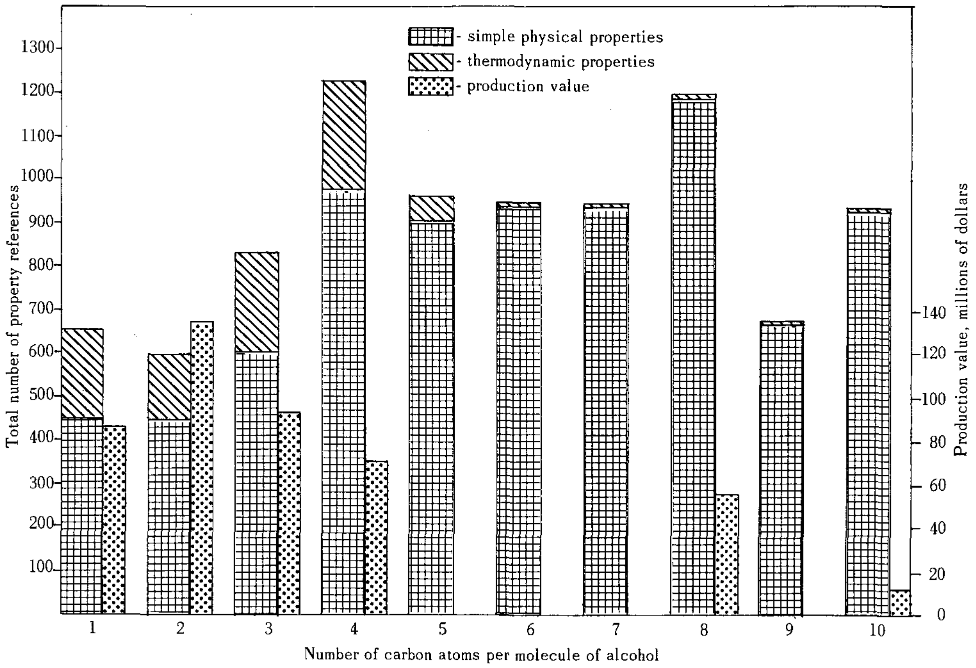

FIGURE 1. Total property references for all isomers.

atoms per molecule. Figure 1 is a graph of the number of references to specific measured properties grouped according to the number of carbon atoms per molecule. Each reference to a given property, not counting measurements at different temperatures or other conditions, was counted as distinct. The simple physical properties are boiling point, density, melting point, and refractive index. Figure 1 further shows the market value of the alcohols in the various carbon ranges which were produced in 1965. Compounds having a value of at least $10,000,000 per year were included. The statistical data were taken from "Chemical Origins and Markets," Stanford Research Institute, Menlo Park, California, 1967. Information in the "Kirk-Othmer Encyclopedia of Chemical Technology" indicates that the production value of alcohols above ten carbon atoms per molecule was $58,000,000 in 1959.

Figure 2 presents the same statistical data on the number of literature property references in a slightly different way. The total number of references divided by the number of isomeric alcohols in each group is plotted versus the carbon range. This graph emphasizes the average number of property references per compound for the various numbers of carbon atoms per molecule.

Except for 2-methyl-1-propanol, the alcohols up through C_4 have been studied extensively, and reasonably reliable information on the more common physical and thermodynamic properties is available. For the C_5 alcohols most of the simple physical property data are of good precision and accuracy. In sharp contrast, the thermodynamic data are of a lower order of precision and few cross checks on any one property are availaible No P-V-T data on the real gas have been published in the open literature on any alcohol containing more than four carbon atoms per molecule. A few scattered measurements on thermodynamic properties such as heat capacity, entropy, heat of fusion and vaporization, and heat of combustion have been made on alcohols above C_5. The scarcity of thermodynamic data on the higher alcohols is clearly shown in figures 1 and 2. There is a definite alteration in the amount of information available for alcohols above C_5. There are more data for compounds containing an even number of carbon atoms than for those containing an odd number. Figure 1 gives only a hint of this situation, but does not show it clearly since it does not indicate the quantity and quality of the data

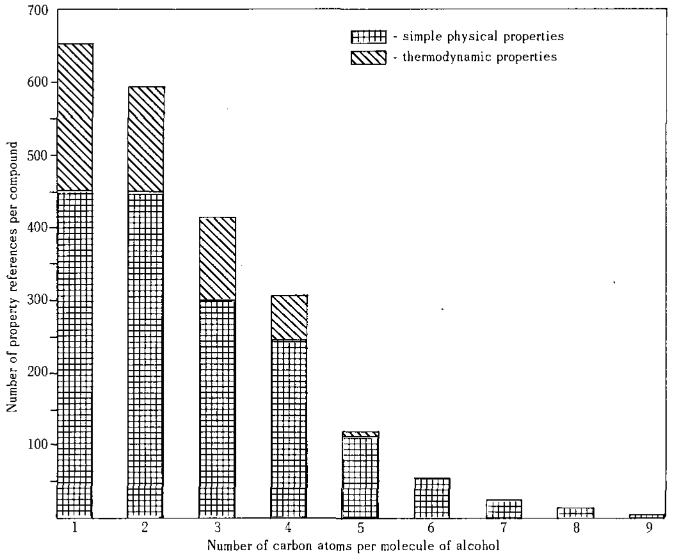

FIGURE 2. Average number of property references for each isomer.

in the references. This distribution is due to the easier synthesis of alcohols containing an even number of carbon atoms, as well as the more frequent occurrence of these compounds in nature and in industrial processes.

Under normal room conditions, alcohols exist either as colorless liquids or solids. As is true for most homologous series, one finds the general trend of increasing melting point, boiling point, and viscosity, and decreasing vapor pressure as the number of carbon atoms in the molecule increases. There is a marked tendency for the higher alcohols to form undercooled liquids, so it is usually difficult to obtain accurate values of melting points for them. The solid forms usually take on a soft "waxy" texture. The boiling points of isomeric alcohols with the same number of carbon atoms generally decrease on going from primary to secondary to tertiary structures for the hydroxyl group, and with increased branching of the hydrocarbon chain.

B. Nature and Scope of the Report

This report consists of an exhaustive and critical review of certain physical and thermodynamic properties of the pure, simple, monohydroxy, aliphatic alcohols (alkanols) in the carbon range of C_1 to C_{50} currently available in the open literature. The principal objective is the tabulation of selected "best" or "standard reference" values of the properties considered. These values are based primarily on the world's scientific literature published through 1967 and part of 1968. The material is arranged to accommodate both those users of data who wish to obtain only the best available numerical values of properties and those who wish to identify the original sources of information and to follow the details of the selection procedure. All literature references have been fully documented, and the reasons for the selections are described within the allowable space limitations. Estimates of uncertainties have been given for the selected basic physical and thermodynamic data.

The report is restricted to values of the equilibrium properties of pure compounds. The properties considered are those frequently required in thermodynamic and thermochemical calculations. The simple physical properties are melting point, boiling point and vapor pressure, liquid density, and refractive index. The basic thermodynamic properties are enthalpies and temperatures of phase transitions, heat capacity, entropy, enthalpies of formation, and Gibbs energy of formation of the various physical states. Critical constants have been selected, but in general, properties at temperatures and pressures much above the normal boiling point were not selected. Although some discussion is presented for the equilibrium properties of the real gas, no final values were recommended except for a few special conditions. Values of the statistical thermodynamic functions of ideal gases as a function of temperature were tabulated where possible. Data on viscosity, thermal conductivity, and surface tension have not been included.

With one exception, all selections are based on direct experimentally observed data or upon reasonable interpolations, extrapolations, or minor adjustments of such data. The exception is the thermodynamic functions of the ideal gases. These values for alcohols containing from one to three carbon atoms were calculated from molecular energy states by the accepted methods of statistical thermodynamics. Values for the higher alcohols were obtained by applying the $-CH_2-$ increments found for the alkanes to the values for the lower alcohols. The selections were made to be "internally consistent" in the sense of satisfying all the thermodynamic relationships among the properties of a single compound. In most cases no attempt was made to adjust or bias the *selected values* to correspond to any preconceived correlation scheme for relating molecular structure to physical and thermodynamic properties. The availability of selected experimental values of properties of the alkanols, many of which are "key" compounds in molecular correlation procedures, should serve as an incentive for the development of more powerful and more precise correlation procedures for predicting thermodynamic data on new or less common compounds where experimental data is currently not available. Some consideration of the enthalpies of formation of the liquid 1-alkanols from this standpoint is presented in appendix F.

Many of the branched-chain alkanols can be resolved into two optically active isomers. These differ in physical properties only in the direction of rotation of polarized light, which is not included in this report. Although there may be differences in the physical properties of a crystalline enantiomorph from those of the racemic mixture of *d*- and *l*- forms, no data of this type have been found for any of the compounds included in the report. Therefore, no distinction has been made between properties of either enantiomorph or the racemic mixture in such cases. Diastereoisomers exist for compounds containing two or more asymmetric centers. The simplest alkanol of this type is 3-methyl-2-pentanol. Physical properties of such isomers are different for the liquid and gaseous states, as well as for the crystalline state. However properties of diastereoisomers of this, or of any of the other alkanols, have not been reported. Presumably in those cases where diastereoisomers exist, the reported properties refer to an undetermined mixture of the isomers.

C. Organization of the Report

The presentation of numerical data and the accompanying discussions in this report are organized on the basis of the individual compounds. Therefore, except for the references to original sources in the Bibliography, all the information for any one compound will be found in the same section of the report. The material is primarily arranged according to the number of carbon atoms per molecule, starting with methanol and proceeding systematically through the higher alcohols.

Within each carbon number, the isomers are arranged first according to the longest straight chain in the molecule, next by position of the hydroxy group, and finally by number and type of side chains. A complete list of all compounds in the order of appearance in the report will be found in table 2a, page 1–23. This table includes the names of the compounds, the Wiswesser line-formula notations, *selected values* of a few simple physical properties, and references to table numbers and page numbers in the report where additional information is located. Table 2b contains a condensed summary of the thermodynamic properties of those alcohols for which appropriate data are available.

Because of the large number of compounds considered and the great variation in amount and kind of information available for each compound, some differences in style of presentation have been adopted. In general, more extensive data are available for the lower alcohols containing one to five carbon atoms per molecule and for the higher normal 1-alkanols up through C_{18} than for the other secondary, tertiary, and branched-chain alcohols. These 26 *well-characterized* alcohols are discussed on an individual basis with material for each such compound arranged as follows: tables of *selected values*; discussion of specific properties; tables of *reported values*; and Index to the Bibliography. The topics in the discussion are listed in the Contents, page 1–5. The particular grouping of properties chosen reflects the usual type of experimental data reported in the literature and the order of discussion follows the approximate order in which they were considered in making the selections. Tables of *selected values* summarize the final recommended values of the standard set of properties and include estimates of the uncertainties in these values. Tables of *reported values* contain numerical data obtained by individual authors as the result of experimental observations. In these tables the sources are identified by the last names of the investigators and the year of publication. Complete references to these sources are given in the Bibliography, page 1–389, at the end of the report. In general only those data considered in the final selections have been included in tables of *reported values*. If necessary, the original data have been corrected to correspond to modern units and to certain standard conditions as defined in Section F and in the headings of the tables. The tables of *reported values* of the *simple physical properties* of the 26 *well-characterized* alcohols consist of a partial list of values of the normal boiling point (760 mmHg), density and refractive index at 20 and 25 °C, and the melting point in air at 1 atm. Boiling points at other pressures and densities and refractive indices at other temperatures and/or wavelengths have not been included. A complete list of references to these properties can be obtained from the identifying numbers given in the Index to the Bibliography which follows the section on each alcohol. These numbers correspond to the numbers in the Bibliography on page 1–389. Sources of data used in fitting constants in the Antoine and Francis equations and in selecting the refractive index data can be identified from the underlined numbers in the Index to the Bibliography. Additional details concerning the selection of data for these and other properties are given in the discussions. The *selected values* of *simple physical properties* are also given at the end of these tables. All tables containing *selected* and *reported values* of properties of the 26 *well-characterized* alcohols have been given individual numbers, and a complete list will be found on page 1–10.

Information on the remaining group of 696 compounds has been put into a more concise format. All isomeric compounds containing the same number of carbon atoms are discussed in one section. Most of the numerical data for these compounds are confined to the *simple physical properties*; *i.e.*, boiling point, refractive index, density, and melting point. All sources of such data, irrespective of whether they were considered in the final selection, are listed in the tables of *reported values*, which, unlike similar tables for the *well-characterized alcohols*, are *not* given individual table numbers but are identified in table 1 by the corresponding page number. Since these tables furnish a complete index to the *simple physical property* data no additional indices are necessary. Values of density or refractive index taken close to 20 or 25 °C have been adjusted to one of these temperatures by applying an experimental or estimated correction. In some cases where the original data are too far away from either of these standard temperatures, the experimental temperature is given in parenthesis following the reported value. In certain cases where extensive tables of vapor pressure have been reported in the literature, only values in the vicinity of 760 or 10 mmHg are listed in the tables, even though all the data were used to fix the values of the Antoine constants. Similar situations, occurring mostly for isomeric hexanols and octanols, were sometimes found for the density and refractive index data at other temperatures or wavelengths, and these data are identified in the discussion.

When justified by the availability of the data, *selected values* of the *simple physical properties* for members of this group of alcohols are given after their *reported values*, in these tables. These *selected values* are accompanied by an estimated uncertainty and a letter superscript which roughly indicates the method of selection. The superscript letters have the following significance:

a—the single underlined value was selected
b—the average of two or more underlined values was selected
c—the *selected value* was obtained by some type of interpolation or extrapolation
d—the *selected value* was calculated from some function of temperature which was adjusted to fit the available data (usually applied to density data)
e—the selected boiling point was calculated from the Antoine equation using the constants shown
f—estimate based on available information.

When there were sufficient data, tables of *selected values* of density, refractive index at the sodium D-line, and vapor pressure were prepared over the temperature range represented by the experimental measurements. These tables also include the values of the Antoine and Francis constants used to calculate the vapor pressure and density, respectively. Finally, additional tables of *selected values* of other properties were included when such data were found in the literature. All tables of *selected values* are numbered and are included in the List of Tables on page 1–10.

D. References and Literature Coverage

All *selected values* of data are based on experimental measurements which have been reported in the world's scientific literature. For the most part these have been published in recognized journals and periodicals. Additional information found in private and government reports, patents, theses, dissertations, and other miscellaneous sources was used whenever it seemed worthwhile to do so. Most of the data were taken from primary sources by examination of the original documents, however, data of lesser importance published in obscure journals were obtained from *Chemical Abstracts.* In some cases authors have been contacted personally for clarification of published material or for additional data not previously published. The Bibliography contains a few references to secondary sources of information and to reviews or correlations of data, but these are used only for comparison with our selections and as a source of additional references.

The 2036 references to the physical and thermodynamic properties of the alcohols are listed in the Bibliography beginning on page 1–389 in alphabetical order of the last name of the first author. The abbreviation of the names of the periodicals follows the usual practice of *Chemical Abstracts.* Each reference is numbered consecutively for identification in the Indices to the Bibliography. The list is complete through 1967, and contains some references to 1968 publications.

In the text and in the tables of the report, citations to the references are by last name of the authors followed by the year of publication in parenthesis. Cases in which the same author, or group of authors, has published more than one report in the same year are distinguished by the letters, a, b, c, . . . following the year. A complete reference list to properties of the 26 *well-characterized* alcohols can be obtained through use of the Indices to the Bibliography at the end of the section for each compound. The citations in the Indices, grouped according to a standard list of properties for each compound, consist of the identification numbers in the Bibliography. Within each compound-property group, these reference numbers are listed in the order of increasing date of publication. Numbers in parenthesis refer to publications which contain theoretical discussions, correlations, or reviews but do not contain new experimental data. In the Indices, the **boldface** numbers identify references to sources of data used in selecting the values of the *simple physical properties* of refractive index, density, boiling point, and melting point and in fixing the values of the Antoine and Francis constants. The numerical values of the refractive index and density at 20 and 25 °C, the boiling point at 760 mmHg and the melting point taken from these sources are given in the tables of *reported values.*

All sources of *simple physical property* data for the other 694 compounds are given in the unnumbered tables of *reported values*, along with the numerical data themselves. References to other properties for these compounds are identified in the discussions.

E. Procedures for the Evaluation, Processing, and Selection of Data

The primary objective of this report is the compilation of an internally consistent set of standard physical and thermodynamic properties of the monohydroxy aliphatic alcohols, which represents the most accurate experimental measurements currently available. In this sense, internal consistency means satisfying all of the known exact requirements of the three laws of thermodynamics at least to within the experimental uncertainties. In order to make valid comparisons possible among the properties of different compounds, systematic selection procedures were followed throughout. The following steps were taken in arriving at the final *selected values.*

(1) Searching the scientific literature, identifying the sources of data, and recording the pertinent numerical values.

(2) Rating and evaluating the available data on the basis of accuracy and reliability, and sorting out the "best" numerical values.

(3) Converting the data to a uniform set of units and conditions, adjusting them to the current set of fundamental constants, and correcting arithmetic and other errors in the published values.

(4) Choosing preliminary values of the primary input data and, where appropriate, fitting them to standard functions of temperature, pressure, or other variables.

(5) Testing the preliminary choices for internal thermodynamic consistency, and making necessary adjustments to achieve consistency to within the experimental uncertainty.

(6) Calculating the values of the derived properties from the final choices of the basic input data.

(7) Estimating the uncertainties in the *selected values.*

(8) Tabulating the final values in a uniform style.

The evaluation of the available data is based entirely on the judgment of the compilers, and no rigorous rules can be stated. Consideration has been given to sample purity and experimental technique as described in the publications, as well as to the reputation of the authors for reliable work. Normally, more weight was given to a value obtained as the principal objective of an investigation rather than as a by-product of some other study. In some cases, the choice of the best value was obvious. However, after culling the less reliable data, it was more common to find that several reported values of about equal reliability were left. In such cases, if no basis for a further choice could be found, a properly weighted average value was chosen. For the lower alcohols, where data were extensive, the final choices depended not only on the directly measured values of any given property but also on the complete network of thermodynamic relations among the properties (see appendix C). In some situations it was necessary to combine data of different reliability to obtain the final selections. For example, one might have a series of accurate measurements of the vapor pressure of a specific compound over a certain range of temperature and another series of less reliable values outside this range. In order to obtain a smoothed set of *selected values* over the extended temperature ranges it is necessary to fit both sets of data to the same function of temperature. It is more common to have several sets of data of varying reliability for various temperature ranges which may partially or completely overlap. In fitting all of these data to a single function of temperature, more weight is given to the more reliable values. However the resulting equation still may not reproduce the best data as well as desired. The discrepancy is dictated, of course, by the choice of input data. While there may be cases in which the values of density or vapor pressure, as calculated from the selected Francis or Antoine constants respectively, do not reproduce all data to the accuracy represented by the original data, such discrepancies are small and not much greater than the experimental uncertainty.

Primary input data consist of directly measured properties such as the *simple physical properties*, heats of phase transitions, heat capacity, third law entropy, heat of combustion, P-V-T data for the gas phase, and equilibrium constants. Once the values of these properties have been fixed, the derived properties, such as entropy of phase transitions, temperature derivative of the enthalpy of phase transitions, Gibbs energy of formation, and ideal gas properties, are calculated from the usual thermodynamic formulae summarized in appendix C. Although various tests of internal consistency have been applied, the results of one type of test are given in the discussion of the individual alcohols which show the net change in enthalpy and entropy on taking one mole of the compound through the cycle,

> liquid, 25 °C→saturated real gas, 25 °C→ideal gas, 25 °C→ideal gas, t_b→ideal gas at 1 atm, t_b→saturated real gas, t_b→liquid, t_b→liquid, 25 °C.

If the heats of vaporization, ideal gas corrections, vapor pressures at 25 °C, boiling point, and heat capacities of liquid and vapor are all self-consistent, the total ΔH and ΔS for the cycle will be zero.

The selected values of the thermodynamic properties are accompanied by estimates of the uncertainties. While these estimates are intended to represent the uncertainty interval[1] in the associated quantities, they are obtained by estimation only and thus have no exact significance.

The selected liquid phase densities of those alcohols for which there are sufficient data have been calculated over a range of temperatures from the Francis equation.

$$d = A - Bt - \frac{C}{E-t} \tag{1}$$

In this equation d is the density in g cm^{-3} at temperature t in °C. A, B, C, and E are empirical constants obtained by a least squares fit to the experimental data. Temperatures have been limited to the range of about 0 to 150 °C or to the limits of the experimental data when they fall within this range. Although, in most cases, a quadratic function of temperature will represent the density data within this range with sufficient fidelity, there are several reasons for adopting eq (1). The Francis equation can be used successfully to represent the density of most organic liquids up to temperatures near the critical point. Thus eq (1) will probably give a more reliable extrapolation above the range of experimental temperatures than will the quadratic function of temperature. In addition it is helpful to have the constants in eq (1) determined for low temperature data when developing equations for representing data at higher temperatures. Finally, it seems likely that correlation and prediction of density data will be easier in terms of the constants in the Francis equation than in terms of some other possible methods of representing liquid densities. Additional details on the use of the Francis equation and on the computational procedure for evaluating the constants will be found in appendix B.

The Antoine equation

$$\log_{10} P = A - \frac{B}{C + t(°\mathrm{C})} \tag{2}$$

has been adopted for representing vapor pressure as a function of temperature. P is the equilibrium vapor pressure of a liquid or solid in millimeters of mercury and t the temperature in °C, A, B, and C are empirical constants. Experience has shown that for many classes of organic and inorganic compounds the Antoine equation can be made to represent experimental vapor pressures as well as any three parameter equation. Whenever the available data warrant, the Antoine constants have been evaluated and the *selected values* calculated from eq (2) in the pressure range of 10 to 1500 mmHg or to within the limit of the experimental data, if they fall within this range. Several procedures have been used for fitting the three parameters to the experimental observations. For most of the 26 alcohols discussed in detail, a nonlinear

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[1] The uncertainty interval, u, assigned to the selected value of a property, x, is such that there is a 95 percent probability that the "true" value of the property lies in the interval, $x \pm u$. In estimating the uncertainty interval, the sources of the original experimental data, the uncertainties in auxiliary data, and in any corrections or conversions which have been applied to the data and the magnitude of the discrepancies among different sources of data are considered. Effects of both random and systematic errors are included in the estimate.

computational technique has been used which minimizes simultaneously the weighted sum of the square deviations of calculated and observed pressures and calculated and observed calorimetric heats of vaporization. In cases where the data were less extensive, least squares calculation based on an equation obtained by rearranging eq (2) to a form which is linear in the parameters was used. Finally, when only a few scattered values were available, the A and B constants were evaluated by a least squares calculation or a graphical procedure for several assigned values of C, and the one which appeared to give the best fit was adopted. These computations are described more fully in appendix B.

Refractive index is very nearly a linear function of temperature, at least over range of 60 to 80 degrees. Experimental values outside the temperature range of 15 to 30 °C are scarce. When experimental values outside the range of 20 to 25 °C were found, the *selected values* were taken from a straight line graph drawn through a plot of the data. At any given temperature, refractive index can be calculated as a function of wavelength of light by the modified Hartman equation.

$$n=n_\infty+\frac{C}{(\lambda-\lambda^*)^{1.6}} \qquad (3)$$

n is the refractive index for light of wavelength λ. n_∞, C, and λ^* are adjustable parameters. *Selected values* of refractive index at wavelengths other than the Na_D line were taken from graphs of experimental values plotted against $1/(\lambda-1000)^{1.6}$ (λ in angstroms). Since these were straight lines, or very nearly straight lines, interpolation was easy. The numerical values are reported at a series of eight standard wavelengths which match common laboratory sources of monochromatic visible light.

F. Definitions and Glossary of Properties, Symbols, and Units

The symbols used throughout the text and tables of the report and their definitions are as follows:

A, B, C, E—Constants in the Antoine equation (equation 2) or the Francis equation (equation 1)
B_p, C_p, D_p—Virial coefficients for the real gas, based on the Berlin expansion (see appendix A for complete definition)
C_p —Heat capacity at constant pressure, cal^{-1} mol^{-1} deg^{-1}
d —Density, g cm^{-3} (of air saturated liquid at 1 atm below t_b and of liquid in equilibrium with vapor above t_b)
G —Gibbs (free) energy, $G=H-TS$, kcal mol^{-1}
H —Enthalpy (heat content, $H=E+PV$, kcal mol^{-1})
K —Equilibrium constant for gas phase reactions, standard state taken as the ideal gas at one atmosphere
M —Molecular weight
n —Refractive index relative to air at 1 atm and at the stated wavelength of light
n_D —Refractive index relative to air at 1 atm at the D-line of the sodium emission spectrum (5892.6 angstroms) which is the weighted average of the D_1 and D_2 lines
P —Pressure, mmHg or atm
R —Gas constant, 1.98717 cal mol^{-1} deg^{-1} or 82.0561 cm^3 atm deg^{-1} mol^{-1}
S —Entropy, cal mol^{-1} deg^{-1}
T —Temperature, Kelvin scale
t —Temperature, Celsius scale
V —Volume, liters mol^{-1} or cm^3 mol^{-1}
Z —Compressibility constant, equals PV/RT for one mole of a real gas

A "Δ" written before a symbol which represents an extensive property signifies a change in that property on going from some initial state to some final state. The kind of change is indicated by one of the following letters written after the property symbol.

m—fusion
v —vaporization
t —transition between crystalline forms
c —combustion
f —formation from the elements in their reference states (C (graphite), O_2(g) and H_2(g))
s —sublimation

Thus, for example, ΔH_m is the enthalpy of fusion, ΔH_f the enthalpy of formation, and ΔH_c the enthalpy of combustion. The products of combustion are gaseous carbon dioxide and liquid water. See appendix A for additional relationships.

The superscript "0" following a property symbol signifies the value of that property in the thermodynamic standard state. For solids and liquids, this is the thermodynamically stable state at a pressure of 1 atm. For gases, it is the hypothetical ideal gas at 1 atm. The superscript "r" signifies the property of the real gas in equilibrium with the condensed phase at the stated temperature. Symbols such as H^r-H^0, S^r-S^0, and $C_p{}^r-C_p{}^0$ represent the difference in properties between the real gas at saturated vapor pressure and ideal gas *at the same pressure.* In quantities such as ΔH_v, ΔS_v, and ΔC_{pv}, it is to be understood that the vapor phase consists of the real gas at saturation pressure even though the superscript "r" is not used.

The physical states are designated by one of the following letters written in parenthesis after a property symbol.
g—gas
l—liquid
c—crystal, if more than one crystalline modification exists, they are distinguished by I, II, III, etc., which indicates the form stable at the highest, next highest, etc., temperatures.
u—unstable or metastable crystalline form.

Therefore $\Delta H_f{}^0$ (g) is the enthalpy of formation of a compound in the ideal gas state from the elements in their reference states, and $\Delta G_f{}^0$ (c) is the Gibbs energy change for the formation of a crystalline substance from the elements.

The subscript "c" written after the symbols T, t, P, or d represents the corresponding critical property. Thus T_c is the critical temperature. The symbols T_b and t_b are the normal boiling points, defined as the boiling temperatures at 760 mmHg (1 atm) pressure, and t_m and T_m are the melting points. The quantity $d\Delta H/dt$ is the change in an enthalpy of a phase transition per degree of change of temperature at the *equilibrium pressure*. This is not the same as $(\partial\Delta H/\partial T)_p$ which is equal to ΔC_p and implies a constant pressure derivative. The quantity dt/dP is the change in the equilibrium temperature for a phase transition (usually vaporization) per unit change in applied pressure. Thermodynamic functions of the ideal gas, such as H^0-H^0 and G^0-G^0, represent the difference in the value of the property of the ideal gas at one atmosphere at the stated temperature and the property of the ideal gas at a temperature of 0 K.

The following abbreviations are used for units:

atm	—atmosphere, pressure equals 101325 Nm^{-2} (exactly).
cal	—thermochemical calorie, energy, equals 4.184 joules (exactly)
cm	—centimeter
deg	—degree Celsius
g	—gram
mmHg	—millimeter of mercury pressure (also written mm)
mol	—gram mole, the amount of a substance containing the same number of formula units as there are in 12 g (exactly) of the pure nuclide ^{12}C
K	—temperature on the Kelvin scale
°C	—temperature on the Celsius scale

The molecular weights were calculated from the following 1961 atomic weights; C, 12.01115; O, 15.9994; and H, 1.00797. Temperatures are reported in degrees Celsius or degrees Kelvin as defined by the IPTS (1948) and text revision of 1960, with the triple point of water taken as 273.16 K (exactly), except that temperatures reported in the tables of ideal gas thermodynamic functions are in the thermodynamic Kelvin scales.

Reported values of densities are given as specific gravity with respect to water at 4 °C (d_4). When necessary, data reported in the literature are converted to this basis for listing in the tables of *reported values*. However, all *selected values* of density are given in units of grams per cubic centimeter (g cm^{-3}) and the constants in the Francis equation have been adjusted to those units. To convert a specific gravity relative to water at 4 °C to g cm^{-3}, multiply by 0.999972.

In the section on "Data for Phase Transitions" in the tables of Selected Data (see table 3, page 1-42 for example), a special convention is adopted for distinguishing between a melting temperature in contact with the air and a triple point. If the pressure for a crystal to liquid transition is listed as "760," the corresponding temperature is to be considered as the melting point of the substance in equilibrium with air at 1 atm. If some other pressure or no pressure is listed, the temperature is to be considered as the triple point for the crystal-liquid-gas equilibrium with no air present. Differences between the melting point in air and the triple point are due not only to the difference in pressure but also to the effect of dissolved air.

The number of significant figures used to report numerical data is rounded either to the first uncertain figure or to one additional digit. In tables where properties are given at a series of temperatures, pressures, or other variables, one additional figure beyond that representing the total uncertainty is usually carried in order to preserve relative values. In rounding off the numerical values, the figure in the last place to be retained is left unchanged when the next figure beyond is less than five but is increased by one if it is more than five. When the figure beyond the last one to be retained is exactly five, then the last figure retained is increased by one if it is odd and is left as is if it is even. Those numbers written without a decimal point are to be interpreted as exact by definition. Thus, for example, in table 3 the vapor pressure of methanol at 25 °C (exactly) is given as 59.8 mmHg. Similarly, the boiling point at 760 mmHg (exactly) is listed as 78.29 °C. The temperatures 273.15 and 298.15 K written in the tables of thermodynamic functions and elsewhere are also to be taken as exact by definition.

The equivalents in the International System of Units (SI) to the units used in this monograph are shown below:

Quantity	Unit	Value in SI Units
mass	g	0.001 kg (kilogram)
energy	cal	4.184 J (joule)
pressure	atm	101325 Nm^{-2} (Newtons per square meter)
pressure	mmHg	133.322 Nm^{-2} (Newtons per square meter)

II. Selected Values of Physical Properties of Aliphatic Alcohols and Compound Index

TABLE 2a. Selected values of physical properties of aliphatic alcohols and compound index

Compound Name	Wiswesser Line-Formula Notation[a]	Density at 25 °C g cm^{-3}	Refractive Index, n_D at 25 °C	Boiling Point, °C at 760 mm Hg	Boiling Point, °C at 10 mm Hg	Index of Page Numbers
CH_4O						
Methanol	Q1	0.78664	1.32652	64.70	−15.42	1-40—1-54
C_2H_6O						
Ethanol	Q2	0.78509	1.35941	78.29	−2.84	1-55—1-66
C_3H_8O						
1-Propanol	Q3	0.79975	1.38370	97.20	14.3	1-66—1-78
2-Propanol	QY	.78126	1.3752	82.26	2.49	1-78—1-87
$C_4H_{10}O$						
1-Butanol	Q4	0.8060	1.3971	117.66	31.58	1-88—1-97
2-Butanol	QY2	.8026	1.3949	99.55	16.4	1-97—1-106
2-Methyl-1-Propanol	Q1Y	.7978	1.3938	107.87	24.4	1-106—1-112
2-Methyl-2-Propanol	QX	[u] .7812	[u] 1.3852	82.42		1-113—1-123
$C_5H_{12}O$						
1-Pentanol	Q5	0.8112	1.4080	137.8	44.7	1-123—1-130
2-Pentanol	QY3	0.8053	1.4044	119.0	32.3	1-131—1-134
3-Pentanol	QY2&2	.8160	1.4079	115.3	27.7	1-134—1-137
2-Methyl-1-butanol	Q1Y2	.8150	1.4086	128.7	40.2	1-138—1-140
3-Methyl-1-butanol	Q2Y	.8070	1.4052	131.2	41.0	1-141—1-145
2-Methyl-2-butanol	QX2	.8044	1.4020	102.0	21.0	1-145—1-150
3-Methyl-2-butanol	QY&Y	.8137	1.4075	111.5	26.	1-150—1-153
2,2-Dimethyl-1-propanol	Q1X			113.1		1-153—1-154
$C_6H_{14}O$						
1-Hexanol	Q6	0.8162	1.4161	157.0	60.1	1-155—1-159
2-Hexanol	QY4	.8105	1.4128	139.9	44.7	1-160, 1-167, 1-168
3-Hexanol	QY3&2	.8144	[c] 1.4140	135.4	36.	1-160, 1-167, 1-169
2-Methyl-1-pentanol	Q1Y3	.8206	1.4172	148.0	50.5	1-160, 1-167, 1-169
3-Methyl-1-pentanol	Q2Y2	.8202	1.4175	152.4	55.9	1-161, 1-167, 1-170
4-Methyl-1-pentanol	Q3Y	.8095	1.4135	151.8	56.9	1-161, 1-167, 1-170
2-Methyl-2-pentanol	QX3	.8095	1.4089	121.4	30.8	1-161, 1-166, 1-167 1-171
3-Methyl-2-pentanol	QY&Y2	.8248	1.4179	134.2	40.8	1-162, 1-167, 1-171
4-Methyl-2-pentanol	QY&1Y	.8033	1.4090	131.7	35.0	1-162, 1-166, 1-167, 1-172
2-Methyl-3-pentanol	QY2&Y	.8198	1.4148	126.5	34.0	1-162, 1-167, 1-171
3-Methyl-3-pentanol	QX2&2	0.8238	1.4163	122.4		1-163, 1-166, 1-167, 1-173
2-Ethyl-1-butanol	Q1Y2&2	.8295	1.4205	146.5	49.8	1-163, 1-167, 1-173
2,2-Dimethyl-1-butanol	Q1X2	.8246	1.4188	136.8	41.1	1-163, 1-167, 1-174
2,3-Dimethyl-1-butanol	Q1Y&Y	.8255	1.4185	149.		1-164, 1-167, 1-174
3,3-Dimethyl-1-butanol	Q2Y	.8097	1.4118	143.		1-169, 1-167, 1-175
2,3-Dimethyl-2-butanol	QY&&Y	.8182	1.4150	118.6	26.8	1-164, 1-167, 1-175
3,3-Dimethyl-2-butanol	QY&X	.8139	1.4132	120.		1-165, 1-167, 1-176
$C_7H_{16}O$						
1-Heptanol	Q7	0.8187	1.4223	176.3	75.4	1-179, 1-185
2-Heptanol	QY5	.8139	1.4190	159.2	59.1	1-185, 1-192, 1-193
3-Heptanol	QY4&2	.8170	1.4200	156.8	58.6	1-186, 1-192, 1-193
4-Heptanol	QY3&3	.8149	1.418	155.0	55.3	1-186, 1-192, 1-194
2-Methyl-1-hexanol	Q1Y4	.823	1.421	164.	65.	1-187, 1-194

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[a] E. G. Smith, The Wiswesser Line-Formula Chemical Notation (McGraw-Hill Book Co., New York, 1968).

* Based on a single experimental value only.

[c] Extrapolated or interpolated from other temperatures.

[u] Under cooled liquid.

TABLE 2a. Selected values of physical properties of aliphatic alcohols and compound index—Continued

Compound Name	Wiswesser Line-Formula Notation[a]	Density at 25 °C g cm^{-3}	Refractive Index, n_D at 25 °C	Boiling Point, °C		Index of Page Numbers
				at 760 mm Hg	at 10 mm Hg	
$C_7H_{16}O$						
3-Methyl-1-hexanol	Q2Y3	.824	1.422	172.	75.	1-187, 1-195
4-Methyl-1-hexanol	Q3Y2	.820	1.423	173.	75.	1-187, 1-195
5-Methyl-1-hexanol	Q4Y	.812	1.422	172.		1-195
2-Methyl-2-hexanol	QX4	.8103	1.4170	142.5	46.4	1-187, 1-192, 1-196
3-Methyl-2-hexanol	QY&Y3	* .822	* 1.421	152.	49.	1-196
4-Methyl-2-hexanol	QY&1Y2	0.817	1.422	151.	60.	1-197
5-Methyl-2-hexanol	QY&2Y	.810	1.417	151.	51.	1-188, 1-197
2-Methyl-3-hexanol	QY3&Y	.820	1.420	147.	50.	1-188, 1-197
3-Methyl-3-hexanol	QX3&2	.8204	1.421	142.4	45.	1-189, 1-192, 1-198
4-Methyl-3-hexanol	QY2&Y2			*150		1-198
5-Methyl-3-hexanol	QY2&1Y	.829	1.417	148.	45.	1-198
2-Ethyl-1-pentanol	Q1Y2&2	.829	1.425	166.	57.	1-198
2,2-Dimethyl-1-pentanol	Q1X3			153.		1-199
2,3-Dimethyl-1-pentanol	Q1Y&Y2	* .834	* 1.429	164.	66.	1-199
2,4-Dimethyl-1-pentanol	Q1Y&1Y	.815	[c] 1.425	159.		1-199
3,3-Dimethyl-1-pentanol	Q2X2			165.	67.	1-199
3,4-Dimethyl-1-pentanol	Q2Y&Y	.827	1.426	165.	60.	1-189, 1-200
4,4-Dimethyl-1-pentanol	Q3X	[c] .811	[c] 1.418	160.		1-200
3-Ethyl-2-pentanol	QY&Y2&2	* .834	* 1.426	152.		1-200
2,3-Dimethyl-2-pentanol	QX&&Y2	.828	1.423	139.7	44.	1-201
2,4-Dimethyl-2-pentanol	QX&&1Y	.808	[c] 1.415	133.	38.	1-189, 1-192, 1-201
3,3-Dimethyl-2-pentanol	QY&X2		[c] 1.428	147.	36.	1-202
3,4-Dimethyl-2-pentanol	QY&Y&Y	[c] .834		153.	49.	1-203
4,4-Dimethyl-2-pentanol	QY&1X	.807	1.417	138.	43.	1-203
3-Ethyl-3-pentanol	QX2&2&2	0.8400	1.4277	142.5	43.7	1-190, 1-192, 1-202
2,2-Dimethyl-3-pentanol	QY2&X	.822	1.421	136.	39.	1-190, 1-203
2,3-Dimethyl-3-pentanol	QX&2&Y	.836	1.426	139.	42.	1-190, 1-204
2,4-Dimethyl-3-pentanol	1Y&YQY	.8253	1.423	138.8	41.3	1-191, 1-192, 1-204
2-Methyl-2-ethyl-1-butanol	Q1X2&2	.824	1.424	156.	62.	1-191, 1-205
3-Methyl-2-ethyl-1-butanol	Q1&2&Y	.833	1.426		60.	1-205
2,2,3-Trimethyl-1-butanol	Q1X&&Y	.843	1.431	157.		1-205
2,3,3-Trimethyl-1-butanol	Q1Y&X	* .824	1.429	160.		1-205
2,3,3-Trimethyl-2-butanol	QX&&X	* .838	* 1.428	131.		1-206
$C_8H_{18}O$						
1-Octanol	Q8	0.8223	1.4276	195.2	88.5	1-211—1-217
2-Octanol	QY6	.8171	1.4241	179.8	74.3	1-218, 1-227, 1-230
3-Octanol	QY5&2	.8176	1.421	174.7	68.1	1-218, 1-227, 1-230
4-Octanol	QY4&3	.8154	1.4227	176.6	71.	1-218, 1-228, 1-231
2-Methyl-1-heptanol	Q1Y5	.7986	1.4219	175.6	65.7	1-219, 1-228, 1-231
3-Methyl-1-heptanol	Q2Y4	.7844	1.4225	186.0	74.6	1-219, 1-228, 1-231
4-Methyl-1-heptanol	Q3Y3	.8064	1.4253	183.2	72.5	1-219, 1-228, 1-232
5-Methyl-1-heptanol	Q4Y2	.8153	1.4272	186.6	79.1	1-220, 1-228, 1-232
6-Methyl-1-heptanol	Q5Y	0.8175	1.4255	187.7	84.1	1-220, 1-228, 1-232
2-Methyl-2-heptanol	QX&&5	.8072	1.4201	156.7	59.5	1-220, 1-228, 1-233
3-Methyl-2-heptanol	QY&Y4	.8177	* 1.4199	166.1	55.1	1-221, 1-228, 1-233
4-Methyl-2-heptanol	QY&1Y3	* .7990	* 1.4225	171.6	66.4	1-221, 1-228, 1-233
5-Methyl-2-heptanol	QY&2Y2	* .8098	* 1.4218	171.9	63.5	1-221, 1-228, 1-234
6-Methyl-2-heptanol	QY&3Y	.8033	1.4209	171.9	68.9	1-222, 1-228, 1-234
2-Methyl-3-heptanol	QY4&Y	.8205	1.4246	167.6	64.2	1-222, 1-228, 1-235
3-Methyl-3-heptanol	QX&4&2	.8251	1.4263	161.	59.2	1-222, 1-227, 1-228, 1-235
4-Methyl-3-heptanol	QY2&Y3	.7940	1.4179	155.4	44.9	1-223, 1-228, 1-236
5-Methyl-3-heptanol	QY2&1Y2	.8143	1.4156	153.6	44.6	1-223, 1-228, 1-236
6-Methyl-3-heptanol	QY2&2Y					1-236
2-Methyl-4-heptanol	QY3&1Y	.8098	1.4196	166.1	65.	1-223, 1-228, 1-237
3-Methyl-4-heptanol	QY3&Y2	.8329	1.4211	164.7	54.4	1-224, 1-228, 1-238
4-Methyl-4-heptanol	QX3&3	.8194	1.4240	161.1	59.0	1-224, 1-227, 1-228, 1-237
2-Ethyl-1-hexanol	Q1Y4&2	.8290	1.4290	184.6	79.3	1-224, 1-228, 1-238
3-Ethyl-1-hexanol	Q2Y3&2	* .831	* 1.4323			1-239
4-Ethyl-1-hexanol	Q3Y2&2				85.	1-239
2,2-Dimethyl-1-hexanol	Q1X4	[c] .822	1.428	172.5	75.	1-239

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* Based on a single experimental value only.

[c] Extrapolated or interpolated from other temperatures.

TABLE 2a. Selected values of physical properties of aliphatic alcohols and compound index—Continued

Compound Name	Wiswesser Line-Formula Notation[a]	Density at 25 °C g cm^{-3}	Refractive Index, n_D at 25 °C	Boiling Point, °C		Index of Page Numbers
				at 760 mm Hg	at 10 mm Hg	
$C_8H_{18}O$						
2,4-Dimethyl-1-hexanol	Q1Y&1Y2			175.		1–239
2,5-Dimethyl-1-hexanol	Q1Y&2Y	* 0.825		* 179.		1–239
3,3-Dimethyl-1-hexanol	Q2X3	^{c} .835	^{c} 1.431			1–239
3,5-Dimethyl-1-hexanol	Q2Y&1Y	* .819	^{c} 1.423	* 183.		1–239
4,4-Dimethyl-1-hexanol	Q3X2		^{c} 1.433			1–239
3-Ethyl-2-hexanol	QY&Y3&2			* 168.		1–240
2,3-Dimethyl-2-hexanol	QX&&Y3	.832	1.432	160.1	62.	1–240
2,4-Dimethyl-2-hexanol	QX&&1&2	.806	1.422	150.7	51.	1–240
2,5-Dimethyl-2-hexanol	QX&&2Y	.812	1.419	152.5	58.	1–240
3,3-Dimethyl-2-hexanol	QY&X3	^{c} .842	^{c} 1.433		71.	1–240
3,4-Dimethyl-2-hexanol	QY&Y&Y2		^{c} 1.434	171.		1–241
3,5-Dimethyl-2-hexanol	QY&Y&1&			* 160.		1–241
5,5-Dimethyl-2-hexanol	QY&2X		^{c} 1.421	* 166.		1–241
3-Ethyl-3-hexanol	QY3&2&2	.8337	^{c} 1.425	159.	55.	1–225, 1–241
4-Ethyl-3-hexanol	QY2&Y2&2		^{c} 1.430	164.	59.	1–241
2,2-Dimethyl-3-hexanol	QY3&X	^{c} .830	^{c} 1.424	156.1	42.	1–242
2,3-Dimethyl-3-hexanol	QX3&&Y	^{c} .833	^{c} 1.428	158.2	52.	1–242
2,4-Dimethyl-3-hexanol	2Y&YQY		^{c} 1.429	160.	48.	1–242
2,5-Dimethyl-3-hexanol	1Y&YQ1Y	.8146	^{c} 1.422	159.	58.	1–225, 1–243
3,4-Dimethyl-3-hexanol	QY2&&Y2	* 0.834	^{c} 1.433	152.	51.	1–243
3,5-Dimethyl-3-hexanol	QX2&&1Y	.823	1.424	152.	43.	1–243
4,4-Dimethyl-3-hexanol	QY2&X2	^{c} .830	1.432	159.	54.	1–244
5,5-Dimethyl-3-hexanol	QY2&1X		1.424	153.	50.	1–244
2-*n*-Propyl-1-pentanol	Q1Y3&3			179.	79.	1–244
2-Methyl-2-ethyl-1-pentanol	Q1X3&2		^{c} 1.434	174.1		1–228, 1–244
4-Methyl-2-ethyl-1-pentanol	Q1Y2&1Y	^{c} .823	* 1.427	177.1	73.2	1–225, 1–245
2,2,3-Trimethyl-1-pentanol	Q1X&&Y2		1.437	174.5	71.	1–245
2,2,4-Trimethyl-1-pentanol	Q1X&&1Y	^{c} .834	1.428	168.3	63.4	1–226, 1–228, 1–245
2,3,4-Trimethyl-1-pentanol	Q1Y&Y&Y	^{c} .846	^{c} 1.437	183.		1–246
3,3,4-Trimethyl-1-pentanol	Q2X&&Y					
2,4,4-Trimethyl-1-pentanol	Q1Y&1X	^{c} .829	1.426	171.	63.	1–246
2-Methyl-3-ethyl-2-pentanol	QX&&Y2&2	.835	* 1.430	157.8	59.	1–246
3-Methyl-3-ethyl-2-pentanol	QY&X2&2	^{c} .854	^{c} 1.447		67.	1–246
4-Methyl-3-ethyl-2-pentanol	QY&Y2&Y		^{c} 1.431	164.		1–246
2,3,3-Trimethyl-2-pentanol	QX&&X2	.815	1.436	160.0	49.	1–247
2,3,4-Trimethyl-2-pentanol	QX&&Y&Y	^{c} .804	^{c} 1.435	158.		1–247
2,4,4-Trimethyl-2-pentanol	QX&&1X	^{c} .819	1.426	146.4	44.	1–247
3,3,4-Trimethyl-2-pentanol	QY&X&&Y	^{c} 0.852	^{c} 1.436	165.		1–247
3,4,4-Trimethyl-2-pentanol	QY&Y&X	^{c} .837	* 1.433	158.	57.	1–248
2-Methyl-3-ethyl-3-pentanol	QX2&2&Y	^{c} .826		160.		1–248
2,2,3-Trimethyl-3-pentanol	QX2&&X	.842	1.433	152.5	45.4	1–226, 1–228, 1–248
2,2,4-Trimethyl-3-pentanol	1Y&YQX	^{c} .828	1.427	151.0	50.2	1–225, 1–228, 1–249
2,3,4-Trimethyl-3-pentanol	1Y&XQ&Y	^{c} .845	1.433	157.	43.	1–249
3-Methyl-2-isopropyl-1-butanol	1Y&Y1QY	* .842	* 1.432	173.		1–249
2,2-Diethyl-1-butanol	Q1X2&2&2		* 1.441		69.	1–250
3,3-Dimethyl-2-ethyl-1-butanol	Q1Y2&X	* .843	* 1.435			1–250
2,2,3,3-Tetramethyl-1-butanol	Q1X&&X					1–250
$C_9H_{20}O$						
1-Nonanol	Q9	0.8247	1.4319	213.1	104.	1–251—1–254
2-Nonanol	QY7	.8195	1.4290	198.5	88.	1–256, 1–260
3-Nonanol	QY6&2	^{c} .8214	1.429	194.7	83.	1–256, 1–260
4-Nonanol	QY5&3	^{c} .822	1.4275	193.	81.	1–260
5-Nonanol	QY4&4	.8183	1.4267	195.1	89.1	1–261
2-Methyl-1-octanol	Q1Y6	^{c} .825			^{c} 91.	1–261
3-Methyl-1-octanol	Q2Y5	* .826	* 1.4328		95.3	1–261
4-Methyl-1-octanol	Q3Y4	* .822	1.4331			1–261
5-Methyl-1-octanol	Q4Y3	* .827			^{c} 95.	1–261
6 Methyl-1-octanol	Q5&2	* .829	^{c} 1.434	206.	85.	1–262
7-Methyl-1-octanol	Q6Y	* .8260	* 1.4316	206.		1–262
2-Methyl-2-octanol	QX6	.8158	1.426	178.	77.	1–256, 1–262
3-Methyl-2-octanol	QY&Y5	* .833	1.431		80.	1–262
l-5-Methyl-2-octanol	QY&2Y3	* .821				1–262

* Based on a single experimental value only.

^{c} Extrapolated or interpolated from other temperatures.

TABLE 2a. Selected values of physical properties of aliphatic alcohols and compound index—Continued

Compound Name	Wiswesser Line-Formula Notation[a]	Density at 25 °C g cm^{-3}	Refractive Index, n_D at 25 °C	Boiling Point, °C		Index of Page Numbers
				at 760 mm Hg	at 10 mm Hg	
$C_9H_{20}O$						
7-Methyl-2-octanol	QY&4Y		^{c} 1.429			1–263
2-Methyl-3-octanol	QY5&Y	^{c} .8249	^{c} 1.429	184.	73.	1–257, 1–263
3-Methyl-3-octanol	QX&5&2	.8279	1.4301	189.	72.	1–257, 1–263
4-Methyl-3-octanol	QY2&Y4	* .8437			^{c} 122.	1–263
6-Methyl-3-octanol	QY2&2Y2	* .8320	* 1.4372		^{c} 76.	1–263
7-Methyl-3-octanol	QY2&3Y	^{c} .830				1–263
2-Methyl-4-octanol	QY4&1Y	.815	1.426	184.	77.	1–264
3-Methyl-4-octanol	QY4&Y2	^{c} .828	^{c} 1.430	* 180.	80.	1–264
4-Methyl-4-octanol	QX4&3	.8237	1.4301	181.		1–257, 1–264
5-Methyl-4-octanol	QY3&Y3	* .816	* 1.4262		76.	1–264
6-Methyl-4-octanol	QY3&1Y2	* .820				1–264
7-Methyl-4-octanol	QY3&2Y	^{c} .810	^{c} 1.424		^{c} 80.	1–265
2-Ethyl-1-heptanol	Q1Y5&2		^{c} 1.432		^{c} 75.	1–265
3-Ethyl-1-heptanol	Q2Y4&2	* 0.832		207.	89.	1–265
5-Ethyl-1-heptanol	Q4Y2&2	* .848	* 1.4350			1–265
2,2-Dimethyl-1-heptanol	Q1X5		^{c} 1.432	192.	80.	1–265
4,6-Dimethyl-1-heptanol	Q3Y&1Y		^{c} 1.430		^{c} 72.	1–265
6,6-Dimethyl-1-heptanol	Q5X	^{c} .840	^{c} 1.441		^{c} 85.	1–265
2-Ethyl-2-heptanol	QX5&2		^{c} 1.436			1–265
3-Ethyl-2-heptanol	QY&Y4&2		^{c} 1.429		^{c} 80.	1–266
2,3-Dimethyl-2-heptanol	QX&&Y4		^{c} 1.438		^{c} 70.	1–266
2,4-Dimethyl-2-heptanol	QX&&1Y3	* .828	* 1.4290			1–266
2,5-Dimethyl-2-heptanol	QX&&2Y2	^{c} .828			^{c} 70.	1–266
2,6-Dimethyl-2-heptanol	QX&&3Y	.815	1.422		^{c} 54.	1–266
4,6-Dimethyl-2-heptanol	QY&1Y&1Y	^{c} .859		* 194.		1–266
5,6-Dimethyl-2-heptanol	QY&2Y&Y	^{c} .829	1.4480	* 192.		1–266
3-Ethyl-3-heptanol	QX4&2&2	.837	1.434	182.2	72.	1–267
2,2-Dimethyl-3-heptanol	QY4&X	* .824	^{c} 1.431		63.	1–267
2,3-Dimethyl-3-heptanol	QY4&Y	^{c} .833	^{c} 1.434	174.	74.	1–267
2,6-Dimethyl-3-heptanol	QYY&2Y	^{c} 0.817	^{c} 1.423	175.	73.	1–267
3,5-Dimethyl-3-heptanol	QX2&1Y2	.820	1.429		40.	1–268
3,6-Dimethyl-3-heptanol	QX2&2Y	^{c} .821	^{c} 1.429			1–268
3-Ethyl-4-heptanol	QY3&Y2&2				* 80.	1–268
4-Ethyl-4-heptanol	QX3&3&2	^{c} .831	^{c} 1.432	179.	73.	1–268
2,2-Dimethyl-4-heptanol	QY3&1X		^{c} 1.425	173.7	61.	1–258, 1–268
2,4-Dimethyl-4-heptanol	QX3&&1Y	^{c} .821	^{c} 1.428	171.4	64.	1–269
2,6-Dimethyl-4-heptanol	1Y&1YQ1Y	^{c} .8061	1.4211	178.0	71.7	1–258, 1–269
3,3-Dimethyl-4-heptanol	QY3&X2			* 176.		1–269
3,5-Dimethyl-4-heptanol	2Y&YQY2	^{c} .855	^{c} 1.426	187.	70.	1–269
2-*n*-Propyl-1-hexanol	Q1Y4&3		* 1.492		^{c} 93.	1–270
3-*n*-Propyl-1-hexanol	Q2Y3&3		^{c} 1.434			1–270
2-Methyl-2-ethyl-1-hexanol	Q1X4&2		^{c} 1.438		* 85.	1–270
2-Methyl-3-ethyl-1-hexanol	Q1Y&Y3&2	^{c} .846	^{c} 1.443	192.	78.	1–270
3-Methyl-2-ethyl-1-hexanol	Q1Y2&Y3	* .836	* 1.436		* 84.	1–270
4-Methyl-2-ethyl-1-hexanol	Q1Y2&1Y2	^{c} .825	^{c} 1.431	* 195.		1–270
5-Methyl-2-ethyl-1-hexanol	Q1Y2&2Y	* .821	* 1.430		* 85.	1–270
3,3,5-Trimethyl-1-hexanol	Q2X&&1Y		^{c} 1.432		* 81.	1–270
3,4,4-Trimethyl-1-hexanol	Q2Y&X2		* 1.431	* 191.		1–271
3,5,5-Trimethyl-1-hexanol	Q2Y&1X	* 0.824	1.4300	193.0	83.	1–271
4,5,5-Trimethyl-1-hexanol	Q3Y&X		^{c} 1.439	* 202.		1–271
2-Methyl-3-ethyl-2-hexanol	QX&&Y3&2	* .8334	* 1.4331	* 178.	^{c} 65.	1–271
2,3,4-Trimethyl-2-hexanol	QX&&Y&Y2	^{c} .827	^{c} 1.438			1–271
2,4,4-Trimethyl-2-hexanol	QX&&1X2	^{c} .844	^{c} 1.440			1–271
2,4,5-Trimethyl-2-hexanol	QX&&1Y&Y	^{c} 0.828	^{c} 1.430			1–271
2,5,5-Trimethyl-2-hexanol	QX&&2X		^{c} 1.424			1–271
2-Methyl-3-ethyl-3-hexanol	QX3&2&Y	.8445	1.4369	184.1	62.0	1–272
2-Methyl-4-ethyl-3-hexanol	2Y2&YQY	^{c} .824	^{c} 1.435			1–272
3-Methyl-4-ethyl-3-hexanol	QX2&&Y2&2	* .8994	* 1.4405		^{c} 45.	1–272
4-Methyl-3-ethyl-3-hexanol	QX2&2&Y2	^{c} .853			69.	1–272
5-Methyl-3-ethyl-3-hexanol	QX2&2&1Y	^{c} .837	^{c} 1.430	172.		1–272
2,2,3-Trimethyl-3-hexanol	QX3&&X	^{c} .842	^{c} 1.437	173.1	63.5	1–258, 1–272
2,2,4-Trimethyl-3-hexanol	2Y&YQX			* 169.		1–273
2,2,5-Trimethyl-3-hexanol	1X&&YQ1Y	^{c} .785	^{c} 1.428	160.	58.	1–273
2,3,4-Trimethyl-3-hexanol	2Y&XQ&Y		^{c} 1.439		49.	1–273

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* Based on a single experimental value only.

[c] Extrapolated or interpolated from other temperatures.

TABLE 2a. Selected values of physical properties of aliphatic alcohols and compound index—Continued

Compound Name	Wiswesser Line-Formula Notation[a]	Density at 25 °C g cm^{-3}	Refractive Index, n_D at 25 °C	Boiling Point, °C		Index of Page Numbers
				at 760 mm Hg	at 10 mm Hg	
$C_9H_{20}O$						
2,3,5-Trimethyl-3-hexanol	1Y&XQ&1Y	[c] .824	[c] 1.430		61.	1–273
2,4,4-Trimethyl-3-hexanol	2X&&YQY	[c] .845	[c] 1.437	171.	62.	1–273
2,5,5-Trimethyl-3-hexanol	1Y&YQ1X	[c] .821	[c] 1.427			1–274
3,4,4-Trimethyl-3-hexanol	QX2&&X2	[c] 0.829	[c] 1.445	166.	52.	1–274
3,5,5-Trimethyl-3-hexanol	QX2&&1X	[c] .831	[c] 1.433		57.	1–274
4-Methyl-2-*n*-propyl-1-pentanol	Q1Y3&1Y	[c] .822	[c] 1.829	* 192.		1–274
4-Methyl-2-isopropyl-1-pentanol	1Y&Y1Q1Y			* 187.		1–274
2,2-Dimethyl-3-ethyl-1-pentanol	Q1X&&Y2&2		[c] 1.430			1–274
2,4-Dimethyl-2-ethyl-1-pentanol	Q1X2&1&1Y	* .837	* 1.438	188.		1–275
3,3-Dimethyl-2-pentanol	QY&X2&2&2		* 1.448		[c] 82.	1–274
2,3-Dimethyl-3-ethyl-2-pentanol	QX&&X2&2		[c] 1.445		[c] 69.	1–275
4,4-Dimethyl-3-ethyl-2-pentanol	QY&Y2&X		[c] 1.442			1–275
2,3,3,4-Tetramethyl-2-pentanol	QX&&X&&Y		[c] 1.446			1–275
2,3,4,4-Tetramethyl-2-pentanol	QX&&Y&X		[c] 1.444			1–275
3,3,4,4-Tetramethyl-2-pentanol	QY&X&&X			* 180.		1–275
2,2-Dimethyl-3-ethyl-3-pentanol	QX2&2&X	.8526	1.4405	174.0	58.1	1–275
2,4-Dimethyl-3-ethyl-3-pentanol	1Y&XQ2&Y	.8543	1.4416	177.9	67.	1–259, 1–276
2,2,3,4-Tetramethyl-3-pentanol	1Y&XQ1&Y	.8523	1.4405	174.2	62.8	1–259, 1–276
2,2,4,4-Tetramethyl-3-pentanol	1Y&XQ&X		[c] 1.441	167.	62.	1–277
$C_{10}H_{22}O$						
1-Decanol	Q10	.8263	1.4353	230.2	114.6	1–277—1–281
2-Decanol	QY8	0.8216	1.432	209.7	104.	1–283, 1–287
3-Decanol	QY7&2	[c] .823	1.432		105.	1–283, 1–288
4-Decanol	QY6&3	[c] .820	[c] 1.431	210.	98.	1–288
5-Decanol	QY5&4	[c] .820	1.431	201.	98.	1–288
2-Methyl-1-nonanol	Q1Y7			* 222.		1–288
3-Methyl-1-nonanol	Q2Y6	.830	1.435		105.	1–289
4-Methyl-1-nonanol	Q3Y5	.828	1.436		110.	1–289
5-Methyl-1-nonanol	Q4Y4	* .830	[c] 1.436		[c] 110.	1–289
7-Methyl-1-nonanol	Q6Y2	.828	* 1.436		[c] 110.	1–289
8-Methyl-1-nonanol	Q7Y		[c] 1.433		[c] 108.	1–289
2-Methyl-2-nonanol	QX7		[c] 1.430		[c] 91.	1–289
3-Methyl-2-nonanol	QY&Y6	[c] .831	[c] 1.436		[c] 90.	1–290
5-Methyl-2-nonanol	QY&2Y4		* 1.432	203.		1–290
6-Methyl-2-nonanol	QY&3Y3	[c] .829	[c] 1.439		[c] 95.	1–290
7-Methyl-2-nonanol	QY&4&2		[c] 1.430		[c] 100.	1–290
8-Methyl-2-nonanol	QY&5Y1	* .821				1–283, 1–290
2-Methyl-3-nonanol	QY6&Y	.8249	1.4320	208.6	94.4	1–284, 1–290
3-Methyl-3-nonanol	QX6&2	[c] .827	1.436		86.	1–284, 1–291
5-Methyl-3-nonanol	QY2&1Y4		1.433	* 198.		1–291
2-Methyl-4-nonanol	QY5&1Y	* 0.820	1.430		90.	1–291
4-Methyl-4-nonanol	QX5&3	.826	1.4332		80.	1–284, 1–291
5-Methyl-4-nonanol	QY3&Y4	* .828	1.434			1–291
7-Methyl-4-nonanol	QY3&2Y2		[c] 1.430	* 199.	92.	1–291
2-Methyl-5-nonanol	QY4&2Y	[c] .817	[c] 1.429			1–292
3-Methyl-5-nonanol	QY4&1Y	* .821	* 1.431		[c] 90.	1–292
5-Methyl-5-nonanol	QX4&4	.8256	1.4326		85.	1–285, 1–292
2-Ethyl-1-octanol	Q1Y6&2		[c] 1.436		* 104.	1–292
3-Ethyl-1-octanol	Q2Y5&2	[c] .831				1–292
4-Ethyl-1-octanol	Q3Y4&2				* 108.	1–292
6-Ethyl-1-octanol	Q5Y2&2				[c] 115.	1–292
2,2-Dimethyl-1-octanol	Q1X6	[c] .826	* 1.435	* 208.		1–292
2,6-Dimethyl-1-octanol	Q1Y&3Y2	[c] .824	[c] 1.435		[c] 105.	1–293
3,3-Dimethyl-1-octanol	Q2X5				[c] 105.	1–293
3,7-Dimethyl-1-octanol	Q2Y&3Y	[c] .832	[c] 1.438	212.	101.	1–293
4,5-Dimethyl-1-octanol	Q3Y&Y3		* 1.442			1–293
4,6-Dimethyl-1-octanol	Q3Y&1Y2		[c] 1.439			1–293
4,7-Dimethyl-1-octanol	Q3Y&2Y		* 1.438			1–294
7,7-Dimethyl-1-octanol	Q6X		* 1.438		[c] 98.	1–294
2,4-Dimethyl-2-octanol	QX&&1Y4	[c] 0.822	[c] 1.431		[c] 77.	1–294
2,6-Dimethyl-2-octanol	QX&&3Y2	[c] .824	[c] 1.428		81.	1–294
2,7-Dimethyl-2-octanol	QX&&4Y		[c] 1.429		83.	1–294

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* Based on a single experimental value only.

[c] Extrapolated or interpolated from other temperatures.

TABLE 2a. Selected values of physical properties of aliphatic alcohols and compound index—Continued

Compound Name	Wiswesser Line-Formula Notation[a]	Density at 25 °C g cm^{-3}	Refractive Index, n_D at 25 °C	Boiling Point, °C		Index of Page Numbers
				at 760 mm Hg	at 10 mm Hg	
$C_{10}H_{22}O$						
3,7-Dimethyl-2-octanol	QY&Y&3Y	^{c} .825	^{c}1.434			1-294
3-Ethyl-3-octanol	QX5&2&2	* .836	^{c}1.437	199.	82.	1-294
6-Ethyl-3-octanol	QY2&2Y2&2		*1.437		^{c}80.	1-295
2,2-Dimethyl-3-octanol	QY5&X		^{c}1.432		^{c}80.	1-295
2,3-Dimethyl-3-octanol	QX5&&Y	.8249	1.4351	189.1	74.0	1-295
2,7-Dimethyl-3-octanol	1Y&YQ3Y	^{c} .811	^{c}1.428	*194.		1-295
3,5-Dimethyl-3-octanol	QX2&&1Y3	* .837	*1.436			1-295
3,6-Dimethyl-3-octanol	QX2&&2Y2	^{c} .829	^{c}1.437	*192.		1-295
3,7-Dimethyl-3-octanol	QX2&&3Y	^{c} .826	1.433	*196.	81.	1-295
3-Ethyl-4-octanol	QY4&Y2&2		*1.439		93.	1-296
4-Ethyl-4-octanol	QX4&3&2	.834	^{c}1.436		^{c}80.	1-296
2,2-Dimethyl-4-octanol	QY4&1X	^{c} .817	^{c}1.428			1-296
2,4-Dimethyl-4-octanol	QX4&&1Y	^{c} .819	^{c}1.431		^{c}83.	1-296
2,5-Dimethyl-4-octanol	3Y&YQ1Y	* .812	*1.426			1-296
2,6-Dimethyl-4-octanol	2Y&1YQ1Y		^{c}1.429		^{c}85.	1-296
2,7-Dimethyl-4-octanol	1Y&2YQ1Y	^{c}0.812	^{c}1.427		^{c}92.	1-296
3,4-Dimethyl-4-octanol	QX4&&Y2		^{c}1.440		^{c}72.	1-297
3,6-Dimethyl-4-octanol	2Y&YQ1Y2	^{c} .833	^{c}1.447		^{c}103.	1-297
4,6-Dimethyl-4-octanol	QX3&&1Y2	* .828	*1.433		^{c}80.	1-297
4,7-Dimethyl-4-octanol	QX3&&2Y	^{c} .822		*192.		1-297
2-*n*-Propyl-1-heptanol	Q1Y5&3	^{c} .828	1.436	217.9	103.	1-285, 1-297
3-Isopropyl-1-heptanol	Q2Y4&Y	* .838	*1.440	215.2	100.	1-297
2,3,6-Trimethyl-2-heptanol	QX&&Y&2Y				^{c}86.	1-297
2,4,6-Trimethyl-2-heptanol	QX&&1Y&1Y		*1.434		^{c}71.	1-298
2,5,6-Trimethyl-2-heptanol	QX&&2Y&Y	^{c} .827	^{c}1.434	*193.		1-298
4,6,6-Trimethyl-2-heptanol	QY&1Y&1X		*1.431		^{c}77.	1-298
2-Methyl-3-ethyl-3-heptanol	QX4&2&Y	^{c} .842	^{c}1.436	*193.		1-298
2-Methyl-5-ethyl-3-heptanol	2Y2&1YQY					1-298
4-Methyl-3-ethyl-3-heptanol	QX2&2&Y3					1-298
4-Methyl-5-ethyl-3-heptanol	QY2&Y&Y2&2	^{c} .859	^{c}1.453		^{c}83.	1-298
6-Methyl-3-ethyl-3-heptanol	QX2&2&2Y	^{c} .832	^{c}1.435		^{c}80.	1-298
2,2,3-Trimethyl-3-heptanol	QX4&&X	^{c} .841	^{c}1.439	186.	77.	1-298
2,2,6-Trimethyl-3-heptanol	1Y&2YQX	^{c}0.820	^{c}1.430			1-299
2,3,6-Trimethyl-3-heptanol	1Y&XQ&2Y	^{c} .836	^{c}1.436		^{c}75.	1-299
3,5,5-Trimethyl-3-heptanol	QX2&&1X2	^{c} .852	^{c}1.443	195.6	60.	1-299
4-*n*-Propyl-4-heptanol	QX3&3&3	.8281	^{c}1.433	194.3	81.	1-285, 1-299
4-Isopropyl-4-heptanol	QX3&3&Y	^{c} .841	^{c}1.437	190.	73.	1-300
2,2,4-Trimethyl-4-heptanol	QX3&&1X	^{c} .829	^{c}1.435	181.	68.	1-300
2,2,5-Trimethyl-4-heptanol	2Y&YQ1X	^{c} .832			^{c}80.	1-300
2,2,6-Trimethyl-4-heptanol	1Y&1YQ1X		^{c}1.422		^{c}60.	1-300
2,4,5-Trimethyl-4-heptanol	2Y&XQ&1Y		^{c}1.436			1-300
2,4,6-Trimethyl-4-heptanol	1Y&1XQ&1Y	^{c} .815	^{c}1.429	182.	68.	1-301
3,3,6-Trimethyl-4-heptanol	2X&&YQ1Y	* .838	*1.438			1-301
2-*n*-Butyl-1-hexanol	Q1Y4&4		1.434	218.	106.	1-286, 1-301
4-Methyl-2-*n*-propyl-1-hexanol	Q1Y3&1Y2	^{c} .825	^{c}1.434	*208.	98.	1-301
4-Methyl-2-isopropyl-1-hexanol	2Y&1Y1QY			*201.		1-301
5-Methyl-2-isopropyl-1-hexanol	1Y&Y1Q2Y	^{c} .829	^{c}1.436	213.	92.	1-302
2,4-Diethyl-1-hexanol	Q1Y2&1Y2&2					1-302
5,5-Dimethyl-2-ethyl-1-hexanol	Q1Y2&2X	^{c} .835	^{c}1.433		^{c}90.	1-302
2,3,4,4-Tetramethyl-2-hexanol	QX&&Y&X2		^{c}1.448	190.		1-302
3,3,5,5-Tetramethyl-2-hexanol	QY&X&&1X		^{c}1.444		^{c}70.	1-302
2-Methyl-3-isopropyl-3-hexanol	1Y&XQ3&Y	^{c}0.846	*1.441	192.	69.	1-302
2,2-Dimethyl-4-ethyl-3-hexanol	2Y2&YQX	^{c} .830	^{c}1.436	187.	65.	1-303
2,4-Dimethyl-4-ethyl-3-hexanol	2X2&&YQY	^{c} .857	^{c}1.444			1-303
5,5-Dimethyl-3-ethyl-3-hexanol	QX2&2&1X	^{c} .836	^{c}1.438		*62.	1-303
2,2,3,4-Tetramethyl-3-hexanol	2Y&XQ&X	^{c} .854	^{c}1.445	192.		1-303
2,2,3,5-Tetramethyl-3-hexanol	1Y&1XQ&X	^{c} .835	^{c}1.435		^{c}70.	1-303
2,2,4,4-Tetramethyl-3-hexanol	2X&&YQX	^{c} .851	^{c}1.444	190.		1-303
2,2,5,5-Tetramethyl-3-hexanol	1X&&YQ1X			170.		1-304
2,3,4,4-Tetramethyl-3-hexanol	2X&&XQ&Y	^{c} .870	^{c}1.451	201.		1-304
2,3,5,5-Tetramethyl-3-hexanol	1Y&XQ&1X	^{c} .834	^{c}1.435		^{c}62.	1-304
2,4,4,5-Tetramethyl-3-hexanol	1Y&YQX&&Y		^{c}1.447		^{c}76.	1-304
3,4,4,5-Tetramethyl-3-hexanol	QX2&&X&&Y	^{c} .870	^{c}1.451	202.		1-304
3,4,5,5-Tetramethyl-3-hexanol	1Y&YQY&X	^{c} .858	^{c}1.447	195.		1-304

* Based on a single experimental value only.

[c] Extrapolated or interpolated from other temperatures.

TABLE 2a. Selected values of physical properties of aliphatic alcohols and compound index—Continued

Compound Name	Wiswesser Line-Formula Notation[a]	Density at 25 °C g cm^{-3}	Refractive Index, n_D at 25 °C	Boiling Point, °C		Index of Page Numbers
				at 760 mm Hg	at 10 mm Hg	
$C_{10}H_{22}O$						
4-Methyl-2-isobutyl-1-pentanol	1Y&1Y1Q1Y	^{c} .83		204.	91.	1–305
4,4-Dimethyl-3-isopropyl-1-pentanol	1Y&Y2QX		^{c} 1.460		^{c} 88.	1–305
3,4-Dimethyl-3-isopropyl-2-pentanol	QY&X&Y&&Y		^{c} 1.460		^{c} 94.	1–305
2,4-Dimethyl-3-*n*-propyl-3-pentanol	1Y&XQ3&Y	^{c} .8518	^{c} 1.442	185.	66.	1–286, 1–305
2,4-Dimethyl-3-isopropyl-3-pentanol	1Y&XQY&&Y	.8591	1.4458	194.5	73.9	1–286, 1–306
2,2,4-Trimethyl-3-ethyl-3-pentanol	1Y&XQ2&X	^{c} .858	^{c} 1.446	191.	67.	1–306
2,2,3,4,4-Pentamethyl-3-pentanol	1X&&XQ1&X			194.6	70.	1–287, 1–306
2,3-Dimethyl-2-*tert*-butyl-1-butanol	1Y&X1Q&X				^{c} 90.	1–306
$C_{11}H_{24}O$						
1-Undecanol	Q11	0.8291	1.4386	242.8	126.2	1–307—1–309
2-Undecanol	QY9	.8233	1.435	230.	114.8	1–310, 1–312
3-Undecanol	QY8&2	^{c} .8253			^{c} 108.	1–310, 1–312
5-Undecanol	QY4&4					1–312
6-Undecanol	QY5&3	^{c} .829	* 1.4334	230.5	109.	1–310, 1–312
2-Methyl-1-decanol	Q1Y8					1–313
4-Methyl-1-decanol	Q3Y6					1–313
5-Methyl-1-decanol	Q4Y5					1–313
2-Methyl-2-decanol	QX8		^{c} 1.434		^{c} 104.	1–313
4-Methyl-2-decanol	QY&1Y6				^{c} 103.	1–313
4-Methyl-3-decanol	QY2&Y6	* .827	^{c} 1.433		^{c} 89.	1–313
6-Methyl-3-decanol	QY2&2Y4	* .828				1–313
2-Methyl-4-decanol	QY6&1Y	* .817	* 1.431		^{c} 123.	1–313
4-Methyl-4-decanol	QY6&3	.8238	* 1.438			1–311, 1–313
2-Methyl-5-decanol	QY5&2Y	^{c} .823	^{c} 1.433			1–314
5-Methyl-5-decanol	QY5&4	* 0.826	^{c} 1.435		^{c} 100.	1–314
2-Ethyl-1-nonanol	Q1Y7&2					1–314
7-Ethyl-1-nonanol	Q6Y2&2		^{c} 1.452			1–314
3,3-Dimethyl-1-nonanol	Q2X6					1–314
4,8-Dimethyl-1-nonanol	Q3Y&3Y	^{c} .829	^{c} 1.437			1–314
4-Ethyl-2-nonanol	QY&1Y5&2	^{c} .831		* 225.4		1–314
5-Ethyl-2-nonanol	QY&2Y4&2	^{c} .831	^{c} 1.438	* 225.4		1–314
6-Ethyl-3-nonanol	QY2&2Y3&2	^{c} .828				1–314
4-Ethyl-4-nonanol	QX5&3&2				^{c} 105.	1–315
2,2-Dimethyl-4-nonanol	QY5&1X	^{c} .818	^{c} 1.432		^{c} 92.	1–315
2,4-Dimethyl-4-nonanol	QY5&&1Y	^{c} .825	^{c} 1.434		* 93.	1–315
3,4-Dimethyl-4-nonanol	QX5&&Y2		^{c} 1.441			1–315
4,8-Dimethyl-4-nonanol	QX3&&3Y					1–315
5-Ethyl-5-nonanol	QX4&4&2	* .8345	^{c} 1.439		^{c} 93.	1–315
2,6-Dimethyl-5-nonanol	3Y&YQ2Y	* .8126	* 1.4296		* 98.	1–315
5,7-Dimethyl-5-nonanol	QX4&&Y2	^{c} .828	* 1.433			1–315
5-*n*-Propyl-1-octanol	Q4Y3&3					1–315
3-*n*-Propyl-2-octanol	QY&Y5&3	^{c} .824		* 234.		1–316
3,7,7-Trimethyl-3-octanol	QX2&&3X		^{c} 1.432			1–316
4-*n*-Propyl-4-octanol	QX4&3&3	* .8319	^{c} 1.437		^{c} 96.	1–316
4-Isopropyl-4-octanol	QX4&3&Y	^{c} .836	^{c} 1.443			1–316
2,2,4-Trimethyl-4-octanol	QX4&&1X	^{c} 0.831	^{c} 1.438		^{c} 83.	1–316
2,4,7-Trimethyl-4-octanol	1Y&2XQ&1Y	^{c} .820	^{c} 1.434			1–316
3,3,6,6-Tetramethyl-1-heptanol	Q2X&&2X					1–316
3-*n*-Butyl-2-heptanol	QY&Y4&4					1–316
2-Methyl-3-isopropyl-3-heptanol	1Y&XQ4&Y	^{c} .847	^{c} 1.444		85.	1–316
2,2,3,4-Tetramethyl-3-heptanol	3Y&XQ&X			* 212.5		1–317
2,2,3,6-Tetramethyl-3-heptanol	1Y&2XQ&X	^{c} .847	^{c} 1.437			1–317
2,3,4,4-Tetramethyl-3-heptanol	3X&&XQ&Y	^{c} .866	^{c} 1.456	* 216.		1–317
2,2,6,6-Tetramethyl-3-heptanol	1X&&YQ2X					1–317
2-Methyl-4-*n*-propyl-4-heptanol	QX3&3&1Y	^{c} 0.829			^{c} 84.	1–317

* Based on a single experimental value only.

^{c} Extrapolated or interpolated from other temperatures.

TABLE 2a. Selected values of physical properties of aliphatic alcohols and compound index—Continued

Compound Name	Wiswesser Line-Formula Notation[a]	Density at 25 °C g cm^{-3}	Refractive Index, n_D at 25 °C	Boiling Point, °C		Index of Page Numbers
				at 760 mm Hg	at 10 mm Hg	
$C_{11}H_{24}O$						
3,5-Diethyl-4-heptanol	2Y2&YQY2&2				^{c}95.	1–317
2,6-Dimethyl-4-ethyl-4-heptanol	1Y&1XQ2&1Y		^{c}1.435			1–317
3,3-Dimethyl-5-ethyl-4-heptanol	2Y2&YQX2	^{c}.847	^{c}1.442			1–317
2,2,4,6-Tetramethyl-4-heptanol	1Y&1YQ&1X	^{c}.824	^{c}1.434			1–317
2,2,5,5-Tetramethyl-4-heptanol	2X&&YQ1X		^{c}1.439		^{c}79.	1–318
3,3,5,5-Tetramethyl-4-heptanol	2X&&YQX2			* 211.		1–318
5-Methyl-3-isobutyl-2-hexanol	1Y&1YYQ&1Y					1–318
2,2-Dimethyl-3-*n*-propyl-3-hexanol	QX3&3&X	^{c}.847	^{c}1.443			1–318
2,4-Dimethyl-3-isopropyl-3-hexanol	2Y&XQY&&Y		^{c}1.450			1–318
2,5-Dimethyl-3-isopropyl-3-hexanol	1Y&1XQY&&Y	^{c}.844	1.4402	197.	78.	1–311, 1–318
2,2,3-Trimethyl-4-ethyl-3-hexanol	2Y2&XQ&X	^{c}0.855	^{c}1.450	* 210.		1–318
2,2,3,4,4-Pentamethyl-3-hexanol	2X&&XQ&X			* 220.		1–319
2,2,3,4,5-Pentamethyl-3-hexanol	1Y&Y&XQ&X			* 208.		1–319
3,4,4,5,5-Pentamethyl-3-hexanol	QX2&&X&&X					1–319
2,2,4,5,5-Pentamethyl-4-hexanol	1X&&XQ&1X	^{c}.837	^{c}1.439		^{c}67.	1–319
2,4-Dimethyl-3-*n*-butyl-3-pentanol	1Y&XQ4&Y	^{c}.856	^{c}1.446			1–319
2,2,4-Trimethyl-3-isopropyl-3-pentanol	1Y&XQY&&X	^{c}.867	1.453	215.7	83.	1–311, 1–319
$C_{12}H_{26}O$						
1-Dodecanol	Q12	0.8308	1.4413		138.2	1–320—1–323
2-Dodecanol	QY10	.8262	* 1.4401	249.	129.	1–323, 1–324, 1–327
3-Dodecanol	QY9&2	.8278	* 1.4402		124.	1–323, 1–324, 1–327
4-Dodecanol	QY8&3	.8255	1.439		122.	1–323, 1–324, 1–327
5-Dodecanol	QY7&4	.8260	* 1.4388		123.	1–323, 1–325, 1–327
6-Dodecanol	QY6&5	^{c}.823	* 1.4386		121.	1–323, 1–325, 1–328
2-Methyl-1-undecanol	Q1Y9				^{c}126.	1–328
3-Methyl-1-undecanol	Q2Y8	* .8309	* 1.4409			1–328
9-Methyl-1-undecanol	Q8Y2	* .8316	* 1.4413			1–328
10-Methyl-1-undecanol	Q9Y		^{c}1.439			1–328
2-Methyl-2-undecanol	QX9				^{c}100.	1–328
2-Methyl-3-undecanol	QY8&Y	^{c}.829	^{c}1.439	* 236.		1–325, 1–328
3-Methyl-3-undecanol	QY8&2		^{c}1.440			1–329
2-Methyl-4-undecanol	QY7&1Y		^{c}1.435			1–329
2-Methyl-5-undecanol	QY6&2Y	^{c}0.822	^{c}1.433			1–329
3-Methyl-5-undecanol	QY6&1Y2	* .826	* 1.437		^{c}110.	1–329
4-Methyl-5-undecanol	QY6&Y3		^{c}1.440			1–329
5-Methyl-5-undecanol	QX6&4	0.8252			* 126.	1–329
6-Methyl-6-undecanol	QX5&5	* .827	^{c}1.437			1–329
2-Ethyl-1-decanol	Q1Y8&2				^{c}133.	1–330
2,2-Dimethyl-1-decanol	Q1X8	^{c}.831	^{c}1.441	* 244.	^{c}122.	1–330
3,3-Dimethyl-1-decanol	Q2X7					1–330
3-Ethyl-3-decanol	QX7&2					1–330
6-Ethyl-3-decanol	QY2&2Y4	^{c}.839	^{c}1.445	* 225.	118.	1–330
3-Ethyl-4-decanol	QY6&Y2					1–330
2,4-Dimethyl-4-decanol	QX6&&1Y	^{c}.824	^{c}1.437			1–330
3,3-Dimethyl-4-decanol	QY6&X2		^{c}1.443			1–330
5-Ethyl-5-decanol	QX5&4&2	.8357	* 1.4401			1–331
6,6-Dimethyl-5-decanol	QY4&X4	^{c}.841	^{c}1.445			1–331
2,6-Dimethyl-6-decanol	QX4&&3Y					1–331
6,8-Dimethyl-6-decanol	QX5&&1Y2	^{c}.831	* 1.440			1–331
2-*n*-Propyl-1-nonanol	Q1Y7&3					1–331
3-Methyl-2-ethyl-1-nonanol	Q1Y2&Y6		* 1.445			1–331
2-Methyl-5-ethyl-3-nonanol	4Y2&1YQY	^{c}0.843	^{c}1.439			1–331

* Based on a single experimental value only.

[c] Extrapolated or interpolated from other temperatures.

TABLE 2a. Selected values of physical properties of aliphatic alcohols and compound index—Continued

Compound Name	Wiswesser Line-Formula Notation[a]	Density at 25 °C g cm^{-3}	Refractive Index, n_D at 25 °C	Boiling Point, °C		Index of Page Numbers
				at 760 mm Hg	at 10 mm Hg	
$C_{12}H_{26}O$						
7-Methyl-5-ethyl-3-nonanol	QY2&1Y2&Y2			* 252.		1–331
3,7,7-Trimethyl-3-nonanol	QX2&&3X2		^{c}1.441			1–332
4-*n*-Propyl-4-nonanol	QX5&3&3	* .832	^{c}1.439			1–332
2,2,4-Trimethyl-4-nonanol	QX5&&1X		^{c}1.441			1–332
2,6,8-Trimethyl-4-nonanol	1Y&1YQ1Y&1Y	^{c} .814		* 225.2		1–332
5-*n*-Propyl-5-nonanol	QY4&4&3	* .834	* 1.440		^{c}109.	1–332
5-Isopropyl-5-nonanol	QX4&&Y	^{c} .840	^{c}1.443		^{c}102.	1–332
2,5,8-Trimethyl-5-nonanol	1Y&2XQ&2Y	^{c} .825	^{c}1.437		^{c}103.	1–332
2-*n*-Butyl-1 octanol	Q1Y6&4	^{c} .832	* 1.440	253.4	127.	1–326, 1–333
4-*n*-Butyl-1-octanol	Q3Y4&4	^{c} .834			^{c}132.	1–333
2,4-Diethyl-1-octanol	Q1Y2&1Y4&2	^{c} .836	* 1.448			1–333
2,5,7,7-Tetramethyl-2-octanol	QX&&2Y&1X		* 1.436			1–333
2-Methyl-3-isopropyl-3-octanol	1Y&XQ5&Y	^{c} .850	^{c}1.446			1–333
2,2-Dimethyl-4-ethyl-3-octanol	4Y2&YQX	^{c} .837	^{c}1.440		^{c}95.	1–333
5-Methyl-5-*n*-propyl-4-octanol	QY3&X3&3					1–333
2,2,7,7-Tetramethyl-4-octanol	1X&&2YQ1X					1–333
4-Methyl-2-*n*-butyl-1-heptanol	Q1Y4&1Y3			* 232.		1–334
2-Isobutyl-6-methyl-1-heptanol	1Y&3Y1QY				* 113.	1–334
3-Methyl-3-*n*-butyl-2-heptanol	QY&X4&4		^{c}1.447		^{c}105.	1–334
2,2-Dimethyl-3-isopropyl-3-heptanol	1Y&XQ4&X	^{c}0.853	^{c}1.456			1–334
2,6-Dimethyl-3-isopropyl-3-heptanol	1Y&XQY&&2Y		^{c}1.440			1–334
2,2,3,4,4-Pentamethyl-3-heptanol	3X&&XQ&X		^{c}1.461	^{c}234.		1–334
2,2,3,6,6-Pentamethyl-3-heptanol	1X&&XQ&2X					1–334
2,2,4,6,6-Pentamethyl-3-heptanol	1X&&YQY&1X	^{c} .835	^{c}1.440			1–334
2,2,5,6,6-Pentamethyl-3-heptanol	1X&&YQ1Y&X	^{c} .838				1–335
2,2-Dimethyl-4-*n*-propyl-4-heptanol	QX3&3&1X	^{c} .834	^{c}1.441		* 95.	1–335
2,6-Dimethyl-4-isopropyl-4-heptanol	1Y&1XQY&&1Y		^{c}1.443			1–335
3,4,5-Trimethyl-3-ethyl-4-heptanol	2Y&XQ&X2&2		^{c}1.459			1–335
2,2,3,3,4-Pentamethyl-4-heptanol	QX3&&X&&X					1–335
3,3,4,5,5-Pentamethyl-4-heptanol	2X&&XQ&X2			* 244.		1–335
5-Methyl-2-(3-methylbutyl)-1-hexanol	1Y&2Y1Q2Y	^{c} .830			^{c}116.	1–335
5,5-Dimethyl-4-*tert*-butyl-1-hexanol	1X&&Y3QX	^{c} .861				1–335
2,5-Dimethyl-3-isobutyl-2-hexanol	1Y&1YXQ&&1Y					1–335
2,2-Dimethyl-3-*tert*-butyl-3-hexanol	1X&&XQ3&X	^{c} .856	^{c}1.454			1–336
2-Methyl-4-ethyl-3-isopropyl-3-hexanol	2Y2&XQY&&Y	^{c}0.849	^{c}1.446		^{c}95.	1–336
2,2,5-Trimethyl-3-isopropyl-3-hexanol	1Y&1XQY&&X	^{c} .851	^{c}1.449			1–336
2,5,5-Trimethyl-3-isopropyl-3-hexanol	1Y&XQY&&1X		* 1.446		^{c}86.	1–336
2,2-Dimethyl-4,4-diethyl-3-hexanol	2X2&2&YQX			* 227.		1–336
2,2,3,4-Tetramethyl-4-ethyl-3-hexanol	2X2&&XQ&X	* .886	* 1.468	* 238.		1–336
2,2,3,4,4,5-Hexamethyl-3-hexanol	1Y&X&&XQ&X			* 236.		1–336
2,2,4,4,5,5-Hexamethyl-3-hexanol	1X&&YQX&&X		* 1.445		^{c}92.	1–336

* Based on a single experimental value only.

^{c} Extrapolated or interpolated from other temperatures.

TABLE 2a. Selected values of physical properties of aliphatic alcohols and compound index—Continued

Compound Name	Wiswesser Line-Formula Notation[a]	Density at 25 °C g cm^{-3}	Refractive Index, n_D at 25 °C	Boiling Point, °C		Index of Page Numbers
				at 760 mm Hg	at 10 mm Hg	
$C_{12}H_{26}O$						
2,3,4,4,5,5-Hexamethyl-3-hexanol	1Y&XQ&X&&X					1–337
4,4-Dimethyl-2-neopentyl-1-pentanol	1X&&1Y1Q1X					1–337
2,4,4-Trimethyl-2-*tert*-butyl-1-pentanol	1X&&X&1Q1X	[c] .871	[c] 1.459			1–337
2,4,4-Trimethyl-3-*tert*-butyl-2-pentanol	QX&&YX&&&X					1–337
2,2,4,4-Tetramethyl-3-isopropyl-3-pentanol	1Y&XQ2&X	[c] 0.884	* 1.4625	234.	95.	1–337
$C_{13}H_{28}O$						
1-Tridecanol	Q13				[c] 148.	1–338, 1–340
2-Tridecanol	QY11	* .8282			146.	1–338, 1–340
3-Tridecanol	QY2&10					1–338, 1–340
4-Tridecanol	QY9&3	[c] .819	[c] 1.436			1–340
7-Tridecanol	QY6&6					1–340
2-Methyl-1-dodecanol	Q1Y10	* .844				1–341
10-Methyl-1-dodecanol	Q9Y2		[c] 1.453			1–341
2-Methyl-2-dodecanol	QX10				* 145.	1–341
6-Methyl-6-dodecanol	QX6&5	.8273				1–338, 1–341
2-Ethyl-1-undecanol	Q1Y9&2	[c] .836	[c] 1.443			1–341
3-Ethyl-3-undecanol	QX8&2&2			* 250.		1–341
6-Ethyl-6-undecanol	QX5&5&2		[c] 1.441			1–341
3,5-Dimethyl-5-undecanol	QX6&&1Y2	* .830	* 1.442			1–341
4-*n*-Propyl-4-decanol	QX6&3&3		[c] 1.441		[c] 122.	1–338, 1–342
5-*n*-Propyl-5-decanol	QX5&4&3	* .8320	* 1.4397			1–338, 1–342
2,5,9-Trimethyl-5-decanol	1Y&3XQ&2Y					1–342
2-*n*-Butyl-1-nonanol	Q1Y7&4	[c] .832	[c] 1.441			1–342
3,6,8,8-Tetramethyl-3-nonanol	QX2&&2Y&1X		* 1.4408			1–342
3,3-Dimethyl-5-ethyl-4-nonanol	4Y2&YQX2	[c] 0.847	[c] 1.447			1–342
5-*n*-Butyl-5-nonanol	QX4&4&4	.8355	[c] 1.4464		119.	1–338, 1–343
2,8-Dimethyl-5-ethyl-5-nonanol	1Y&2XQ2&2Y	[c] .864				1–343
5,7,7-Trimethyl-3-ethyl-3-octanol	QX2&2&1Y&1X		* 1.4431			1–343
2,2,3,3,4-Pentamethyl-4-octanol	QX4&&X&&X	[c] .872	[c] 1.460			1–343
2,2-Dimethyl-3-*n*-butyl-3-heptanol	QX4&4&X	[c] .845	[c] 1.447		* 105.	1–343
2,2-Dimethyl-3-*tert*-butyl-3-heptanol	1X&&XQ4&X	[c] .856	[c] 1.452	240.4	108.1	1–339, 1–344
2,2,3-Trimethyl-4-*n*-propyl-3-heptanol	3Y3&XQ&X			* 236.	* 103.	1–344
2,6-Dimethyl-4-isobutyl-4-heptanol	1Y&1XQ3&1Y		[c] 1.432			1–344
3,3,6-Trimethyl-4-*n*-propyl-4-heptanol	2X&&XQ3&1Y	[c] .856	[c] 1.452	240.4	110.0	1–339, 1–344
3,3,6-Trimethyl-4-isopropyl-4-heptanol	2X&&XQY&&1	[c] .861	[c] 1.453	239.4	108.0	1–339, 1–344
3,3,5-Triethyl-4-heptanol	2Y&YQX2&2&2					1–345
3,3,5,5-Tetramethyl-4-ethyl-4-heptanol	2X&&XQ2&X2	[c] .888	[c] 1.468	252.6	118.0	1–339, 1–395
2,3,3,5,5,6-Hexamethyl-4-heptanol	1Y&X&&YQX&&Y					1–345
5,5-Dimethyl-2-neopentyl-1-hexanol	2X&&Y1Q2X2	[c] .843	[c] 1.447			1–345
3,5,5-Trimethyl-3-*tert*-butyl-2-hexanol	2X&&1X&YQ&X		[c] 1.467			1–345
2,2,5-Trimethyl-3-*tert*-butyl-3-hexanol	2Y&1XQX&&&X	[c] .863	[c] 1.455	240.5	104.0	1–345
2,2,3-Trimethyl-4,4-diethyl-3-hexanol	3X2&2&XQ&X					1–345

* Based on a single experimental value only.

[c] Extrapolated or interpolated from other temperatures.

TABLE 2a. Selected values of physical properties of aliphatic alcohols and compound index—Continued

Compound Name	Wiswesser Line-Formula Notation[a]	Density at 25 °C g cm^{-3}	Refractive Index, n_D at 25 °C	Boiling Point, °C at 760 mm Hg	Boiling Point, °C at 10 mm Hg	Index of Page Numbers
$C_{13}H_{28}O$						
2,2,4,4-Tetramethyl-3-*tert*-butyl-3-pentanol	1X&&XQX&&&X					1–345
$C_{14}H_{30}O$						
1-Tetradecanol	Q14	[c] 0.833		263.5	158.	1–346—1–348
2-Tetradecanol	QY12					1–350
3-Tetradecanol	QY2&11				* 146.	1–349, 1–350
4-Tetradecanol	QY3&10					1–350
5-Tetradecanol	QY9&4					1–350
6-Tetradecanol	QY8&5					1–350
11-Methyl-1-tridecanol	Q10Y2	* .8344	* 1.4455			1–350
12-Methyl-1-tridecanol	Q11Y		* 1.4464		* 161.	1–350
2-Methyl-2-tridecanol	QX11	[c] .823	[c] 1.442			1–349, 1–350
2-Methyl-3-tridecanol	10YQY	[c] .8340	[c] 1.444	* 274.		1–349, 1–351
2-Methyl-4-tridecanol	QY9&1Y		* 1.4404			1–351
4-Methyl-4-tridecanol	QX9&3	* .8284	* 1.4430			1–349, 1–351
6-Methyl-6-tridecanol	QX7&5					1–351
2,2-Dimethyl-1-dodecanol	Q1X10	[c] .832		* 272.		1–351
4,10-Dimethyl-1-dodecanol	Q3Y&5Y2		[c] 1.444			1–351
3,10,10-Trimethyl-3-undecanol	QX2&&6X2		[c] 1.442			1–351
2-Methyl-7-ethyl-4-undecanol	4Y2&2YQ1Y	[c] .830		264.3		1–351
6-*n*-Propyl-6-undecanol	QX5&5&3	* .834	[c] 1.443		[c] 93.	1–352
6-Isopropyl-6-undecanol	QX5&5&Y	[c] .839	[c] 1.446			1–352
2,2,6-Trimethyl-6-undecanol	QX5&&3X		[c] 1.440		* 126.	1–352
5-*n*-Butyl-5-decanol	QX5&4&4	.8370	* 1.4434		[c] 120.	1–352
2-*n*-Pentyl-1-nonanol	Q1Y7&5	* .837	[c] 1.444	240.	150.	1–352
2-Methyl-4-iosbutyl-4-nonanol	1Y&XQ5&1Y					1–352
2,2,3,3,4-Pentamethyl-4-nonanol	QX5&&X&&X	[c] .871	[c] 1.462			1–352
4,4,5,6,6-Pentamethyl-5-nonanol	3X&&XQ&X3		[c] 1.468	* 268.		1–353
7,7-Dimethyl-6-*tert*-butyl-1-octanol	1X&&Y5QX		[c] 1.419			1–353
2,2-Dimethyl-4-*n*-butyl-4-octanol	QX4&4&1X	[c] .836	[c] 1.444		[c] 120.	1–353
3,3-Dimethyl-4-*tert*-butyl-4-octanol	2X&&XQ4&X	[c] .868	[c] 1.460	260.	126.	1–349, 1–353
3,3-Dimethyl-4-isobutyl-4-octanol	2X&&XQ4&1Y	[c] .852	[c] 1.451	* 246.	[c] 116.	1–349, 1–353
2,2,6-Trimethyl-4-isobutyl-4-heptanol	1Y&1XQ1X&&&1Y	[c] .827	[c] 1.437			1–353
3,3,6-Trimethyl-4-isobutyl-4-heptanol	3X&&XQ1X&&1Y	[c] .849	[c] 1.450	* 240.	* 112.	1–349, 1–354
3,3,6-Trimethyl-4-*tert*-butyl-4-heptanol	2X&&XQX&&&1Y	[c] .874	[c] 1.463	* 260.	* 119.	1–349, 1–354
3,3,5,5-Tetramethyl-4-*n*-propyl-4-heptanol	2X&&XQ3&X2	[c] 0.884	[c] 1.467			1–354
2,2-Di-*n*-butyl-1-hexanol	Q1X4&4&4		[c] 1.451			1–354
$C_{15}H_{32}O$						
1-Pentadecanol	Q15	[c] 0.834	[c] 1.446			1–354, 1–355
2-Pentadecanol	QY13				[c] 149.	1–355
3-Pentadecanol	QY2&12				[c] 153.	1–355, 1–358
4-Pentadecanol	QY3&11					1–355
6-Pentadecanol	QY9&5				* 159.	1–355
8-Pentadecanol	QY7&7				[c] 152.	1–356
2-Methyl-1-tetradecanol	Q1Y12					1–356
12-Methyl-1-tetradecanol	Q11Y2		[c] 1.447			1–356
2-Methyl-2-tetradecanol	QX12	[c] .834	[c] 1.442			1–356
5-Methyl-5-tetradecanol	QX9&4					1–356
6,10-Dimethyl-2-tridecanol	QY&3Y&3Y3	[c] .884	[c] 1.445		* 144.	1–356
9-Ethyl-6-tridecanol	QY5&2Y4&2			* 276.	[c] 147.	1–356

* Based on a single experimental value only.

[c] Extrapolated or interpolated from other temperatures.

TABLE 2a. Selected values of physical properties of aliphatic alcohols and compound index—Continued

Compound Name	Wiswesser Line-Formula Notation[a]	Density at 25 °C g cm^{-3}	Refractive Index, n_D at 25 °C	Boiling Point, °C		Index of Page Numbers
				at 760 mm Hg	at 10 mm Hg	
$C_{15}H_{32}O$						
2,3,6-Trimethyl-1-dodecanol	Q1Y&Y&2Y6	* .835	* 1.447			1–356
3,7,11-Trimethyl-3-dodecanol	QX2&&3Y&3Y	^{c} .836	^{c} 1.444			1–357
2,6,10-Trimethyl-6-dodecanol	2Y&3XQ&3Y					1–357
2,7,10-Trimethyl-6-dodecanol	2Y&2Y&YQ3Y					1–357
5,7-Diethyl-4-undecanol	QY3&Y2&1Y4&2			* 264.	* 113.	1–357
6-*n*-Butyl-6-undecanol	QX5&5&4	* 0.834	^{c} 1.445			1–357
6-Isobutyl-6-undecanol	QX5&5&1Y	^{c} .833	^{c} 1.444			1–357
2,2-Dimethyl-3-*tert*-butyl-3-nonanol	1X&&XQ6&X	^{c} .856	^{c} 1.455			1–357
2,8-Dimethyl-5-isobutyl-5-nonanol	1Y&2XQ1Y&&2Y					1–357
3,3-Di-*n*-butyl-2-heptanol	QY&X4&4&4		* 1.455			1–357
3,3,5,5-Tetramethyl-4-*n*-butyl-4-heptanol	2X&&XQ4&X2	^{c} .881	^{c} 1.467		^{c} 136.7	1–358
3,3,5,5-Tetraethyl-4-heptanol	2X2&2&2YQ					1–358
$C_{16}H_{34}O$						
1-Hexadecanol	Q16				^{c} 177.	1–358—1–363
2-Hexadecanol	QY14					1–365
3-Hexadecanol	QY2&13					1–364, 1–365
4-Hexadecanol	QY3&12					1–365
5-Hexadecanol	QY4&11					1–366
6-Hexadecanol	QY5&10					1–366
7-Hexadecanol	QY9&4					1–366
8-Hexadecanol	QY8&7					1–366
14-Methyl-1-pentadecanol	Q13Y					1–366
2-Methyl-2-pentadecanol	QX13	* .827	^{c} 1.433			1–364, 1–366
6-Methyl-6-pentadecanol	QX9&5	* .8316	* 1.4446			1–366
9-Methyl-7-pentadecanol	QY6&1Y6		^{c} 1.446		^{c} 165.	1–366
8-Methyl-8-pentadecanol	QX7&7					1–366
2-Ethyl-1-tetradecanol	Q1Y2&12	* 0.8371				1–364, 1–367
2,2-Dimethyl-1-tetradecanol	Q1X12	^{c} .836	* 1.448	* 293.		1–367
2,2-Dimethyl-3-tetradecanol	11YQX	^{c} .832	^{c} 1.446			1–367
3-Ethyl-3-tetradecanol	QX2&2&11		1.451			1–364, 1–367
2-*n*-Propyl-1-tridecanol	Q1Y3&11	* .8353				1–364, 1–367
5-*n*-Propyl-4-tridecanol	QY3&Y8&3				* 153.	1–367
5-Methyl-9-ethyl-6-tridecanol	4Y2&2YQY4			* 288.	* 157.	1–367
2-*n*-Butyl-1-dodecanol	Q1Y4&10	* .8347				1–364, 1–368
2-*n*-Pentyl-1-undecanol	Q1Y9&5	* .8343				1–365, 1–368
6-*n*-Pentyl-6-undecanol	QX5&5&5	* .8293	^{c} 1.445		^{c} 150.	1–365, 1–368
2,2,6,10,10-Pentamethyl-6-undecanol	1X&&3XQ&3X					1–368
2-*n*-Hexyl-1-decanol	Q1Y8&6	* .8343	^{c} 1.449		^{c} 172.	1–365, 1–368
2,4,6-Triethyl-1-decanol	Q1Y2&1Y2&1Y4&2		* 1.467			1–368
2-Heptyl-1-nonanol	Q1Y7&7	* .8343				1–365, 1–369
2,8-Dimethyl-5-isopentyl-5-nonanol	1Y&23XQ					1–369
2,2,6,6-Tetramethyl-4-neopentyl-3-heptanol	1X&&YQY1X&&&1X					1–369
$C_{17}H_{36}O$						
1-Heptadecanol	Q17			* 333.		1–369
2-Heptadecanol	QY15		^{c} 1.448		* 177.	1–370
8-Heptadecanol	QY9&7					1–370
9-Heptadecanol	QY8&8					1–370
14-Methyl-1-hexadecanol	Q13Y2		^{c} 1.451			1–370
3,3-Dimethyl-4-pentadecanol	11YQX2	^{c} 0.840	^{c} 1.450			1–370
6-Methyl-6-*n*-propyl-4-tridecanol	QY3&1X7&3					1–370
3,9-Diethyl-6-tridecanol	4Y2&2YQ2Y2&2	^{c} .842		* 309.		1–370
8-Methyl-8-isobutyl-6-dodecanol	QY5&1X4&&1Y	^{c} .842	^{c} 1.452			1–370

* Based on a single experimental value only.

[c] Extrapolated or interpolated from other temperatures.

TABLE 2a. Selected values of physical properties of aliphatic alcohols and compound index—Continued

Compound Name	Wiswesser Line-Formula Notation[a]	Density at 25 °C g cm^{-3}	Refractive Index, n_D at 25 °C	Boiling Point, °C		Index of Page Numbers
				at 760 mm Hg	at 10 mm Hg	
$C_{18}H_{38}O$						
1-Octadecanol	Q18				^{c}203.	1–371—1–374
2-Octadecanol	QY16					1–375
3-Octadecanol	QY2&15					1–375
6-Methyl-1-heptadecanol	Q5Y11		^{c}1.452			1–375
16-Methyl-1-heptadecanol	Q15Y					1–375
2-Methyl-2-heptadecanol	QX15					1–375
3-Ethyl-3-hexadecanol	QX13&2&22	^{c}0.839				1–375
2,2-Dimethyl-3-hexadecanol	13YQX		^{c}1.447			1–376
6,10,14-Trimethyl-2-pentadecanol	QY&3Y&3Y&3Y					1–376
2,2,6-Trimethyl-6-pentadecanol	QX9&&3X		1.450			1–376
7-*n*-Butyl-7-tetradecanol	QX7&6&4		1.440			1–376
3,3,7,11,11-Pentamethyl-7-tridecanol	2X&&3XQ&3X2					1–376
2-*n*-Heptyl-1-undecanol	Q1Y9&7					1–376
$C_{19}H_{40}O$						
1-Nonadecanol	Q19					1–376
2-Nonadecanol	QY17					1–377
4-Nonadecanol	QY3&15					1–377
10-Nonadecanol	QY9&9					1–377
2-Methyl-1-octadecanol	Q1Y16					1–377
16-Methyl-1-octadecanol	Q15Y2					1–377
3-Methyl-3-octadecanol	QX2&&15					1–377
4-Methyl-4-octadecanol	QX3&&14	^{c}.835	^{c}1.456			1–377
5-Methyl-5-octadecanol	QX4&&13	^{c}.833	^{c}1.449			1–377
6-Methyl-6-octadecanol	QX5&&12	^{c}.835	^{c}1.449			1–377
9-Methyl-9-octadecanol	QX9&8	^{c}0.832	^{c}1.449			1–378
9-Ethyl-9-heptadecanol	QX8&8&2					1–378
2,2-Dimethyl-3-*tert*-butyl-3-tridecanol	1X&&XQ10&X	^{c}.866	^{c}1.465			1–378
7-*n*-Hexyl-7-tridecanol	QX6&6&6	^{c}.837	^{c}1.447		^{c}175.	1–378
$C_{20}H_{42}O$						
1-Eicosanol	Q20				^{c}251.	1–378, 1–379, 1–380
2-Eicosanol	QY18					1–379
4-Eicosanol	QY3&16					1–379
5-Eicosanol	QY5&15					1–379
6-Eicosanol	QY5&14					1–380
8-Eicosanol	QY7&12					1–380
10-Eicosanol	QY9&10					1–380
18-Methyl-1-nonadecanol	Q17Y					1–380
2-Methyl-2-nonadecanol	QX17					1–380, 1–381
3-Ethyl-3-octadecanol	QX2&2&15					1–380, 1–381
2,6,11,15-Tetramethyl-8-hexadecanol	1Y&3Y&2YQ1Y&3Y	0.889				1–380
2,2,4,7,10,12,12-Heptamethyl-7-tridecanol	1X&&1Y&2XQ&2Y&1X					1–381
2-*n*-Octyl-1-dodecanol	Q1Y8&10	^{c}0.842	^{c}1.452			1–381
$C_{21}H_{44}O$						
1-Heneicosanol	Q21					1–382
18-Methyl-1-eicosanol	Q17Y3					1–382
$C_{22}H_{46}O$						
1-Docosanol	Q22					1–381, 1–382
20-Methyl-1-heneicosanol	Q19Y					1–383
11-Methyl-11-heneicosanol	QX10&10					1–383
3-Ethyl-3-eicosanol	QX2&2&17					1–381, 1–383

* Based on a single experimental value only.

[c] Extrapolated or interpolated from other temperatures.

TABLE 2a. Selected values of physical properties of aliphatic alcohols and compound index—Continued

Compound Name	Wiswesser Line-Formula Notation[a]	Density at 25 °C g cm^{-3}	Refractive Index, n_D at 25 °C	Boiling Point, °C		Index of Page Numbers
				at 760 mm Hg	at 10 mm Hg	
$C_{22}H_{46}O$						
8-*n*-Heptyl-8-pentadecanol	QX7&7&7					1-383
2-*n*-Nonyl-1-tridecanol	Q1Y9&11					1-383
2,2,10,10-Tetramethyl-6-(4,4-dimethyl-*n*-pentyl)-6-undecanol	1X&&3XQ5&3X					1-383
$C_{23}H_{48}O$						
1-Tricosanol	Q23					1-382, 1-383
20-Methyl-1-docosanol	Q19Y2					1-383
2-*n*-Nonyl-2-tetradecanol	QX9&&12					1-384
3-*n*-Decyl-1-tridecanol	Q2Y10&10					1-384
$C_{24}H_{50}O$						
1-Tetracosanol	Q24					1-382, 1-384
2-Tetracosanol	QY22					1-384
6-Tetracosanol	QY5&18					1-384
22-Methyl-1-tricosanol	Q21Y					1-384
4-*n*-Propyl-4-heneicosanol	QX3&3&17					1-381, 1-385
2-Methyl-4-isobutyl-4-nonadecanol	1Y&1XQ5&1Y	[c] .837	[c] 1.453			1-385
2-*n*-Decyl-1-tetradecanol	Q1Y12&10	[c] .845	[c] 1.457			1-385
$C_{25}H_{52}O$						
1-Pentacosanol	Q25					1-382, 1-385
22-Methyl-1-tetracosanol	Q21Y2					1-385
9-*n*-Octyl-9-heptacosanol	QX8&8&8					1-385
$C_{26}H_{54}O$						
1-Hexacosanol	Q26					1-382—1-385
24-Methyl-1-pentacosanol	Q23Y					1-386
$C_{27}H_{56}O$						
1-Heptacosanol	Q27					1-382, 1-386
24-Methyl-1-hexacosanol	Q23Y2					1-386
$C_{28}H_{58}O$						
1-Octacosanol	Q28					1-382, 1-386
10-*n*-Nonyl-10-nonadecanol	QX9&9&9					1-386
2,2,4,10,12,12-Hexamethyl-7-(3,5,5-trimethyl-1-hexyl)-7-tridecanol	1X&&1Y&23XQ		[c] 1.454			1-386
$C_{29}H_{60}O$						
1-Nonacosanol	Q29					1-382, 1-386
26-Methyl-1-octacosanol	Q25Y2					1-387
6-Pentyl-6-tetracosanol	QX5&5&18					1-387
$C_{30}H_{62}O$						
1-Triacontanol	Q30					1-382, 1-387
$C_{31}H_{64}O$						
1-Hentriacontanol	Q31					1-382, 1-387
16-Hentriacontanol	QY15&15					1-387
28-Methyl-1-triacontanol	Q27Y2					1-387
11-Decyl-11-heneicosanol	QX10&10&10					1-387

[a] Based on a single experimental value only.

[c] Extrapolated or interpolated from other temperatures.

TABLE 2a. Selected values of physical properties of aliphatic alcohols and compound index—Continued

Compound Name	Wiswesser Line-Formula Notation[a]	Density at 25 °C g cm^{-3}	Refractive Index, n_D at 25 °C	Boiling Point, °C		Index of Page Numbers
				at 760 mm Hg	at 10 mm Hg	
$C_{32}H_{66}O$						
1-Dotriacontanol	Q32					1-382, 1-387
$C_{33}H_{68}O$						
1-Tritriacontanol	Q33					1-382, 1-388
17-Tritriacontanol	QY16&16					1-388
$C_{34}H_{70}O$						
1-Tetratriacontanol	Q34					1-382, 1-388
12-Undecyl-12-tricosanol	QX11&11&11					1-388
$C_{35}H_{72}O$						
1-Pentatriacontanol	Q35					1-382, 1-388
18-Pentatriacontanol	QY17&17					1-388
$C_{36}H_{74}O$						
1-Hexatriacontanol	Q36					1-382, 1-388
$C_{37}H_{76}O$						
1-Heptatriacontanol	Q37					1-382, 1-388
13-Dodecyl-13-pentacosanol	Q12&12&12					1-388
$C_{41}H_{84}O$						
1-Hentetracontanol	Q41					1-389
$C_{49}H_{100}O$						
17-Hexadecyl-17-tritriacontanol	Q16&16&16					1-389
$C_{50}H_{102}O$						
1-Pentacontanol	Q50					1-389

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* Based on a single experimental value only.

[c] Extrapolated or interpolated from other temperatures.

TABLE 2b. Summary of selected values of the thermodynamic properties of the well-characterized group of alcohols

Formula	Name	State	Formula Weight	0 K	298.15 K				
				ΔH_f^0	ΔH_f^0	ΔG_f^0	$H_{298}^0—H_0^0$	S^0	C_p^0
					kcal mol^{-1}			cal deg^{-1} mol^{-1}	
CH_4O	Methanol	liq	32.042		−57.13	−39.87		30.41	19.40
		g	32.042	−45.46	−48.06	−38.82	2.73	57.29	10.49
C_2H_6O	Ethanol	liq	46.070		−66.20	−41.63		38.49	26.76
		g	46.070	−51.81	−56.03	−40.13	3.39	67.54	15.64
C_3H_8O	1-Propanol	liq	60.097		−72.66	−40.78		46.5	33.7
		g	60.097	−55.71	−61.28	−38.67	4.32	77.61	20.82
	2-Propanol	liq	60.097		−75.97	−43.09		43.16	36.06
		g	60.097	−59.33	−65.11	−41.44	4.11	74.07	21.21
$C_4H_{10}O$	1-Butanol	liq	74.124		−78.18	−38.84		54.1	42.31
		g	74.124	−58.80	−65.65	−36.04	5.31	86.7	26.29
	2-Butanol	liq	74.124		−81.88	−42.31		53.8	47.5
		g	74.124	−62.96	−69.94	−40.06	5.18	85.8	27.08
	2-Methyl-1-propanol	liq	74.124		−79.85				43.1
		g	74.124		−67.69				26.6
	2-Methyl-2-propanol	c	74.124		−87.45	−44.14		40.77	34.92
		liq	74.124		−85.86	−44.14		46.10	52.61
		g	74.124	−67.43	−74.67	−42.46	4.92	77.98	27.10
$C_5H_{12}O$	1-Pentanol	liq	88.151		−85.0	−38.3		62.0	49.8
		g	88.151	−63.27	−71.4	−34.9	6.30	96.2	31.8
	2-Pentanol	liq	88.151		−87.70				
	3-Pentanol	liq	88.151		−88.5	−40.4		57.4	60.0
		g	88.151		−75.7	−37.8		91.3	
	2-Methyl-1-butanol	liq	88.151		−85.2				52.6
		g	88.151		−72.3				
	3-Methyl-1-butanol	liq	88.151		−85.2				50.3
		g	88.151		−72.2				
	2-Methyl-2-butanol	liq	88.151		−90.7	−41.9		54.8	59.2
		g	88.151		−78.8	−39.5		86.7	
	3-Methyl-2-butanol	liq	88.151		−87.5				55.5
		g	88.151		−75.2				
$C_6H_{14}O$	1-Hexanol	liq	102.178		−90.7	−36.4		69.2	56.6
		g	102.178	−66.5	−75.9	−32.4	7.30	105.5	37.2
$C_7H_{16}O$	1-Heptanol	liq	116.205		−95.8	−34.0		76.5	66.5
		g	116.205	−68.6	−79.3	−28.9	8.29	114.8	42.7
$C_8H_{18}O$	1-Octanol	liq	130.232		−101.6	−34.2		90.2	77.7
		g	130.232	−74.0	−86.0	−28.7	9.28	124.14	48.2

TABLE 2b. Summary of selected values of the thermodynamic properties of the well-characterized group of of alcohols—Continued

Formula	Name	State	Formula Weight	0 K	298.15 K				
				ΔH_f^0	ΔH_f^0	ΔG_f^0	$H^0_{298}-H_0^0$	S^0	C_p^0
					kcal mol^{-1}			cal deg^{-1} mol^{-1}	
$C_9H_{20}O$	1-Nonanol	liq	144.259		−109.2	−32.4		91.3	
		g	144.259	−77.3	−90.6	−26.4	10.27	133.5	53.6
$C_{10}H_{22}O$	1-Decanol	liq	158.286		−114.6	−31.6		102.9	
		g	158.286	−81.5	−96.0	−24.9	11.27	142.8	59.1
$C_{16}H_{34}O$	1-Hexadecanol	c, II	242.45		−163.4	−23.6		108.	104.8
		g	242.45		−122.9	−11.7		204.	

III Discussion and Selection of Physical and Thermodynamic Properties

Methanol

Properties of the Liquid Phase at Various Temperatures

Refractive Index

The Index to the Bibliography for methanol on page 1-53 identifies a total of 72 references to the refractive index. Those references specifically considered in choosing the selected values in tables 3 and 5 are underlined. Some reported values of n_D at 20 and 25 °C are given in table 6. The most accurate measurements of n_D have been made by Reisler and Eisenberg [1965], who used a Rayleigh interference refractometer throughout the range from 10 to 25 °C. Although their samples were degassed, little direct information was given to establish their purity. They also found that the piezo-optic coefficient, $(\partial n/\partial P)_T$, is 40.56×10^{-6} atm^{-1} for methanol at 22.8 °C. Wood, Langer, and Battino [1960] have also made accurate measurements at 25 °C and various wavelengths from 6563.1 to 4046.9 Å. Their value at the sodium D-line agrees exactly with that of Reisler and Eisenberg but is appreciably lower than most of the other values reported in table 6. However, the data of Reisler and Eisenberg have been selected for the 10 to 35 °C range.

Measurements at wavelengths other than the sodium D-line have been reported by Dale and Gladstone [1863], Gladstone [1884], Jahn [1891], Landolt and Jahn [1892], Brühl and Schröder [1904], Eykman [1919], Timmermans and Hennaut-Roland [1930], Pesce [1940], Vogel [1948], and Wood, Langer, and Battino [1960]. The selected smoothed values in table 5 were taken from plots of refractive index against $1/(\lambda-1000)^{1.6}$. The data of Wood, Langer, and Battino were weighted heavily in this selection. The uncertainties of the values in this table are estimated to be in the range of 0.0002 to 0.0005. Everett and Munn [1963] have determined the refractive index of methanol in the vapor phase.

Density

A complete identification of sources of density data is shown in the Index on page 1-53, and a portion of these observed values is given in table 6. The final selected values of the density at various temperatures are shown in tables 3 and 6. They were calculated from the Francis equation, equation (1) with the constants shown in table 3. The sources of density data used in the least squares calculations of the constants are underlined in the Index. The observed data could not be fit satisfactorily to a single set of constants over the entire temperature range from −20 to +180 °C. Therefore two sets of constants covering the range from −20 to +50 °C and from 40 to 180 °C, respectively, were calculated. Data from 40 to 50 °C were included in both sets. The standard deviations of the calculated from the observed values are 0.000031 g cm^{-3} for the low temperature set and 0.000337 g cm^{-3} for the high temperature set. The selected values in table 3 from −20 to +40 °C and from 60 to 120 °C were calculated from the corresponding sets of Francis constants. At 50 °C the densities calculated by the two sets of equations differs by 0.00077 g cm^{-3}. An average value is given for this temperature in table 3. Yamamoto and Kunimoto [1958] have made accurate measurements at 10, 15, and 20 °C. After converting their data to units of g cm^{-3}, the maximum deviation from the ones calculated from the selected Francis constants occurs at 15 °C, where their observed density is 0.00018 g cm^{-3} below the calculated one. In general the scatter of the density data for methanol from a smooth function of temperature is somewhat greater than for the other lower alcohols. The uncertainty in the selected densities is estimated to be 0.0001 g cm^{-3} in the range from 0 to 30 °C, and 0.0002 to 0.0004 g cm^{-3} outside this range.

Vapor Pressure and Boiling Points

As shown by the Index on page 1-53, the literature is very extensive. The vapor pressure data of Dever, Finch, and Grunwald [1955] represent accurate measurements made in recent years. However, they agree quite well with the older measurements of Ramsay and Young [1887]. Vapor pressure data from 10 to 1500 mmHg have been represented by the Antoine equation, equation (2), with the constants listed in table 3. These were calculated using a nonlinear least squares procedure, described in appendix B, from the data identified by the underlined references in the Index, along with calorimetric heats of vaporization and vapor phase volumes calculated from equations of state. Two separate sets of Antoine constants were evaluated for the low temperature data, −14 to +65 °C, and the high temperature data, 64 to 110 °C. These two sets of constants generate essentially the same vapor pressure values in the range from 60 to 85 °C.

The best values of the normal boiling point are summarized in table 6. Most of these fall within a range of temperature of about 0.2 °C. The selected boiling point, as calculated from the Antoine equation, lies in the upper end of this range. The discrepancies in the observed data are rather large, considering the importance of this compound. The estimated uncertainty of 0.03 °C of the selected boiling point was based on the overall fit of the Antoine constants to the vapor pressure data. Mündel [1913] and Miller, G. A. [1964] have measured the vapor pressure at low temperatures. Those of Miller go down to the triple point. Ramsay and Young [1887], Young, S. [1910], and Kay and Donham [1955] have reported vapor pressure data at temperatures up to the critical point.

Critical Properties

Critical Temperature

The value reported by Kay and Donham [1955] was selected. Critical temperatures reported by Young [1910], Salzwedel [1930], and Fischer and Reichel [1943] are higher than that of Kay and Donham but are within about one degree of their value. The value reported by Ross is about 1.5 degrees lower. Kay and Donham used carefully purified methanol and derived the critical constants from measurements of pressure-volume-temperature data. See table 6 for summary of reported values.

Critical Pressure

Kay and Donham's value was again selected. It is close to the measurement of Nadezhdin [1882] and about 1.5 atm higher than the value of Young. Salzewdel obtained a much higher value.

Critical Density

Kay and Donham's value was selected. It agrees well with the value of Centnerszwer and Young, but differs considerably from that of Salzwedel.

Solid-Solid Phase Equilibria

Transition Temperature

Solid methanol exists in at least two crystalline forms; crystal II is orthorhombic, and crystal I is monoclinic. The transition temperature reported by Carlson [1962] was selected. This is very close to the measurement of Kelley. Both of these values were obtained in the process of measuring specific heats in a calorimeter. Davidson [1957] detected this transition at −113.2 °C from a measurement of dielectric constant and also possibly another transition around −118 °C. Westrum [1962] gives a brief description of the transition at −113.2 °C and has described some of the difficulties in measuring the properties of the monoclinic modification.

Murti [1959] finds that there are two methanol molecules in the unit cell of the monoclinic crystal and gives the following dimensions: $a=4.59$ Å; $b=4.68$ Å; $c=4.92$ Å; and $\mathrm{B}=97°30'$. Falk and Whalley [1961] discuss further the crystal structures of the two forms and interpret the infrared spectra in terms of the lattice vibrational modes.

Heat Capacity of Solid Phases (c, I and II)

The data of Carlson (1962) were used.

Heat of Transition

Four values have been reported in the literature. The value of Carlson [1962] was selected. The accurate measurement of this property requires a sample of very high purity.

Solid-Liquid Phase Equilibria

Normal Melting Point

The value reported by Roper [1938] was selected. Most of the other values in the literature lie within about a two degree range.

Triple Point

The value of Carlson [1962] was selected. Stavely and Gupta [1949] report a value which is 0.22 °C lower. Both these values were obtained from a melting curve in an adiabatic calorimeter. The vapor pressure at the triple point was calculated from the data of Miller, G. A. [1964].

Heat Capacity of Solid Phase (c, I) at the Melting Point

The data of Carlson [1962] were used.

Heat Capacity of the Liquid at the Melting Point

The value was taken from a smooth curve through the data of Carlson [1962], Stavely and Gupta [1949] and Eucken [1948]. Greatest weight was given to the data of Carlson.

Heat of Fusion

The value reported by Carlson [1962], corrected to a temperature of −97.68 °C, was adopted.

Heat of Vaporization at the Triple Point

The selected value was calculated from the heat of vaporization at 25°, and the heat capacity of the liquid and gaseous phases between 25 and −97.56 °C. Applying the Clausius-Clapeyron equation to the vapor pressures reported by Miller gives a heat of vaporization of 10.8 kcal mol^{-1}.

Properties of the Liquid at 25 °C

Absolute Entropy

Four sets of heat capacity measurements, suitable for calculation of the absolute entropy of the liquid at 25 °C through use of the third law, have been reported in the literature. The measurements of Parks [1925] extend only down to 88.7 K. His extrapolation below this temperature was revised by Parks, Kelley, and Huffman [1929], but

TABLE 3. Methanol. Selected values, physical and thermodynamic properties

Temp. °C	Refractive Index, n_D	Density g cm^{-3}	Vapor Pressure, mmHg
−20		0.8287	
−15.42			10
−15			10.3
−10		.8194	14.8
− 5			20.9
0	1.3361	.8100	29.1
+ 5			40.0
10	1.33224	.8007	54.1
15	1.33034		72.3
20	1.32840	.79131	95.6
20.81			100
25	1.32652	.78664	125.4
30	1.32457	.78196	161.8
34.26			200
35	1.32264		207.3
40	1.3207	.7726	263.2
45	1.3189		331.3
49.23			400
50	1.3169	.7633	413.5
55			512.2
60		.7546	629.8
64.70			760
65			768.8
70		.7448	932.4
75			1123.6
80		.7347	1346.
90		.7242	
100		.7132	
110		.7016	
120		.6894	

Data For Phase Transitions

Initial	Final	Temp. °C	dt/dP deg mm^{-1}	Pressure mmHg	ΔH kcal mol^{-1}	$d\Delta H/dt$	ΔS cal deg^{-1} mol^{-1}	ΔC_p cal deg^{-1} mol^{-1}
c,II	c,I	−115.8±0.1			0.152±0.001	−2.0±1	0.966±0.005	−3.0±1
c,I	liq	−97.68±0.04		760	0.768±0.001	9.5±0.1	4.377±0.005	5.2±0.1
c,I	liq	−97.56±0.02		$(1.137\pm0.05)10^{-3}$				
liq	g	−97.56±0.02		$(1.137\pm0.05)10^{-3}$	10.03±0.05		57.1±0.2	
liq	g	25	0.1516	125.45±0.1	8.94±0.03	−11.2±0.5	30.0±0.1	−2.5±2
liq	g	64.70±0.05	.03347	760	8.24±0.01	−15.3±0.5	24.92±0.03	13.5±1

Condensed Phase Heat Capacity

State		Temp. °C	C_p cal deg^{-1} mol^{-1}
c,I		−97.56	11.77±0.1
liq		−97.56	16.92±0.05
liq		64.70	21.5±0.1

Properties of the Saturated Real Gas

Temp. °C	H^r-H^0 kcal mol^{-1}	S^r-S^0 cal deg^{-1} mol^{-1}	$C_p^r-C_p^0$ cal deg^{-1} mol^{-1}
25	−0.13±0.03	−0.46±0.05	6.5±2
64.70	−.29±0.02	−.80±0.05	24.0±1

Data for the Standard States at 25 °C

State	Heat of Combustion ΔH_c^0 kcal mol^{-1}	Heat of Formation ΔH_f^0 kcal mol^{-1}	Entropy S^0 cal deg^{-1} mol^{-1}	Gibbs Energy of Formation ΔG_f^0 kcal mol^{-1}	Heat Capacity, C_p cal deg^{-1} mol^{-1}
liq	−173.55±0.1	−57.13±0.1	30.41±0.05	−39.87±0.1	19.40±0.01
g	−182.62±0.1	−48.06±0.1	57.29±0.05	−38.82±0.1	10.49±0.03

Critical Constants

Temp. 239.43 °C, 512.58 K	Pressure 79.9 atm,	Density 0.272 g cm^{-3}

			Constants in Vapor Pressure and Density Equation								
			Antoine Equation				Francis Equation				
			Temp. Range	*A*	*B*	*C*	Temp. Range	*A*	$B \times 10^3$	*C*	*E*
			−14–65 °C	7.89750	1474.08	229.13	−20–50 °C	0.84638	0.9321	423.28	11641.
			64–110 °C	7.97328	1515.14	232.85	40–180 °C	.86867	.6111	17.267	283.08

TABLE 4. Methanol. Selected values, thermodynamic functions of the ideal gas at one atmosphere

Temperature K	Entropy S^0 cal deg^{-1} mol^{-1}	Heat Capacity C_p^0 cal deg^{-1} mol^{-1}	Enthalpy Function $(H^0-H^0_0)/T$ cal deg^{-1} mol^{-1}	Gibbs Energy Function $(G^0-H^0_0)/T$ cal deg^{-1} mol^{-1}	Heat of Formation ΔHf^0 kcal mol^{-1}	Gibbs Energy of Formation ΔGf^0 kcal mol^{-1}
0	0	0	0	0	−45.46	−45.46
273.15	56.39	10.15	9.05	−47.33	−47.84	−39.58
298.15	57.29	10.49	9.16	−48.13	−48.06	−38.82
300	57.36	10.52	9.17	−48.19	−48.08	−38.76
400	60.61	12.29	9.71	−50.90	−48.93	−38.52
500	63.51	14.22	10.42	−53.14	−49.69	−32.08
600	66.32	16.02	11.21	−55.11	−50.33	−28.50
700	68.91	17.62	12.01	−56.90	−50.86	−24.82
800	71.36	19.04	12.81	−58.55	−51.29	−21.06
900	73.67	20.29	13.56	−60.11	−51.65	− 17.26
1000	75.87	21.38	14.30	−61.58	−51.91	−13.43

TABLE 5. Methanol. Selected values, refractive index at various temperatures and wavelengths

Symbol	Wavelength, Å	15 °C	20 °C	25 °C	30 °C
He_{red}	6678.1	1.3298	1.3273	1.3248	1.3231
H_c	6562.8	1.3290	1.3274	1.3250	1.3233
Na_D	5892.6	1.33034	1.32840	1.32652	1.32457
Hg_e	5460.7	1.33211	1.32981	1.32792	1.32597
He_{blue}	5015.7	1.3337	1.3316	1.3291	1.3278
H_F	4861.3	1.3344	1.3323	1.3303	1.3285
Hg_g	4358.3	1.3375	1.3356	1.3333	1.3315
$H_{G'}$	4340.5	1.3379	1.3361	1.3337	1.3318
	4046.9			1.3361	

the entropy based on these measurements is uncertain because of the required long extrapolation to 0 K. The low temperature limits of measurement of the other investigations are: Kelley [1929], 16.5 K; Ahlberg, Blanchard and Lundberg [1937], 3.68 K; and Carlson [1962], 4.9 K. The recent measurements of Carlson were carried out at the thermochemistry laboratory of Dr. Westrum at the University of Michigan and furnished the most reliable data. His value, after slight adjustment to achieve internal consistency, was selected.

Heat of Combustion

Eight values of the heat of combustion of methanol have been reported. For two of these, Thomsen [1886] and Rossini [1932], the methanol was burned in a gas flow calorimeter. The data shown in table 12 have been converted to correspond to the liquid. All of the values in this table have been corrected to current energy units and molecular weights. In the measurements of Rossini [1932] and of Chao and Rossini [1965], the quantity of sample burned was based on the mass of carbon dioxide produced, while the mass of the methanol was used in all of the others. The following procedure was used in converting the published values to the new molecular weight. If the quantity of material was based on the mass of the sample, the heat of combustion, in calories per gram, was multiplied by the new molecular weight. If it was based on the mass of carbon dioxide, the heat of combustion, in calories per mole, was multiplied by the ratio of the new molecular weight of carbon dioxide (44.00995) to the molecular weight of carbon dioxide used in the original publication.

The two most reliable values are those of Rossini [1932] and of Chao and Rossini [1965]. Rossini found the heat of combustion of gaseous methanol to be -182.596 kcal mol^{-1} in a flame calorimeter. He burned a mixture of methanol vapor saturated at 23 °C and air at a total pressure of one atmosphere. The change in enthalpy on converting this result to pure methanol gas at a pressure of 125.5 mmHg, the vapor pressure of the liquid at 25 °C, is 0.0098 kcal mol^{-1}. The heat of vaporization was taken to be 8.94 kcal mol^{-1} in calculating the value shown in table 12. This differs from the result of Chao and Rossini [1965], who burned the liquid directly, by 0.2 kcal mol^{-1}. This is greater than the estimated uncertainty in either measurement. In both sets of measurements, the amount of sample burned was determined by the amount of carbon dioxide produced. Since there did not appear to be any way of deciding between these two results at this time, an average value was selected.

Properties of the Real Gas

Equation of State

Gaseous methanol, as well as the other alcohols, shows appreciable deviation from the ideal gas. Equations of state of gaseous alcohols have been derived from measurements of pressure, volume, and temperature of the gas and from measurements of the vapor heat capacity as a function of temperature and pressure. There are numerous experimental difficulties involved in the measurement of these properties with sufficient accuracy to identify the nature of the intermolecular interactions responsible for the nonideal behavior. For this purpose accurate data at pressures below 1 atm are required. Ramsay and Young [1887] have reported values of molar volume of the saturated vapor of methanol from 0 °C to the critical temperature. However, these are not adequate by themselves to establish an equation of state. Lashakov [1939] has reported values of the molar volume in the temperature range of 170 to 290 °C and the pressure range of 10 to 95 atm. These do not extend into the low pressure region. Ingle and Cady [1938] calculated apparent molecular weights from experimental vapor density in the vicinity of the normal boiling point. They indicate some degree of association in the vapor state.

Properties of gaseous alcohols in the low pressure range have usually been reported in terms of the virial equation of state in the form[2]

$$PV=RT+B_p'P+C_p'P^2+D_p'P^3+\ldots$$

Lambert, Roberts, Rowlinson, and Wilkinson [1949] reported values of the second virial coefficient, B_p', derived from P-V-T data but did not report their experimental data directly. They ascribed these results to the existence of an equilibrium between monomers and dimers in the gas phase. They show that if there is only a small amount of association, the gaseous mixture should follow the virial equation of state, with a second virial coefficient only, and that,

$$B_p'=B_{p0}'-RTK_2$$

where B_{p0}' is the effective second virial coefficient for the monomers alone, and K_2 is the equilibrium constant for the association reaction.

$$K_2=\frac{P_{\text{dimer}}}{(P_{\text{monomer}})^2}.$$

They also report values of K_2 over the temperature range of 322 to 410 K. A plot of log K_2 versus $1/T$ gives a heat of association which varies from -3200 to -7300 cal mol^{-1} over this range. Rowlinson [1949] calculated the parameters in the Stockmayer potential which fits their values of B_p'.

Weltner and Pitzer [1951] related the available properties of gaseous methanol to the virial equation in the form,

$$PV=RT+B_p'P+JP^n.$$

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[2] See Appendix C for a discussion of various forms of the virial equation and for relations among the virial coefficients.

TABLE 6. Reported values. Simple physical properties

Investigators	Vapor Pressures and Boiling Points		Freezing Point	Density, d g cm^{-3}		Refractive Index, n_D	
	°C	mmHg	t_m, °C	20 °C	25 °C	20 °C	25 °C
Methanol, CH_4O, mol wt. 32.042, state at 25 °C liq							
Ramsay and Young [1887b]	64.7	760		0.7905	0.7872		
Loomis [1900]				.79133			
Young and Fortey [1902]	64.70	760					
Crismer [1904]				.79141			
Klason and Norlin [1906]				.79134			
Doroshevskii [1909]	64.53	760					
Doroshevskii and Polyanskii [1910a]	64.57	760					
Timmermans [1910]	64.70	760		.79151	.78697		
Dawson [1910]				.79734			
Young [1910]	64.7	760		.79203			
Timmermans [1911]	64.7	760	−97.05				
Atkins and Wallace [1913]	64.65	760					
Tyrer [1914]	64.72	760					
Hartung [1917]	65.28–65.37	760			.78740		
Jaeger [1917]	65.8–66.1	760		.793			
Barr and Bircumshaw [1921]	64.5	760			.78658		
McKelvey and Simpson [1922]			−97.7		.78658		
Keyes, Townshend, and Young [1922]			−98.53				
Willard and Smith [1923]	64.89–65.09	760			.7872		
Hartley and Raikes [1925]					.78641		
Norris and Ashdown [1925]	64.7–64.8	760			.78866		
Parks [1925]			−97.7	.7985			
Perrakis [1925]			−94.0				
Ewart and Raikes [1926]					.78641		
Mathews [1926]	64.65–64.70	760		.7917		1.32863	
Kelley [1929b]			−97.94		.78675		
Rakovskii and Frost [1930]	64.37	760		.79128	.78654	1.3286	
Timmermans and Hennaut-Roland [1930]	64.65	760	−97.0				
Fiock, Ginnings and Holton [1931]				.79133			
Lund and Bjerrum [1931]					.78651		
Butler, Thomson, and Maclennan [1933]	64.46	760			.78643		
Vosburgh, Connell, and Butler [1933]					.78652		
Washburn and Spencer [1934]					.78673		1.32660
de Brouchere and Gillet [1935]	64.62	760					
Gibson [1935]					.78655		
Keffler and Maclean [1935]	64.73–64.78	760					
Wojciechowski [1936]	64.509	760					
Tomonari [1936]				.7913		1.32911	
Betts and Hammett [1937]					0.78668		
Stark and Gilbert [1937]					.78664		
Jones and Fornwalt [1938]			−97.68		.78652		
Roper [1938]			−97.68				
Pesce [1940]					.78662		1.3263
Washburn, Graham, Arnold, and Transue [1940]					.7866		1.32659
Briscoe and Rinehart [1942]	64.75	760			.7866		
Eckfeldt and Lucasse [1943]					.78654		
Pesce and Lago [1944]					.78664		1.32650
Dulitskaya [1945]	64.68	760					
Kretschmer, Nowakowska, and Wiebe [1946]	64.50	760			.78650		
Scatchard, Wood, and Mochel [1946]	64.51	760			.78654		
Vogel [1948]	64.7	760		0.7924		1.32855	
Griswold and Buford [1949]	64.70	760			.7870		1.32657
McKenna, Tartar, and Lingafelter [1949]	64.60	760	−98.02				
Tschamler, Richter, and Wettig [1949b]			−97.5		.7846		
Carr and Riddick [1951]					.7879		

Table 6—Continued

Investigators		Vapor Pressures and Boiling Points		Freezing Point	Density, d g cm^{-3}		Refractive Index, n_D	
		°C	mmHg	t_m, °C	20 °C	25 °C	20 °C	25 C°
Methanol, CH_4O, mol wt. 32.042, state at 25 °C liq								
Scatchard and Ticknor	[1952]	64.509	760			.78653		1.3267
Staveley and Spice	[1952]	64.59	760		.7914			
Corcoran, Kruse, and Skolnik	[1953]			−98.2				
Amer, Paxton, and Van Winkle	[1953]	64.6	760			.7865	1.32904	
McKenna, Tartar, and Lingafelter	[1953]	64.6	760			.78660		1.32777
Griffiths	[1954]	64.73	760			.78654		
Kretschmer and Wiebe	[1954]					.78653		
Sadek and Fuoss	[1954]					.7864		1.3266
Denney and Cole	[1955]					.78665		
Dever, Finch, and Grunwald	[1955]	64.7	760					1.3267
Ling and Van Winkle	[1958]	64.75	760				1.32895	1.32707
Yamamoto and Kunimoto	[1958]				.79134			
Wood, Langer, and Battine	[1960]							1.32652
Mikhail and Kimel	[1961]					.7869		
Brown and Smith	[1962b]	64.54	760			.78683		1.32662
Paraskevopoulos and Missen	[1962]	64.57	760			.78653		
Reisler and Eisenberg	[1965]						1.32840	1.32652
Selected value	[1967]	64.70 ±0.03 −15.42 ±0.05	760 10	−97.68 ±0.04	.79131 ±.0001	.78664 ±.0001	1.32840 ±0.0001	1.32652 ±0.0001

Antoine constants: A 7.89750, B 1474.08, C 229.13

dt/dp at 760 mmHg, 0.03347 °C/mmHg

They first evaluated B_p' from the P-V-T data of Eucken and Meyer [1929], and by assuming that the vapor consisted of an equilibrium mixture of monomers and dimers only, calculated K_2 *in a manner similar to that* of Lambert et al. They then determined the values of the exponent, n, and the constant, J, which best fit the vapor phase heat capacity measured by them and by DeVries and Collins [1941]. Experimental data covered the temperature range of about 345 to 520 K. They found that the value $n=3$ gave the best fit, and thus J corresponds to the fourth virial coefficient, D_p'. This is related to the equilibrium constant for the formation of tetramers from monomers by

$$D_p' = -3RTK_4.$$

Their equilibrium constants are equivalent to $1/K_2$ and $1/K_4$, as defined above. They concluded, therefore, that methanol vapor consisted only of the monomer, dimer, and tetramer, and that trimers are not present. Assuming that the change in heat capacity for polymerization is zero, they also calculated the heats and entropies for the formation of dimers and tetramers from the monomers. Their final equation of state is,

$$PV = RT + [80 - 0.0206T \exp(3220/RT)]P$$
$$-[4.36\times10^{-16}T \exp(24200/RT)]P^3$$

in which the volume is in cubic centimeters and pressure is in atmospheres.

Based on P-V-T measurements from 40 to 120 °C, Kretschmer and Wiebe [1954] published the equation of state,

$$PV = RT - [100 + 2.148 \exp(1986/T)]P$$
$$-[8.34\times10^{-14} \exp(10750/T)]P^3$$

Since that time a number of investigators have expressed experimental measurements on several of the lower alcohols in terms of a virial equation of state containing only the terms $B_p'P$ and $D_p'P^3$, and this has been cited as evidence that there are no trimers in the vapor state of these alcohols.

TABLE 7. Methanol. Reported values. Critical properties

Investigator	t_c, °C	P_c, atm	d_c g cm^{-3}
Ramsay and Young [1887]	240.	78.55	0.2715
Young, S. [1910]	240.	78.50	.2722
Salzwedel [1930]	240.	99.	
Fischer and Reichel [1943]	240.6		
Ross, H. K. [1954]	238.		
Kay and Donham [1955]	239.43	79.9	.272
Efremov [1966]	240.	78.7	.272

Foz Gazulla, Morcillo, Masia, and Mendes [1954] have reported results of P-V-T measurements and have calculated values of the second virial coefficient. Recent investigations of gaseous methanol have been made by Bottomly and Spurling [1968] and by Kudchadker [1968]. The measurements of Kudchadker cover a wide range of temperature and pressure. A comparison of the results of these various investigations is shown in table 13. For purposes of more ready comparison, the published data have been converted to the virial coefficients, B_p', C_p', and D_p' (See appendix C for definitions). In order to compare the corresponding properties of methanol directly, values of $(1-Z)100$, where $Z=PV/RT$, have been calculated from the various sets of virial coefficients at various temperatures and pressures. Values in parenthesis have been extrapolated outside the experimental range of temperature or pressure. Kudchadker [1968] has made the only measurements which extend down to 25 °C. However, the uncertainty of correcting for the effect of adsorption of the vapor on the walls of the vessel throws some doubt on the validity of the low temperature data.

Woolley [1953] derived a virial equation of state for a gaseous equilibrium mixture of monomers, dimers, trimers, tetramers, etc., assuming that each species behaved as an ideal gas. He gave general relationships between the virial coefficients and the equilibrium constants for association. For example,

$$B_p=B_p'/RT=-K_2$$

$$C_p=C_p'/RT=3K_2^2-2K_3$$

$$D_p=D_p'/RT=-10K_2^3+12K_2K_3-3K_4.$$

Table 8. Methanol. Reported values. Condensed phase transitions

Investigator	Transition, c, II→c, I		Fusion		
	t_t, °C	ΔH_t	t_{tp}, °C	t_m, °C	ΔH_m
Keyes, Townshend, and Young [1922]				−98.54	
Parks [1925]	−112.1	0.141		−97.9	0.759
Kelley [1929]	−115.8	.1543	−97.94		.756
Timmermans and Hennaut-Roland [1930]				−97.0	
Roper [1938]				−97.68	
McKenna, Tartar, and Lingafelter [1949]				−98.02	
Staveley and Gupta [1949]	−115.4	.170	−97.79		.7552
Davidson [1957]	−113.6				
Carlson [1962]	−115.81	.1520	−97.56		.7685

Although the assumption that there are no trimers in the gas phase of methanol or other alcohols has been frequently made, it must be considered as questionable at this time. In spite of the numerous experimental studies, the P-V-T and vapor heat capacity data are still not sufficiently accurate over a sufficiently wide range to establish reliably the values of any of the virial coefficients beyond the second. Even if C_p' can be shown to be zero, the equations of Woolley show that $K_3=\frac{3}{2}K_2^2$ rather than zero. Irrespective of the effect of association, the monomeric form of the alcohols, as well as the polymeric species, would be expected to show appreciable nonideal character as the result of the usual dispersion forces and dipole-dipole interactions between molecules. No rigorous calculations which allow for the nonideality of the various polymeric species have yet been carried out. Some further discussion of association in alcohols is given in appendix A.

Heat Capacity

References to measurements of the heat capacity of methanol in the gas phase will be found in the Index. The effect of pressure on the heat capacity of a gas is related to the equation of state through familiar thermodynamic formulae, and these data have been used in evaluating the constants in the equation of state of methanol. At pressures greater than the micron range, heat capacities have been obtained by the use of a gas flow calorimeter. De Vries and Collins [1941] have made such measurements at a pressure of 750 mmHg in the range from 76.5 to 169.5 °C. They found a minimum in the vicinity of 125 °C and explained it as due to association in the vapor state. As of the present, all experimental measurements have been made at pressures below the saturated vapor pressure at any given temperature. The heat capacity of methanol gas is strongly dependent on pressure in the vicinity of the saturated vapor pressure. This is illustrated by the following results obtained by Weltner and Pitzer (1951), at 72.4 °C:

		pressure, mmHg		
0	260	500	755	
		$C_p(g)$, methanol		
11.46	12.18	14.72	21.03	cal deg^{-1} mol^{-1}.

The extrapolation of these and similar data to the equilibrium vapor pressure is quite uncertain, even when done on the basis of an equation of state which has been fitted to experimental data.

Corrections to the Ideal Gas State

The differences between the enthalpy, entropy, and heat capacity of the real gas and ideal gas at 25 °C and at 64.51 °C, the normal boiling point, are shown in table 14. The selected values were based largely on the two equations of state listed. Since the original data used to develop these equations did not extend down to 25 °C, these equations cannot be considered to be very reliable at this temperature. The agreement between the values calculated from the two equations of state is poor at 25 °C.

Vapor-Liquid Equilibrium at 25 °C

Vapor Pressure

Since the vapor pressure at 25 °C is in the range of pressures used in evaluating the Antoine constants, it was calculated from the Antoine equation.

Heat of Vaporization

The only reliable calorimetric measurements at 25 °C are those of McCurdy and Laidler [1963] and Wadso [1966]. The difference between them, as shown in table 9, is somewhat larger than the estimated uncertainties in the individual measurements, but not unexpectedly large for data of this type obtained by quite different kinds of calorimeters. The heat of vaporization calculated from the selected Antoine constants and the equation of state of Weltner and Pitzer is also listed in table 9. The selected value was from the work of Wadso, with minor adjustments for internal consistency.

Temperature Derivative of the Heat of Vaporization

$d\Delta H_v/dT$ was calculated from ΔC_p, (the change in heat capacity on vaporization), the equations of state listed previously, and the Antoine constants.

TABLE 9. Methanol. Reported values. Heats of vaporization

Investigator	ΔH_v at 25 °C	ΔH_v at t_b	Method and Remarks
Ramsay and Young [1887]	9.042	8.525	Calculated from vapor pressure.
Brown, J. C. (s) [1903]		8.446	Calorimetric.
Mathews [1926]		8.426	Calorimetric.
Bartoszewiczowna [1931]	9.13		Calorimetric, corrected to 25 °C.
Fiock, Ginnings, and Holtan [1931]	8.949	8.431	Calorimetric, extrapolated by equation to 25 °C.
Bennewitz and Rossner [1938]		8.420	Calorimetric.
Staveley and Gupta [1949]	8.88		Calorimetric, corrected to 25 °C.
Weltner and Pitzer [1951]		8.44	Calorimetric.
Plewes, Jardine and Butler [1954]		8.462	Calorimetric.
Green [1960]	8.94		Calculated from published vapor pressure.
McCurdy and Laidler [1963]	9.010		Calorimetric.
Wadso [1966]	8.911		Calorimetric.
Selected Antoine Constants	9.08	8.454	

TABLE 10. Methanol. Reported values. Heat capacity and entropy of the liquid at 25 °C

Investigator	C_p^0(l)	Remarks	S^0(l), Third Law
Bose and Müller [1907]	19.5	From equation	
Parks [1925]	19.6	Extrapolated	
Parks, Kelley and Huffman [1929]			31.0 (revision of Parks)
Kelley [1929]	19.5	Extrapolated	30.3
Ahlberg, Blanchard and Lundberg [1937]			30.3
Fiock, Ginnings, and Holtan [1931]	19.15	Extrapolated by Equation	
Eucken [1948]	19.2		
Hough, Mason and Sage [1950]	18.7	Extrapolated	
Carlson [1962]	19.40		30.40

Vapor-Liquid Equilibrium at the Normal Boiling Point

Normal Boiling Point

This was calculated from the selected Antoine constants.

Heat of Vaporization

Values of Fiock, Ginnings, and Holtan [1931] and Bennewitz and Rossner [1938] were considered principally. The value selected was based on internal consistency.

Heat Capacity of the Liquid

This was calculated from the equation of Fiock, Ginnings, and Holtan [1931].

Properties of the Ideal Gas State

Molecular Parameters

Numerous studies of the molecular properties of methanol, in the gas, liquid, and liquid solution phases have been made. These include infrared, Raman, microwave, and nuclear magnetic resonance spectra. A partial list of references to information on fundamental vibration frequencies may be found in the index, and table 16 shows a selection of reported values of frequencies, other than torsional motion of the $-OH$ group with respect to the $-CH_3$ group. Some references to association may be found in appendix A. Measurement of spectra in the far infrared and microwave region permits calculation of moments of inertia which can be used to derive bond distances and angles in the molecule. This information is also included in many of the publications referred to in the Index. The publication of Zerbi, Overend, and

Crawford [1963] is an example of a recent vibrational analysis in which Urey-Bradley force constants are assigned. Kimura and Kubo [1959] have calculated molecular geometry from measurements of electron diffraction of the gas. In the spectroscopic studies, considerable attention has been paid to the study of the effect of hydrogen bonding on the O—H vibrational frequency. Whalley and Falk [1961] compare the intermolecular potential of CH_3OH with that of CH_3OD in the crystal and find that the potential for the deuterium is larger by about 2000 cal per mole. Their calculations are based on heat capacity and infrared spectra of the crystalline phases.

TABLE 11. Methanol. Reported values. Heat capacity and entropy of the ideal gas at 25 °C

Investigator	$C_p^0(g)$	Method	$S^0(g)$ from molecular parameters
Halford [1934]			57.6
Smith, J. M. [1948]	10.80	Molecular parameters.	56.7
Eucken and Franck [1948]	10.6	Extrap. exp. meas.	
Halford [1950]			57.14
Weltner and Pitzer [1951]	10.8	Extrap. exp. meas.	57.21
Barrow [1952]			57.58
Ivash, Pitzer and Li [1955]	10.5	Molecular parameters.	57.29
Halford and Miller [1957]	10.1 (at 6 °C)	From thermal cond.	

TABLE 12. Methanol. Reported values. Heat of combustion of the liquid at 25 °C

Investigator	$-\Delta H_c^0(l)$, kcal mole^{-1}
Thomsen [1886]	*173.4
Stohman, Kleber and Langbein [1889]	170.4
Richards and Davis [1920]	170.8
Roth [1926]	171.9
Roth and Muller [1927]	171.8
Roth and Banse [1931]	173.9
Rossini [1932]	*173.65
Chao and Rossini [1965]	173.45

* ΔH_c of gas measured. Value corrected to the liquid.

The torsional motion of the $-OH$ group on methanol may be considered approximately either as a hindered internal rotation or as a torsional vibration with considerable anharmonic character. The potential barrier for this internal rotation may, in principle, be derived from an analysis of the microwave spectrum, by comparison of the entropy of the ideal gas based on the third law with the entropy calculated from statistical thermodynamics, or by a similar comparison of experimental and calculated heat capacities of the ideal gas. The use of microwave spectra involves many difficulties of measurement and interpretation. The use of entropy or heat capacity rests upon a relatively small difference between two quantities. Calorimetric entropy and heat capacity included the usual experimental uncertainties, which are particularly great for methanol. Calculation of entropy or heat capacity from statistical thermodynamics requires an accurate knowledge of vibrational frequencies and molecular geometry. All of these difficulties have resulted in confusion and in poor agreement among values of the potential barrier reported by different investigators. Table 17 summarizes most of the values which have been published. A reduced moment of 1.009×10^{-40} g cm^2 was used to convert torsional frequency to potential energy.

Entropy at 25 °C

The principal difficulty encountered in calculating the thermodynamic properties of methanol in the ideal gas state by the methods of statistical mechanics is due to the internal rotation (or torsional frequency). Not only is the potential barrier difficult to determine, but it exerts a comparatively large effect on the thermodynamic properties. Furthermore, the moment of inertia of the $-OH$ group about the C—O axis is so small that it falls outside the range of the tables of Pitzer and Gwinn [1942] for the calculation of the contribution of internal rotation to the partition function. A special theory has been developed by Koehler and Dennison [1940], Burkhard and Dennison [1951], Ivash and Dennison [1953], Halford [1950a, c] and Ivash, Li, and Pitzer [1955] to compute the rotational energy levels and their contribution of the partition function. The selected value was obtained by applying a correction of -0.0025 cal deg^{-1} mol^{-1} to the value calculated by Ivash, Li, and Pitzer. The correction was applied to convert their value to the current values of the fundamental constants.

Heat Capacity at 25 °C

The selected value is from the calculations of Ivash, Li, and Pitzer [1955]. Other values, both experimental and calculated, are shown in table II.

Thermodynamic Functions

These were all taken from Ivash, Li, and Pitzer [1955], which was also the source of the tables published by Green [1961]. The values of $\Delta H^\circ_f(g)$ and $\Delta G^\circ_f(g)$ at various temperatures were calculated from the selected values at 25 °C.

TABLE 13. Methanol. Comparison of virial coefficients and compressibility factor, Z, derived from experimental measurements

Investigators	Virial coefficients			Pressure, atmospheres						
	B_p' cm^3	C_p' $cm^3\ atm^{-1}$	D_p' $cm^3\ atm^{-2}$	0.15	0.25	1	2	5	10	20
				Values of $(1-Z)\times 100$						
				Temperature = 25 °C						
Weltner and Pitzer [1951]	(−1328)		(-7.129×10^4)	(1.798)						
Kretschmer and Wiebe [1954]	(−1778)		(-3.805×10^4)	(1.615)						
Kudchadker [1968]*	−2075	−16380	-4.853×10^5	15.14						
				Temperature = 50 °C						
Lambert, Roberts, Rowlinson, and Wilkinson [1949]	−1380			0.781	1.301					
Weltner and Pitzer [1951]	(−921)		(−3278)	(.563)	(1.062)					
Kretschmer and Wiebe [1954]	−1103		−2338	.654	1.178					
Bottomly and Spurling [1968]	−1144	−440		.684	1.182					
Kudchadker [1968]	−1185	−2863	-1.076×10^5	2.282	8.130					
				Temperature = 100 °C						
Eucken and Meyer [1929]	−533			0.261	0.435	1.741	(3.48)			
Russell and Maas [1931]	−432	−132		(.221)	(.379)	1.838	(4.54)			
Lambert, Roberts, Rowlinson, and Wilkinson [1949]	−790			.387	.645	2.580	5.16			
Weltner and Pitzer [1951]	−511		−24.3	(.251)	.427	1.748	(3.97)			
Kretschmer and Wiebe [1954]	−540		−27.1	.265	.442	1.852	(4.24)			
Foz Gazulla, Morcillo, Masia, and Mendes [1954]	−657			.332	.536	2.146	(4.29)			
Petty and Smith [1955]	−909			(.446)	(.743)	2.97	5.94			
Bottomly and Spurling [1968]	−691	+496		.302	.463	(0.637)	(−1.97)			
Kudchadker [1968]	−535	−654		.310	.570	3.885	12.05			

* Fifth virial coefficient, $E_p' = -27.39\times10^5\ cm^3\ atm^{-3}$ included

Temperature = 150 °C

Russell and Maas [1931]	−153	−280		(0.084)	(0.160)	1.244	(4.10)	(22.3)		
Weltner and Pitzer [1951]	−321		−0.582	(.139)	.231	0.926	(1.862)	(4.83)	(10.92)	
Kretschmer and Wiebe [1954]	(−335)		(−0.901)	(.145)	(.241)	(.967)	(1.950)	(5.15)	(12.24)	
Foz Gazulla, Morcillo, Masia, and Mendes [1954]	−400			.173	.288	1.152	(2.304)	(5.76)	(11.52)	
Bottomly and Spurling [1968]	−412	+312		.158	.240	(0.259)	(−1.22)			
Kudchadker [1968]	−321	−41.25		.141	.239	1.043	2.324	7.592	21.13	

Temperature = 200 °C

Russell and Maas [1931]	−57.2	−149		(0.031)	(0.060)	0.529	(1.822)	(10.3)	(39.7)	
Weltner and Pitzer [1951]	−219		−0.0311	(.085)	.141	.564	(1.129)	(2.830)	(5.72)	(11.92)
Kretschmer and Wiebe [1954]	(−243)		(−0.0615)	(.094)	(.256)	(.626)	(1.253)	(3.15)	(6.42)	(13.79)
Foz Gazulla, Morcillo, Masia, and Mendes [1954]	−300			.116	.193	.773	(1.545)	(3.86)	(7.73)	(15.45)
Kudchadker [1968]	−185	−4.19		.071	.120	.487	0.996	2.652	5.84	13.85

Values in parenthesis have been extrapolated outside the experimental range of temperature or pressure.

TABLE 14. Methanol. Differences in properties between real gas and ideal gas

Sources	At 25 °C and 126.9 mmHg			At 64.51 °C and 760 mmHg		
	H^r-H^0	$C_p{}^r-C_p{}^0$	S^r-S^0	H^r-H^0	$C_p{}^r-C_p{}^0$	S^r-S^0
Estimated by Ito [1951]			−0.61			−0.91
Calculated from equation of state of Weltner and Pitzer [1951]	−0.140	15.6	−0.44	−0.294	22.5	−0.80
Calculated from equation of state of Kretschmer and Wiebe [1954]	−0.105	7.9	−0.33	−0.354	24.3	−0.97
Miller, G. A. [1964]	−0.153					

Chemical Equilibria

There are relatively few quantitative studies of gas phase reactions involving methanol. Newton and Dodge [1933] studied the reaction,

$$HCHO(g)+H_2(g)\rightarrow CH_3OH(g)$$

from 117 to 237 °C. They report an equilibrium constant of,

$$K_p=\frac{P_{CH_3OH}}{P_{HCHO}P_{H_2}}=2090\ \text{atm}^{-1}$$

at 197 °C.

Test of Internal Consistency

A test of the internal consistency of some of the selected values of thermodynamic properties of methanol consists of adding up the changes in enthalpy and entropy on carrying out the cycle shown below which starts and ends with 1 mol of the liquid at 25 °C and 1 atm. These quantities should add up to zero. The uncertainty in the sum has been calculated from the estimated uncertainties in each individual term by the usual statistical formula for the propagation of errors.

Enthalpy and Entropy Balance for Methanol

Transformation	ΔH, kcal $mole^{-1}$	ΔS, cal deg^{-1} mol^{-1}	
liquid(25 °C)→gas(25 °C, 125.5 mmHg)	8.94±0.03	30.0±0.1	Heat of vaporization.
real gas (25 °C)→ideal gas (25°)	0.13±0.03	0.46±0.05	Ideal gas correct.
ideal gas (25 °C)→ideal gas (64.7°)	0.435±0.005	1.30±0.05	Thermodynamic funct.
ideal gas (64.7 °C, 125.5 mmHg)→ideal gas (64.7 °C, 760 mmHg)	0.0	−3.58±0.005	Calc. for ideal gas.
ideal gas (64.7 °C)→real gas (64.7 °C)	−0.29±0.02	−0.80±0.05	Ideal gas correct.
real gas (64.7 °C)→liquid (64.7 °C)	−8.42±0.01	−24.92±0.03	Heat of vaporization.
liquid (64.7 °C)→liquid (25 °C)	−0.809±0.003	−2.55±0.01	Calc. from $C_p(1)$.
Sum	−0.014±0.05	−0.09±0.14	

Thus the sums are equal to zero, within the estimated uncertainties.

Miscellaneous

Smith, J. M. [1948] has given tables and graphs of volume, heat capacity, entropy, and enthalpy at various temperatures in the range of 0 to 240 °C and 0 to 80 atmospheres, in engineering units. He also shows a Mollier diagram. Petty and Smith [1955] have measured the volume of gaseous methanol at various pressures from 0.68 atm to saturation pressure in the range from 93 to 138 °C. Davidson [1957] reports the dielectric constant of liquid and solid methanol from −97 to 25 °C and at 40 to 10^6 Hz. Dannhauser and Bahe [1964] report values of the dielectric constant of the liquid from 25 to 240 °C. Liebermann [1949] has measured the dilational viscosity of the liquid at 17.4 °C. Katti and Shil [1966] have measured the compressibility coefficient of the liquid at several temperatures from 30 to 60 °C.

TABLE 15. Methanol. Enthalpies and entropies of formation of dimers and tetramers from the monomer in the ideal gas state

Investigator	Dimer (kcal per mol)		Tetramer (kcal per mol)	
	ΔH_2	ΔS_2	ΔH_4	ΔS_4
Weltner and Pitzer [1951] PVT and vapor heat cap.	−3.22	−16.5	−24.2	−81.3
Kretschmer and Wiebe [1954] PVT data	−3.95	−18.6	−21.4	−70.8
Inskeep, Kelliher, McMahon and Somers [1958] IR spectrum	−2.9	−16.2	−17.	−56.
Inskeep, Dickson, and Olson [1960] IR spectrum	−4.9		−14.	
FozGazulla, Garcia de la Banda, and Perez Masia [1952] thermal conductivity	−7.1	−9.5		
Lambert, Roberts, Rowlinson and Wilkinson [1949] PVT data	−3.2 to −7.3			

TABLE 16. Methanol. Reported values. Fundamental vibration frequencies

in cm^{-1}

Normal Vibration Mode	Smith, J. M. [1948]	Plyler [1952]	Ivash, Li, and Pitzer [1952]	Falk and Whalley [1961]	Kecki and Bernstein [1965]	Shimanouchi [1966]
a' ν_1 OH stretch	3683	3682	3682	3687	3683	3681
ν_2 CH_3 "degenerate" stretch	2978	2976	2976	2973		3005
ν_3 CH_3 symmetrical stretch	2845	2846	2846	2845	2846	2844
ν_4 CH_3 "degenerate" deformation	1477	1479	1479	1477		1477
ν_5 CH_3 symmetrical deformation	1430	1427	1427	1455	1460	1455
ν_6 OH bending	1340	1346	1346	1346	1071	1345
ν_7 CH_3 rocking	1209	1056	1075	1116		1060
ν_8 CO stretch	1029	1033	1033	1034	1033	1033
a' ν_9 CH_3 "degenerate" stretch	2978	2976	2976	2973		2965
ν_{10} CH_3 "degenerate" deformation	1455	1455	1455	1415		1477
ν_{11} CH_3 rocking	1240	1171	1230	1233		1165

TABLE 17. Methanol. Reported values. Barriers to internal rotation

in cal mol^{-1}

Investigator	Potential Barrier	Method of Estimation
Crawford, B. L. [1940]	3500	Third law.
French and Rasmussen [1946]	1350	Third law.
Eucken and Franck [1948]	1800	Vapor heat capacity.
Rowlinson [1948]	*1300*	Vapor heat capacity.
Pitzer [1948]	2500	Third law.
Halford [1950]	1600	Spectroscopic, third law, and vapor heat capacity.
Burkhard and Dennison [1951]	*1090*	Microwave spectrum.
Ivash and Dennison [1953]	1072	Microwave spectrum.
Shimanouchi [1966]	835	Normal coordinate analysis.

Recommendations for Future Work

Although the physical and thermodynamic properties of methanol have been studied more extensively than those of any of the other alkanols, there are still several questions which have not been adequately resolved. The heat of formation at 25 °C, as derived from the heat of combustion, is still uncertain by about 0.1 kcal per mol. A more accurate measurement, either by combustion or by some other reaction, should be undertaken. The nature of the solid transition at −115.8 °C is not well understood and further study of the solid forms is needed. The properties of the gas phase, especially at saturation, are still not known with sufficient accuracy to establish the nature and extent of association. The kind of association in liquid phases is still less certain but poses a much more difficult problem.

Index to the Bibliography

References to Properties of Methanol

Numbers refer to Bibliography, page 1–389.

References to data used in the selection of refractive index, density, boiling point, vapor pressure, and melting point are in boldface type.

Numbers in parentheses refer to sources of reviews, or theoretical calculations only.

Reference numbers under each property are listed in the order of date of publication.

Refractive Index

378, **608**, 1434, 607, **840**, **990**, **237**, **289**, **438**, **509**, **1140**, 1227, **1780**, **1447**, **1239**, 1634, **1887**, 1891, 858, 1708, **1792**, **1843**, **1886**, **1354**, 532, **1355**, **6**, 1404, 1985, **1856**, **1963**, 1000, **1893**, **721**, **644**, 991, 1240, **201**, 1377, **780**, 996, 22, 1388, 1102, **1547**, 575, **1621**, **76**, 796, 414, **1552**, **760**, **338**, **24**, **35**, 1906, **1152**, **319**, 1437, **763**, **1528**, **417**, **628**, **1292**, 25, **1186**, **1069**, **231**, **1982**, 507, 293, **1473**

Density at 20 to 30 °C Only

608, 989, 1453, 1556, 840, 272, 592, 1481, 771, 1817, 1087, 1479, 1482, 1992, **716**, **88**, **1151**, 750, 1959, **715**, 1448, 1350, **1272**, 1317, **508**, 1140, 1227, 1075, **886**, 148, **1447**, **531**, **1096**, 113, 1067, **254**, 1867, 1887, 344, 739, **594**, 1792, **140**, 1678, **855**, 997, 1886, 1207, 1222, **478**, **1355**, 6, 1553, **965**, **1528**, 1878, 1893, 1963, 853, 1680, 644, 1744, 1377, 835, 1529, 1745, 1621, 1102, **1552**, 796, 1682, 24, 1338, 1823, 1528, 319, 368, 965, 635, 1437, 409, 628, **231**, **1313**

Density at all Temperatures

940, 941, 1434, **1559**, 607, 1560, 1349, **2012**, 1453, **426**, **1457**, 576, **990**, **1452**, 2017, **1081**, **2002**, **363**, 237, **912**, 273, 289, **667**, 435, 440, **1999**, **1771**, 393, **436**, 1775, **1688**, **55**, 1165, 1816, **839**, **838**, 509, 1471, 1776, 1569, **1489**, **42**, **1780**, 1239, 1634, **739**, 880, 1371, **1354**, **213**, 460, **1856**, 1807, 721, 1820, **780**, **271**, **1152**, 35, 25, 514, 1186, 1823, (347), **1069**, **1996**, **1154**, **1178**, 293, 1147, 481, 876, 2032

Normal Boiling Point

940, 941, 1465, 989, 1434, 1561, 1559, 1398, 1560, 2012, 1483, 1216, 1453, 1556, 1572, 1571, 990, 1765, 2017, **2002**, 272, 1395, 667, 1481, 771, 435, 1771, **440**, 1999, 1768, 1817, 55, 211, 1230, 1816, 839, 1479, 1482, 1960, 838, 716, 361, 88, 1471, 750, 1776, 1959, 1272, 1227, 1140, 1009, 42, 148, **1447**, **1780**, 1794, 254, 1634, **396**, 880, **1977**, 1708, 125, 820, 591, 1134, 213, 6, **460**, **963**, 1006, 1404, 1985, 1000, 1856, 721, 1807, **1153**, 644, 1820, 991, 1744, 1377, 1240, 1007, 1745, 22, 1102, 752, 1393, 1621, 76, 1902, **1552**, 414, **1682**, 796, 760, **1152**, **24**, 1906, 1437, 635, 368, 244, 628, 701, 417, 1292, 25, 1823, 347, 1069, 913, **1313**, **231**

Vapor Pressure and Boiling Points at Other Pressures
935, **1483**, **1453**, **1571**, **1081**, **1999**, **440**, 1230, **1991**, **1799**, **260**, 1480, **1570**, **1569**, **858**, **1446**, **1207**, 1553, **460**, **1818**, **523**, **1897**, **1823**, **319**, **417**, 878, **1313**, (23), 1184, **1103**, 910, 764

Critical Temperature
1453, 1999, 748, (1433), 1533, 532, (852), (649), (915), 1501, 347, 878, 499

Critical Pressure
1238, 1453, 1999, 748, 1533, (915), 878, 499

Critical Volume and Density
1453, 1999, 1533, (915), 878, 481

Crystallography
385, 1234

Transition Temperature
1873, 1317, 886, 1680, 385, 270

Heat Capacity of the Solid
1317, 886, 15, 1680, 270

Heat of Transition
1317, 886, 1680, 270

Normal Melting Point
983, 982, 272, 665, 1768, 1728, 105, 106, 107, **897**, 1105, 1151, 1776, 1107, **1317**, 1350, 1194, 1195, **886**, 1538, 148, **1780**, 858, 1708, **1497**, 1172, **1153**, 1680, **1807**, 1527, **575**, 338, 342, 1823

Triple Point
1873, 886, 1680, 270

Heat of Fusion
1317, 886, 1680, 270

Heat Capacity of the Liquid
183, 1317, 886, 531, 501, 1680, 780, 270

Heat Capacity of the Real Gas
125, 418, 1513, 503, 834, 1897, 1627, 1185, 690, 19, 1179

P-V-T Data and Equation of State of the Real Gas
1453, 504, 1523, 820, 999, 986, (1514), (1513), (1897), (831), 965, (1369), 1826, (144), 187, 975

Calorimetric Heat of Vaporization at 25 °C
1147, 1870

Calorimetric Heats of Vaporization at Other Temperatures
219, 1141, 1140, 97, 531, 125, 1680, 1897, 1398, (1184)

Thermodynamic Functions of the Liquid and Real Gas at Various Temperatures and Pressures
1453, 999, (1636), (878), 1362, 1179, (144), 876

Heat of Combustion
1762, 1698, 1480, 1508, 1511, 1509, 1505, 1510, 1506, (1507), (626), 287, 288, (1871), 876

Equilibrium Constants of Gas Phase Reactions
1265, (1636)

Third Law Entropy of the Liquid at 25 °C
1317, 886, (15), 270, (1184)

Molecular Vibration Frequencies and Spectra
(685), 1636, 604, 795, 492, (90), 671, 1190, 833, 91, 528, 537, 1196, 1735, 530, 541, 228, 726, 1108, 251, 1376, 1285, 1012, 1126, 1516, 1625, 663, 672, 968, 516, 932, 1659, 379, 61, (410), 421, 1844, 456, 1600, 1127, 2022, 668, 669, 470, 879, (1609)

Internal Rotation
(685), 360, 561, 1513, 1393, 503, 137, (684), (1897), 250, 376, 492, (90), 77, 833, 1270, 1109, 689, 1717, 251, 1376, 1285, 1012, 1126, 1516, 1625, 663, 672, 968, 516, 932, 1659, 379, 61, (410), 421, 1844, 456, 1660, 1127, 2022, 668, 669, 470, 879, (1609)

Molecular Geometry
(684), 575, 250, 832, 905, 251, (1609)

Thermodynamic Functions of the Ideal Gas
685, 1636, 684, 1897, 90, 833, (624), (291)

Association in the Gas Phase
997, 1897, 552, 965, 824, 823, 507, (1184), 879, 975

Association in the Liquid Phase
158, 769, (1754), 1160, 1540, 1706, 1705, 182, 316, 1683, 529, 489, 1109, 1056, 1835, 530, 1545, 115, 102, 1546, 392, 842, 697, 1451, 1757, 1758, 1845, 380, 470, 78

Ethanol

Properties of the Liquid Phase at Various Temperatures

Refractive Index

The refractive index data for ethanol covers a wider range of temperature and wavelength than for any of the other alcohols. The Index on page 1–65 lists 82 references. The more reliable values of n_D at 20 and 25 °C have been collected in table 21, and the selected values lie within the experimental uncertainties of most of these. The estimated uncertainty is about 0.00005 to 0.0001. A graph of n_D versus temperature shows a slight curvature. Smoothed values of refractive index at various temperatures and wavelengths are given in table 20. Dale and Gladstone [1858], Ketteler [1888], Doroshevskii and Dvorzhanhik [1908], Cheneveau [1907], Schwers [1912], Eykman [1919], Guillery [1930], Venkataraman [1939] and Hatem [1949] have reported refractive index data over wide ranges of temperature and wavelength. The measurements of Guillery extend all the way to 2655 Å

Density

The literature on density of ethanol is very extensive, as reflected in the Index to the Bibliography and the data in table 21. Table 18 lists constants in the Francis equation for three temperature ranges. The constants for the intermediate and high range generate essentially the same values of density from 40 to 60 °C. Maximum deviations of the values calculated from the Francis equation from values determined directly by several investigators are shown below.

Investigators	Temperature Range deg.C	Maximum difference between calculated and observed densities, g cm^{-3}
McKinney, Skinner, and Stavely [1959]	0	0.00015
Fioch, Ginnings, and Holtan [1931]	20–25	.00007
Dreisbach and Martin [1949]	20–25	.00006
Ling and Van Wickle [1958]	30–75	.0003
Ramsay and Young [1889]	0–180	.0014

Vapor Pressure and Boiling Point

The Antoine constants, obtained by fitting vapor pressure data identified in the Index, are given in table 18. Reports by Scatchard and Raymond [1938], Dreisbach and Shrader [1949], Kretschmer [1949] and Plewes [1950] represent careful measurements which have been made in recent years. Below 1000 mm the calculated and observed vapor pressures agree, for the most part, within about 1 mm. The principal exceptions are the data of Ramsay and Young (1885), which are about 1 to 2 mm Hg low in the range of 40 to 80 °C, Winkler (1905), which are about 2 mm Hg too low in the vicinity of the normal boiling point, and Smyth and Engel (1929), which range up to 6 mm Hg too low between 22 and 78 °C. The scatter becomes greater for data about 1000 mmHg, with deviations of 2 to 4 mmHg from the calculated curve common. Most of the experimental measurements of vapor pressure are less than the calculated values at about 1000 mmHg. The Antoine constants used for the calculated values are based on both vapor pressure and heats of vaporization measurements. Most of the calorimetric heats of vaporization are within about 200 cal per mol of the calculated values at the same temperature.

Critical Properties

Critical Temperature, Pressure, and Density

The experimental values are shown in table 22. The recent measurements of Efremov [1966] agree with the older data to within the experimental uncertainty, and the values selected by Kobe and Lynn [1953] were retained.

Solid-Liquid Phase Equilibria

Normal Melting Point

The values of melting points shown in table 21 are within a range of about 0.7 °C, except for two which obviously contain considerable error. The selected value is closer to the more reliable values. No measurements of the triple point have been located.

Heat Capacity of the Solid and Liquid at the Melting Point

The selected values were based primarily on the smoothed values published by Green [1961], which were based on data in the literature.

Heat of Fusion

The selected value was slightly less than that reported by Kelley [1929a].

TABLE 18. Ethanol. Selected values physical and thermodynamic properties

Temp. °C	Refractive Index, n_D	Density g cm^{-3}	Vapor Pressure, mmHg
−20		0.821	
−10	1.3738	.813	
− 2.84			10
0	1.3695	.8062	12.2
+ 5			17.3
10	1.3656	.7979	24.0
15			32.9
20	1.36143	.78937	44.6
25	1.35941	.78509	59.8
30	1.3575	.7808	79.2
34.23			100
35			103.9
40	1.3536	.7721	135.0
45			173.7
47.87			200
50	1.3488	.7636	221.6
55			280.3
60	1.3439	.7550	351.9
62.90			400.
65			438.3
70	1.3390	.7459	542.2
75			666.1
78.29			760
80		.7362	813.0
85			986.2
90		.7260	1189.3
100		.7151	
110		.7036	
120		.6913	

Data For Phase Transitions

Initial	Final	Temp. °C	dt/dP deg mm^{-1}	Pressure mmHg	ΔH kcal mol^{-1}	$d\Delta H/dt$	ΔS	ΔC_p
						cal deg^{-1} mol^{-1}		
c	liq	−114.1±0.2		760	1.198±0.01	13.37±0.14	7.53±0.07	5.84±0.12
liq	g	−114.1			11.51±0.1		72.4±0.7	
liq	g	25	0.2914	59.77±0.2	10.11±0.02	−12.7±1.0	33.91±0.1	−7.7±0.5
liq	g	78.29±0.05	.03317	760	9.255±0.01	−20.1±1.0	−26.33±.05	−5.6±0.5

Condensed Phase Heat Capacity

State	Temp. °C	C_p
		cal deg^{-1} mol^{-1}
c	−114.1	14.80±0.05
liq	−114.1	20.64±0.1
liq	78.29	33.10±0.1

Properties of the Saturated Real Gas

Temp. °C	H^r-H^0	S^r-S^0	$C_p{}^r-C_p{}^0$
	kcal mol^{-1}	cal deg^{-1} mol^{-1}	
25	−0.060±0.02	−0.190±0.05	3.5±0.5
78.29	0.216±0.010	−0.546±0.02	9.90±0.5

Data for the Standard States at 25 °C

State	Heat of Combustion $\Delta H_c{}^0$ kcal mol^{-1}	Heat of Formation $\Delta H_f{}^0$ kcal mol^{-1}	Entropy S^0 cal deg^{-1} mol^{-1}	Gibbs Energy of Formation $\Delta G_f{}^0$ kcal mol^{-1}	Heat Capacity, C_p cal deg^{-1} mol^{-1}
liq	−326.85±0.05	−66.20±0.05	38.49±0.10	−41.63±0.05	26.76±0.10
g	−337.02±0.07	−56.03±0.07	67.54±0.05	−40.13±0.07	15.64±0.05

Critical Constants

Temp. 243.1 °C, 516.3 K	Pressure 63.0 atm	Density 0.276 g cm^{-3}

				Constants in Vapor Pressure and Density Equation								
				Antoine Equation				Francis Equation				
				Temp. Range	*A*	*B*	*C*	Temp. Range	*A*	$B\times10^3$	*C*	*E*
				−2 to 100 °C	8.32109	1718.10	237.52	0 to 55 °C −24 to 55 °C 40 to 180 °C	1.13378 1.16261 1.17171	0.4324 0.0413 −0.1460	267.96 173.37 175.57	818.06 485.70 472.62

Table 19. Ethanol. Selected values, thermodynamic functions of the ideal gas at one atmosphere

Temperature K	Entropy S^0 cal deg^{-1} mol^{-1}	Heat Capacity $C_p{}^0$ cal deg^{-1} mol^{-1}	Enthalpy Function $(H^0-H_0{}^0)/T$ cal deg^{-1} mol^{-1}	Gibbs Energy Function $(G^0-H_0{}^0)/T$ cal deg^{-1} mol^{-1}	Heat of Formation $\Delta H_f{}^0$ kcal mol^{-1}	Gibbs Energy of Formation $\Delta G_f{}^0$ kcal mol^{-1}
0	0	0	0	0	−51.81	−51.81
273.15	66.23	14.78	11.03	−55.20	−55.71	−41.45
298.15	67.54	15.64	11.37	−56.17	−56.03	−40.13
300	67.64	15.71	11.40	−56.24	−56.05	−40.03
400	72.66	19.36	12.93	−59.73	−57.23	−34.50
500	77.34	22.77	14.59	−62.75	−58.21	−28.69
600	81.77	25.69	16.18	−65.59	−59.02	−22.73
700	85.93	28.19	17.73	−68.20	−59.67	−16.62
800	89.85	30.33	19.19	−70.67	−60.16	−10.44
900	93.53	32.19	20.53	−73.00	−60.55	−4.19
1000	97.00	33.83	21.77	−75.24	−60.83	+2.08

TABLE 20. Ethanol. Selected values, refractive index at various temperatures and wavelengths

Symbol	Wavelength, Å	Refractive Index, n									
		0 °C	10 °C	15 °C	20 °C	25 °C	30 °C	40 °C	50 °C	60 °C	70 °C
	7607	1.3657	1.3618	1.3598	1.3578	1.3556	1.3537	1.3498	1.3451	1.3407	1.3358
He_{red}	6678.2	1.3674	1.3635	1.3613	1.3594	1.3573	1.3553	1.3513	1.3468	1.3421	1.3372
H_c	6562.8	1.3676	1.3637	1.3616	1.3596	1.3575	1.3556	1.3516	1.3470	1.3423	1.3374
Na_D	5892.6	1.3695	1.3656	1.3633	1.36143	1.35941	1.3575	1.3536	1.3488	1.3439	1.3390
Hg_e	5460.7	1.3710	1.3671	1.3648	1.3629	1.3609	1.3589	1.3548	1.3503	1.3455	1.3406
He_{blue}	5015.7	1.3730	1.3691	1.3669	1.3649	1.3628	1.3609	1.3567	1.3522	1.3474	1.3425
H_F	4861.3	1.3739	1.3699	1.3677	1.3657	1.3637	1.3617	1.3575	1.3530	1.3482	1.3433
Hg_g	4358.3	1.3773	1.3733	1.3712	1.3692	1.3670	1.3650	1.3608	1.3564	1.3516	1.3466
H_G'	4340.5	1.3775	1.3734	1.3713	1.3693	1.3672	1.3652	1.3609	1.3565	1.3517	1.3467
	4046.6	1.3802	1.3760	1.3741	1.3720	1.3698	1.3678	1.3633	1.3590	1.3542	1.3493
	3968.5	1.3812	1.3770	1.3750	1.3729	1.3707	1.3688	1.3642	1.3600	1.3552	1.3502
	3342				1.3817	1.3798	1.3776	1.3728	1.3684	1.3638	1.3587
	2967				1.3905	1.3885	1.3862	1.3814	1.3767	1.3723	1.3670

Heat of Vaporization at the Triple Point

The heat of vaporization of the liquid at 159 K was calculated from the selected value at 25 °C and the enthalpy changes of liquid and gas. Data for the liquid from 298 to 159 K were taken from the table of Green [1961]. Data for the ideal gas were taken from the selected thermodynamic functions at 298 K and from a calculation based on the partition function at 159 K. The correction to the ideal gas was applied at 298 K. Because of the low vapor pressure, it was assumed that no correction would be needed at 159 K. No vapor pressure was found for this temperature.

Properties of the Liquid at 25 °C

Heat Capacity

The selected value was from Green [1961]. A graph drawn through all available data gave 26.80 cal deg^{-1} mol^{-1} at 25 °C.

Absolute Entropy

Based on the heat capacity data of Gibson, Parks, and Latimer [1920], Parks [1925], and Kelley [1929a], Green reports a value of 38.53 cal deg^{-1} mol^{-1} for the liquid at 25 °C. A value slightly different from this was selected in order to attain internal consistency.

Heat of Combustion

Experimental heats of combustion are summarized in table 27. The last three values listed show fairly good agreement. The selected value was based primarily on the measurement of Chao and Rossini [1965].

Properties of the Real Gas

Equation of State

The saturated vapor volume was measured by Ramsay and Young [1886] from 0 to 240 °C. These data at low temperatures were later revised by Young, [1910]. Russell and Maas [1931], Steurer and Wolf [1938] and Ingle and Cady [1938] calculated the degree of association in gaseous ethanol from experimental vapor density data. Following the model proposed by Weltner and Pitzer for methanol, Barrow [1952] derived the equation of state,

$$PV = RT + B_p'P + D_p'P^3$$

$$B_p' = 100 - 0.02023T\exp(1710/T) \qquad \text{ml mol}^{-1}$$

$$D_p' = -4.27\times10^{-16}T\exp(12460/T) \qquad \text{ml atm}^{-2}\,\text{mol}^{-1}$$

from heat capacity and heat of vaporization data available at that time. Kretschmer and Wiebe [1954] carried out P-V-T measurements in the range 40 to 120 °C and 0 to 1 atm and expressed their results in terms of the virial coefficients,

$$B_p = -290 - 0.284\exp(2730/T) \qquad \text{ml mol}^{-1}$$

$$D_p = -5.7 - 4.38\times10^{-12}\exp(11144/T)\ \text{ml atm}^{-2}\,\text{mol}^{-1}.$$

A comparison of the compressibility coefficients calculated from these two sets of constants and from the data of Russell and Maas is given in table 28. Barua, Chakraborti, and Saran [1965] calculated the proportion of dimers present in ethanol vapor in their theoretical discussion of the second virial coefficients of polar gases.

TABLE 21. Ethanol. Reported values. Simple physical properties

Investigators		Vapor Pressures and Boiling Points		Freezing Point	Density, d g cm^{-3}		Refractive Index, n_D	
		°C	mm Hg	t_m, °C	20 °C	25 °C	20 °C	25 °C
Ethanol. C_2H_6O, mol wt. 46.070, state at 25 °C liq								
Mendeleev	[1865]	78.303	760		0.78945	0.78552		
Dupre and Page	[1869]	78.41	760		.78932			
Perkin	[1884]	78.5	760			.78589		
Ramsay and Young	[1885]	78.30	760					
Rudolphi	[1901]				.79117		1.36171	
Crismer	[1904]				.78948	.78522		
Winkler	[1905]	78.37	760		.78938			
Klason and Norlin	[1906]				.78938			
Walden	[1906]					.7853		
Holmes and Sageman	[1909]	78.38				.78661		
Doroshevskii and Polyanskii	[1910a]	78.23	760					
Young	[1910]				.78939			
Kailan	[1911]					.78513		
Timmermans	[1911]			−114.15				
Wade and Merriman	[1911]	78.39	760					
Schwers	[1912a]				.78969			
Robertson and Acree	[1913]					0.78506		
Osborne, McKelvy, and Bearce	[1913]					.785058		
Tyrer	[1914]	78.32	760					
Price	[1915]				.79085			
Wroth and Reid	[1916]					.78543		
Gibson, Parks, and Latimer	[1920]			−117.0				
Richards and Davis	[1920]	78.55–78.60	760					
Barr and Bircumshaw	[1921]	78.3	760			.78752		
Brunel, Crenshaw, and Tobin	[1921]	78.32	760			.78505		1.3595
McKelvy and Simpson	[1922]					.78506		
Grimm and Patrick	[1923]	78.32						
Willard and Smith	[1923]	78.29–78.31	760			.78516		
Riiber	[1923]				.789334			
Norris and Ashdown	[1925]	78.3–78.4	760			.78506		
Parks	[1925]			−114.5				
Parks and Kelley	[1925a]					.78516		1.3595
Richards and Chadwell	[1925]				.78922			
Barbaudy	[1926]	78.30	760					1.3592
Mathews	[1926]				.78992		1.36175	
Mitsukuri	[1926]			−115.23				
Barbaudy	[1927]					.78506		
Krchma and Williams	[1927]					.7862		1.35894
Parks and Nelson	[1928]					0.78549		
Smyth and Engel	[1929]	78.4	760				1.36130	
Smyth and Stoops	[1929]	78.4	760		0.7901		1.36139	
Kelley	[1929a]			−114.7		.78520		
Sapgir	[1929]			−114.1				
Fiock, Ginnings, and Holton	[1931]				.78946			
Lund and Bjerrum	[1931]					.78503		
Swietoslawski, Zmaczynski, and Usakiewicz	[1932]	78.318	760			.78521		
Solana and Moles	[1932]				.78934			
Harris	[1933]	78.37	760			.78507		
Vosburgh, Connell, and Butler	[1933]					.78535		
de Brouchere and Gillet	[1935]	78.3	760					
Pearce and McDowell	[1936]	78.82	760					
Tomanari	[1936]				.7909		1.36181	
Wojciechowski	[1936]	78.325	760					
Zepalova-Mikhailova	[1937]	78.35	760					
Scatchard and Raymond	[1938]					.78562		
Washburn, Graham, Arnold, and Transue	[1940]					.7851		1.35942
Dulitskaya	[1945]	78.35	760					
Kretschmer, Nowakowska, and Wiebe	[1948]					.78506		
Vogel	[1948]	78	760		.7910		1.36139	
Hatem	[1949a]	78.35			.7901		1.3614	
Hatem	[1949b]				.7901	.7861	1.3615	1.3596
Dreisbach and Martin	[1949]	78.27	760	−114.49	.78933	.78505	1.36155	1.35941

TABLE 21. Ethanol. Reported values. Simple physical properties—Continued

Investigators		Vapor Pressures and Boiling Points		Freezing Point	Density, d g cm^{-3}		Refractive Index, n_D	
		°C	mm Hg	t_m, °C	20 °C	25 °C	20 °C	25 °C
Ethanol, C_2H_6O, mol wt. 46.070, state at 25 °C liq								
Tschamler, Richter, and Wettig	[1949b]	78.2	760	−114.8		.7852		
Griswold, Chu, and Winsauer	[1949]					.78459		1.35931
Kretschmer and Wiebe	[1949b]					.78505		
Dreisbach and Shrader	[1949]	78.27	760					
Kretschmer and Wiebe	[1949a]	78.33	760					
Sackman and Sauerwald	[1950]			−114.2				
Vierk	[1950]				.7894		1.361124	
Cook	[1952]	78	760	−113	.7895		1.3614	
Ballard and Van Winkle	[1952]	78.5	760				1.36120	
Staveley and Spice	[1952]	78.36	760		.7894			
Amer, Paxton, and Van Winkle	[1953]	78.3				.7850	1.36152	
Barker, Brown, and Smith	[1953]	78.29	760			.78511		1.3596
Corcoran, Kruse, and Skolnik	[1953]			−114.0				
Hellwig and Van Winkle	[1953]	78.4	760				1.361514	
McKenna, Tartar, and Lingafelter	[1953]	78.5	760			0.78510		1.35951
Griffiths	[1954]					.78508		
Brown and Smith	[1954]	78.29	760			.78511		1.35820
Purnell and Bowden	[1954]	78.4	760			.78504		1.3596
Kretschmer and Wiebe	[1954]					.78506		
Amer, Paxton, and Van Winkle	[1956]	78.3	760			.7850	1.36152	
Costello and Bowden	[1958]	78.3	760		0.7894			
Ling and Van Winkle	[1958]	78.35	760				1.36132	1.35937
Brown and Smith	[1962b]	78.29	760			0.78511		1.35926
Selected value	[1967]	78.29±0.05	760	−114.1	0.78937	0.78509	1.36143	1.35941
		−2.84±0.07	10	±0.2	±0.00007	±0.00007	±0.0001	±0.0001

Antoine constants: *A* 8.32109, *B* 1718.10, *C* 237.52

dt/dp at 760 mm Hg, 0.03473 °C/mm Hg

TABLE 22. Ethanol. Reported values. Critical properties

Investigator	t_c, °C	P_c, atm	d_c, g cm^{-3}
Ramsay and Young [1886]	243.6	62.8	0.29
Young, S. [1910]	243.1	62.96	0.2755
Khalilov [1939]	248.5		
Fischer and Reichel [1943]	241.7		
Ross [1954]	243.		
Efremov [1966]	243.	63.0	0.275

Heat Capacity

Sinke and DeVries [1953] report the only available direct experimental data on the heat capacity of the real gas. Their values range from 81 to 164 °C at a pressure of 750 mmHg. This does not include the saturated vapor. Deviations from the ideal gas are large but not as large as for methanol. Eucken and Franck [1948] and Halford and Miller [1957] have published values of heat capacity measured at low pressures.

Corrections to the Ideal Gas State

Differences between thermodynamic properties of the real gas and of the ideal gas are shown in table 29. The values at 25 °C are uncertain because they depend upon the extrapolation of the equations of state below the temperatures of experimental measurements. The data calculated from the equation of state of Kretschmer and Wiebe were given the greatest weight in the selected values.

TABLE 23. Ethanol. Reported values. Condensed phase transitions

Investigator	Fusion	
	t_m, °C	ΔH_m, kcal mol^{-1}
Timmermans [1911]	−114.15	
Gibson, Parks and Latimer [1920]	−117.0	1.106
Parks [1925]	−114.5	1.186
Kelley [1929]	−114.7	1.201
Sapgir [1929]	−114.1	
Dreisbach and Martin [1949]	−114.49	
Sackman and Sauerwald [1950]	−114.2	
Cook [1952]	−113.	
Corcoran, Kruse and Skolnik [1953]	−114.0	

Vapor-Liquid Equilibrium at 25 °C

Vapor Pressure

The value shown was calculated from the Antoine constants.

Heat of Vaporization

The value measured by Wadso [1966] was adopted. This agrees closely to the result of McCurdy and Laidler [1963] and the extrapolated measurements of Fiock, Ginnings and Holtan [1931].

Temperature Derivative of the Heat of Vaporization

This was calculated from the differences in heat capacities of the ideal gas and liquid, the Antoine constants and the equation of state of the vapor. The equation of state of Barrow gave -6.11 cal deg^{-1} mol^{-1} and of Kretschmer and Wiebe gave -4.91 cal deg^{-1} mol^{-1} for $d\Delta H/dT-\Delta C_p$.

Vapor-Liquid Equilibrium at the Normal Boiling Point

Normal Boiling Point

The boiling point at 1 atm was calculated from the Antoine constants.

Heat of Vaporization

The selected value was calculated from the equation of Fiock, Ginnings, and Holtan [1931]. Other data are shown in table 24.

TABLE 24. Ethanol. Reported values. Heats of vaporization

Investigator	ΔH_v at 25 °C	ΔH_v at t_b	Method and Remarks
Ramsay and Young [1886]	10.11	9.54	Calculated from vapor pressure.
Louguinine [1889]		9.28	Calorimetric.
Bartoszewiczowna [1931]	10.26		Calorimetric.
Parks and Nelson [1928]		9.61	Calorimetric.
Fiock, Ginnings and Holtan [1931]	10.13	9.255	Calorimetric, extrapolated by equation to 25 °C.
Plewes, Jardine and Butler [1954]		9.45	Calorimetric.
Green [1960]	10.12		Calculated from published vapor pressure.
McCurdy and Laidler [1963]	10.09		Calorimetric.
Kollar and Proszt [1963]		9.55	Calorimetric.
Wadso [1966]	10.11		Calorimetric.
Selected Antoine constants	10.03	9.30	Calculated.

Heat Capacity of the Liquid

The equation of Fiock, Ginnings, and Holtan (1931) gives the heat capacity of 33.08 cal deg^{-1} mol^{-1} at 78.29°, while 33.11 is obtained by a graphical extrapolation of the values listed by Green [1961]. Williams and Daniels [1924], Blacet, Leighton, and Bartlett [1931], and Eucken [1948] have measured the heat capacity of liquid ethanol in the vicinity of the normal boiling point.

TABLE 25. Ethanol. Reported values. Heat capacity and entropy of the liquid at 25 °C

Investigator	$C_p{}^0(1)$	Remarks	$S^0(1)$, Third Law
Bose and Muller [1907]	26.8	From equation	
Gibson, Parks and Latimer [1920]	26.5	Extrapolated	42.6.
Williams and Daniels [1924]	26.80	From equation	
Parks [1925]	27.1		
Parks, Kelley and Huffman [1929]			38.4 (revision of Parks).
Kelley [1929]	26.56	Extrapolated	38.4.
Blacet, Leighton and Bartlett [1931]	27.0	Extrapolated	
Fiock, Ginnings, and Holtan [1931]	26.91	Extrapolated by Equation	
Eucken [1948]	26.90		
Green [1961]			38.53 (recalculated from published data).

Temperature Derivative of the Heat of Vaporization

This was calculated in the same manner as it was for 25 °C. $d\Delta H/dT-\Delta C_p$ was -16.87 cal deg^{-1} mol^{-1} as calculated from the equation of state of Barrow, and -13.66 cal deg^{-1} mol^{-1} from the equation of state of Kretschmer and Wiebe.

Properties of the Ideal Gas State

Molecular Parameters

Many studies have been carried out on the vibrational and rotational spectra of ethanol, in the gas, liquid, and solution states. Green [1961] has summarized some of these investigations and has selected a set of parameters needed to calculate the thermodynamic functions. Some examples of vibration frequencies, other than those for CH_3- and OH-torsion, which have been selected are given in table 31. There are two degrees of freedom for internal rotation, and some of the suggested values for barriers to internal rotation are shown in table 32. As can be seen, there are considerable discrepancies, especially for the rotation of the hydroxyl group. Part of the difficulty lies in selecting a suitable potential function for these rotations. Some of the earlier studies used unsymmetrical functions in an attempt to allow for the interaction between the two rotating groups. However, Green concluded that symmetrical functions gave a better fit to the observed entropy and heat capacities.

Michielson-Effinger [1964 and 1965] has studied the microwave spectrum of ethanol and has identified two stable rotational isomers, *trans* and *gauche*. Although no quantitative data on the potential function of the OH group were obtained, a tentative value of 0.8 kcal was given to the potential barrier for the rotation of the $-CH_3$ group. This probably applies to the *trans* isomer.

Entropy at 25 °C

The calculations of Green [1961] are the best available at this time. His value of the entropy of the ideal gas at 25 °C differs from the third law value by only 0.04 cal deg^{-1} mol^{-1}. The statistical value was selected.

Heat Capacity

Values of observed and calculated ideal gas heat capacities are listed in table 22. Since their measured values cannot be considered as very accurate, the agreement is about as good as could be expected. Jatkar [1939] has measured the speed of sound in ethanol vapor. The heat capacity ratio, C_p/C_v, calculated from their results is 1.1179 at 97.1 °C and 1.1239 at 134 °C.

TABLE 26. Ethanol. Reported values. Heat capacity and entropy of the ideal gas at 25 °C

Investigator	$C_p^0(g)$	Method	$S^0(g)$ from molecular parameters
Aston [1942]			67.26
Brickwedde, Moscow, and Aston [1946]	17.59	From molecular parameters	66.45
Eucken and Franck [1948]	14.0	Thermal conductivity, extrapolated	
Halford [1949]			66.75
Barrow [1952]	14.0	Extrapolated, exp. meas.	67.58
Ito [1952]			67.30 (recalculated data of Barrow).
Halford and Miller [1957]	14.9 (at 6 °C)	Thermal conductivity	
Green [1961]	15.64	From molecular parameters	67.54

TABLE 27. Ethanol. Reported values. Heat of combustion of the liquid at 25 °C

Investigator	$-\Delta H_c^0(1)$, kcal mol^{-1}
Thomsen [1886]	340.7
Berthelot and Matignon [1892]	−325.4
Atwater and Rosa [1899]	−325.2
Atwater and Snell [1903]	−325.9
Emery and Benedict [1911]	−326.1
Richards and Davis [1920]	−327.3
Roth and Muller [1927]	−328.8
Rossini [1932]	*−326.72
Verkade and Coops [1927] (recalculated by Green [1960]	−326.71
Chao and Rossini [1965]	−326.86

* ΔH_c of gas measured. Value corrected to the liquid.

Thermodynamic Functions

The values published by Green [1961] were adopted but his value of $\Delta G_f^0(g)$ for ethanol at 273.16 K is wrong. It should be −41.58. Tables of thermodynamic functions have also been published by Chermin [1961].

Chemical Equilibria

Rideal [1921] and Suen, Chiën, and Chu [1942] have studied the reaction

$$C_2H_5OH(g) \rightarrow CH_3CHO(g) + H_2(g)$$

at equilibrium. Rideal measured the equilibrium constant by a static method in the range of 105 to 275 °C and calculated a value for the heat of reaction of 11.5 kcal mol^{-1} at 18 °C from these measurements. Suen, Chien, and Chu made approximate measurements of the equilibrium composition at 230 and 235 °C using a flow method with a copper catalyst. Several investigators have measured the equilibrium constant for the reaction,

$$C_2H_4(g) + H_2O(g) \rightarrow C_2H_5OH(g).$$

The average values of ΔH^0 and ΔS^0 for this reaction over the range of experimental temperatures, calculated from the equilibrium constants, are shown in table 33. The thermodynamic quantities, corrected to 25 °C by use of the selected thermodynamic functions of ethanol and the thermodynamic functions of water and ethene reported in "Selected Values of Properties of Hydrocarbons and Related Compounds," American Petroleum Institute Research Project 44, Texas A&M University, College Station, Texas (loose-leaf data sheets, extant, 1966), are also given in this table. These data may be compared with the corresponding quantities of this reaction at

TABLE 28. Ethanol. Comparison of virial coefficients and compressibility factor, Z, derived from experimental measurements

	Virial coefficients			Pressure, atmospheres					
	B_p' cm^3	C_p' cm^3 atm^{-1}	D_p' cm^3 atm^{-2}	0.15	0.25	1	2	5	10
				Values of $(1-Z)\times 100$					
Temperature = 50 °C									
Barrow [1952]	(−1199)		(−7679)	(0.776)	(1.583)				
Kretschmer and Wiebe [1954]	−1615		−4158	.967	1.768				
Temperature = 100 °C									
Russell and Maas [1931]	−556	−184		0.285	0.490	2.411	(6.02)		
Barrow [1952]	−638		−50.6	.313	.523	2.249	(5.49)		
Kretschmer and Wiebe [1954]	−717		−46.58	.352	.588	2.494	(5.90)		
Temperature = 150 °C									
Russell and Maas [1931]	−353	−125		0.160	0.276	1.375	(3.47)	(14.08)	
Barrow [1952]	−387		−1.11	.167	.279	1.118	(2.26)	(5.97)	
Kretschmer and Wiebe [1954]	(−470)		(−6.90)	(.203)	(.339)	(1.373)	(2.87)	(9.25)	
Temperature = 200 °C									
Russell and Maas [1931]	−190	−82		0.078	0.135	0.699	(1.818)	(7.70)	(25.89)
Barrow [1952]	−255		−0.0552	.099	.164	0.657	(1.315)	(3.30)	(6.71)
Kretschmer and Wiebe [1954]	(−381)		(−5.77)	(.147)	(.256)	(0.996)	(2.082)	(6.76)	(24.67)

Values in parenthesis have been extrapolated outside the experimental range of temperature or pressure

TABLE 29. Ethanol. Differences in properties between real and ideal gas

Source	at 25 °C and 59.77 mmHg			at 78.29 °C and 760 mmHg		
	H^r-H^0	$C_p{}^r-C_p{}^0$	S^r-S^0	H^r-H^0	$C_p{}^r-C_p{}^0$	S^r-S^0
Estimated by Ito [1951]			−0.05			−0.86
Calculated from the equation of state of Barrow [1952]	−0.049	4.40	−.15	−0.213	13.16	−.54
Calculated from the equation of state of Kretschmer and Wiebe [1954	−.063	3.14	−.20	−.218	9.84	−.55

TABLE 30. Ethanol. Enthalpies and entropies of formation of dimers and tetramers from the monomer in the ideal gas state

Investigator	Dimer (kcal per mol)		Tetramer (kcal per mol)	
	ΔH_2	ΔS_2	ΔH_4	ΔS_4
For Gazulla, Garcia de la Banda and Perez Masia [1952] thermal conductivity	−7.0	−27.3		
Barrow [1952], heat capacity and heat of vaporization	−3.4	−16.6	−24.8	−81.5
Kretschmer and Wiebe [1954], *PVT* data	−5.42	−23.0	−22.14	−74.6

25° calculated from the tabulated values of $\Delta H_f°$, $\Delta G_f°$, and $S°$ from these same sources. They are $\Delta H° = -10.73$ kcal, $\Delta G° = -1.777$ kcal mol^{-1} and $\Delta S° = -30.01$ cal deg^{-1} mol^{-1}. Certainly some of this discrepancy may be ascribed to the difficulty in correcting the experimental measurements to the ideal gas state. The measurements of Stanley, Youell, and Dymock[3] [1934] were made at one atmosphere, but the others were at higher pressures. Gilliland, Gunness, and Bowles [1936] worked in the range of 83 to 200 atm and applied a correction for deviations from ideal behavior. However, this introduces considerable uncertainty into the results.

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[3] Thus these data are internally consistent well within the estimated uncertainties.

TABLE 31. Ethanol. Reported values. Fundamental vibration frequencies

Normal Vibrational Mode	Brickwedde, Moscow and Aston [1946]	Barrow [1952]	Plyler [1952]	Green [1961]
a' ν_1 OH stretch	3359	3660	3689	3689
ν_2 CH stretch(3)	2930	2940	2978	2983
ν_3 CH_2, CH_3 bending(2)	1455	1450	1464	1456
ν_4 CH_3 symmetric deformation	1387	1398	1393	1391
ν_5 CH_2 wag		1300		1320
ν_6 COH deformation	1274	1242	1218	1242
ν_7 CO stretch	1096	1070	1066	1067
ν_8 CH_3 rock	1051	1040	1013	1040
ν_9 CC stretch	883	895		877
ν_{10} CCO deformation	433	433	463	427
a'' ν_{11} CH stretch(2)	2930	2940	2978	2789
ν_{12} CH_3 antisymmetric deformation	1455	1450	1464	1456
ν_{13} CH_2 twist	1125	1270		1270
ν_{14} CH_3 rock	1160	1104		1104
ν_{15} CH_2 rock	814	805	971	801

TABLE 32. Ethanol. Barrier to internal rotation

Investigator	Type of Potential Function	Potential Barriers, cal mol^{-1}	
		$-CH_3$ Group	$-OH$ Group
Schumann and Aston [1938]	Symmetrical	3000	10,000
Brickwedde, Moscow and Aston [1949]	Unsymmetrical	1000, 3000	2375, 1560, 5930
Halford [1949]	Unsymmetrical	1800, 3000	2375, 4410
Barrow [1952]	Symmetrical	3300	800
Ito [1952]	Unsymmetrical	3000, 4000	2900, 1170
Green [1961]	Symmetrical	3300	800

Tests of Internal Consistency

The changes in enthalpy and entropy for the steps in the cycle, which consists of starting with liquid ethanol at 25 °C, converting to gas at the boiling point, back to the liquid at the boiling point, and then back to the initial state, are shown below. These quantities have been calculated from the selected values for ethanol in a manner similar to that done for methanol.

	ΔH kcal mol^{-1}	ΔS cal deg^{-1} mol^{-1}
liquid (25 °C)→real gas (25 °C, 59.77 mm Hg)	10.110±0.030	33.91±0.01
real gas (25 °C)→ideal gas (25 °C)	0.060±0.020	0.19±0.05
ideal gas (25 °C)→ideal gas (78.29 °C)	.893±0.020	2.68±0.10
ideal gas (59.77 mm Hg)→ideal gas (760 mm Hg)	.0	−5.05±0.02
ideal gas (78.29 °C, 760 mm Hg)→real gas (78.29 °C, 760 mm Hg)	−.216±0.010	−0.553±0.0
real gas (78.29 °C)→liquid (78.29 °C)	−9.255±0.010	−26.3±0.052
liquid (78.29 °C)→liquid (25 °C)	−1.590±0.020	−4.86±0.05
Sum	0.002±0.048	−0.01±0.17

TABLE 33. Ethanol. Summary of thermodynamic data derived from equilibrium constant for the reaction

$$C_2H_4\ (g)+H_2O\ (g)\rightarrow C_2H_5OH\ (g)$$

Investigator	Temperature Range, °C	Experimental Temperature		Corrected to 25 °C		
		ΔH^0 kcal mol^{-1}	ΔS^0 cal deg^{-1} mol^{-1}	ΔH^0	ΔG^0	ΔS^0
				kcal mol^{-1}		cal deg^{-1} mol^{-1}
Gilliland, Gunness, and Bowles [1936]	167–307	−7.78	−26.20	−7.42	+0.10	−25.23
Bliss and Dodge [1937]	320–378	−9.61	−28.23	−9.29	−1.18	−27.21
Applebey, Glass and Horsley [1937]	175–275	−9.88	−29.0	−9.53	−2.01	−28.0
Stanley, Youell, and Dymock [1934]	150–250	−9.61	−28.35	−9.28	−1.10	−27.45

Miscellaneous

Storvick and Smith [1960] have published a table of the enthalpy at various pressures and temperatures in the range of 136 to 243 °C for the saturated liquid and vapor and from 121 to 260 °C and 0 to 1000 atm for the superheated vapor. These data were based partly on their own measurements and partly on previously published data. They also published similar tables of ethanol-benzene and ethanol-*n*-pentane mixtures. Dannhauser and Bahe [1964] have measured the dielectric constant of the liquid from 25 to 240 °C and discuss the results in terms of the structure of polymeric species in the liquid. Liebermann [1949] has measured the dilational viscosity of the liquid at 17.4 °C. Gasparyan and Akopyan [1956] have measured the viscosity of the liquid at temperatures up to 190 °C. Sanyal and Mitra [1956] have discussed several semiempirical relations between viscosity and surface tension of ethanol. References to other viscosity measurements will be found in the Index.

Recommendations for Future Work

On the whole, the data on the thermodynamic properties of ethanol in the liquid and gas states are somewhat more consistent than they are for methanol. The same kind of uncertainty concerning the molecular species present in the gas phase exists for ethanol as it does for methanol. Additional experimental measurements of pressure, volume, and temperature in the gas phase are desirable, especially at high temperatures and pressures. Additional measurememts of vapor heat capacity at both low and high pressures are needed. There have been no measurements of the heat capacity of the liquid and solid at low temperatures, suitable for calculation of the absolute entropy by the third law, since the work of Kelley in 1929. Although there is no reason to believe that these data are seriously in error, a more recent study, comparable to the measurements of Carlson on methanol, would be helpful. This should include a careful study of the crystalline solid by both calorimetric and x-ray diffraction methods to determine whether or not the solid undergoes any phase transitions.

Index to the Bibliography

Numbers refer to the Bibliography, page 1–389.

References to data used in the selection of refractive index, density, boiling point, vapor pressure, and melting point are in boldface type.

Numbers in parentheses refer to sources of reviews, or theoretical calculations only.

Reference numbers under each property are listed in the order of date of publication.

Refractive Index
378, **895**, **840**, **990**, 510, **2014**, **1517**, 237, 773, **289**, **290**, **439**, 33, 1588, 1223, 770, 1345, **509**, **239**, 1333, **1324**, **80**, 1227, 1140, **406**, 8, **956**, 1201, **1646**, **1645**, **661**, 1080, **1724**, **712**, 1891, **1792**, **1843**, **1886**, 532, 248, 6, 1404, 1615, **1500**, 1856, **1893**, **966**, 1791, 721, **722**, **723**, **452**, **645**, 1377, **1853**, 201, **338**, **76**, 796, 1906, **24**, **737**, **1152**, **35**, 36, 85, 1139, 1437, 112, **229**, **1139**, **1586**, 719, 540, 25, 1292, **1069**, 1400, **231**

Density at 20 to 30 °C Only
989, 840, 290, 289, 1481, 33, 464, 592, 771, 1405, **869**, 1817, 1199, **1491**, 1087, 1345, 1479, 1482, **1992**, **239**, 88, **1151**, 750, **1959**, **1486**, 1333, **1448**, **1478**, **1272**, **1324**, **1140**, **80**, 1227, 956, 1201, 1075, **1331**, **1646**, **885**, 1202, 148, **531**, **1096**, 113, **1724**, **1656**, **1867**, **712**, 708, 984, 1792, **1551**, 997, 1886, 1222, 241, 6, 963, 1615, 1893, 853, 1810, 645, **452**, **966**, 1377, 1853, 835, 1745, 1682, 796, **338**, 1298, 24, **36**, 286, 1823, **85**, **1152**, **635**, **1437**, **965**, **229**, 540, 877, 1221, **231**

Density at all Temperatures
940, 941, **1163**, **469**, 1561, 1559, 1349, **1456**, 895, 576, 1556, **990**, 510, 2014, **1081**, **1517**, **2000**, **272**, **363**, 237, **1969**, **912**, **1875**, **33**, **1999**, 393, 440, 1868, 408, **436**, **1588**, **1295**, **1869**, **1688**, 1164, **1816**, 1165, **1425**, 838, 509, 1471, **1574**, **1804**, 1770, **646**, 1350, 1308, 1569, 42, **406**, **569**, 984, 142, 739, **2021**, **460**, **962**, **2013**, **1856**, 1823, **722**, 721, 723, **35**, (347), 25, 514, **1069**, 1281, 1147, **1154**, 1743, 481

Normal Boiling Point
940, 941, 1465, 989, 1163, 469, 1561, 1559, 868, 1349, 1560, 118, 1556, 990, 1765, 119, 1083, 2014, 1277, 2000, 272, 1395, 771, 1868, 1817, 1230, 211, **1816**, 1479, 1482, 1960, 814, 361, 509, **1480**, **88**, 239, 1471, 750, 1104, **642**, 1959, 1961, 1333, 1272, 1308, 1227, 1009, 42, 82, 9, **1646**, 148, 569, 1080, **1724**, 1722, 712, 1794, 396, 880, 1346, **1977**, **2021**, 125, 820, 591, 1134, 1161, 6, 1404, 1006, 1615, 1856, 1791, 1807, 1007, **452**, **453**, **721**, 1744, 1377, 452, 1745, 752, 1197, 338, 76, 1902, **1682**, 796, 737, 1297, **85**, **24**, 1906, 286, 1152, 808, **229**, 112, 244, 719, 701, 25, 1292, 1281, 1823, **1069**, 347, **231**

Vapor Pressure and Boiling Points at Other Pressures
1465, **935**, **866**, **1456**, **1454**, **1483**, **1571**, **1969**, 1481, **1999**, **440**, **408**, 1901, **1164**, 1230, **1799**, **120**, **1425**, **260**, **1798**, **1570**, 1082, **1569**, **1645**, **1723**, **1579**, **1551**, **1207**, **460**, **1818**, **453**, **964**, **1397**, **1853**, **85**, **1823**, 1400, (23), 910

Critical Temperature
1453, 1999, (282), (748), (1433), 898, 532, (852), (649), 1501, (347), (499)

Critical Pressure
1453, 1999, (282), (747), (915), (499)

Critical Volume and Density
1456, 1999, (747), (915), 481

Heat Capacity of the Solid
595, 1317, 885, 915

Normal Melting Point
983, 982, 272, 665, 408, **1768**, 1106, 1468, **595**, 1104, **1317**, 1194, 1195, **885**, **1538**, 148, 984, 210, **1807**, **452**, **1527**, 338, 1823, **342**

Heat of Fusion
595, 1317, 885

Heat Capacity of the Liquid
1083, 183, 595, 1961, 1317, 885, 155, 531, 501, 358, 1444, (2024)

Heat Capacity of the Real Gas
501, 125, 820, 1627, 690

P-V-T Data and Equation of State for the Real Gas
1456, 920, 1689, (831), 965

Calorimetric Heat of Vaporization at 25 °C
1147, 1870

Calorimetric Heat of Vaporization at Other Temperatures
1555, 1083, 219, 97, 1331, 885, 531, 125, 1398, (626), 923

Thermodynamic Functions of the Liquid and Real Gas at Various Temperatures and Pressures
1702, (625)

Heat of Combustion
1762, 138, 56, 57, 487, 1480, 1511, 1505, (1506), (1504), 287, 288

Equilibrium Constants of Gas Phase Reactions
1485, 162, 597, 41, 1687, 1676

Third Law Entropy of the Liquid at 25 °C
595, 1317, (1327), 885, (625)

Molecular Vibration Frequencies and Spectra
1399, (53), (90), (1190), 91, 529, 812, 530, 1740, 541, 1376, 1012, 1108, 619, (625), (1583), 46, 968, 818, 898, 379, 1844, 816, 1734, 456, 817, 1127, 814, 815, 668, 669, 470

Internal Rotation
686, 137, 830, 90, 1740, 1285, (625), 1583, 1, 1175

Molecular Geometry
812, 1175, 817, 813, 815

Thermodynamic Functions of the Ideal Gas
1583, 53, 209, 291, 673, 90, 830, 2026, 625, (624)

Association in the Gas Phase
1689, 90, 552, 965, (1258)

Association in the Liquid Phase
842, 769, (1754), 86, 1683, 114, 489, 314, 1706, 1048, 614, 1706, 182, 316, 529, 530, 1109, 1056, 115, 116, 102, 392, 898, 1451, 1758, 1757, 380, 78

1-Propanol

Properties of the Liquid Phase at Various Temperatures

Refractive Index

Refractive index data are not as extensive for 1-propanol as they are for ethanol. Some of the more reliable values of n_D at 20 and 25 °C are shown in table 37 and values at these and other temperatures listed in table 34. Smoothed values at other wavelengths are given in table 36. The agreement among different investigators in general is similar to that for ethanol.

Density

The selected densities were calculated from the Francis equation, with the constants listed in table 34. Ramsay and Young [1889] measured the density in the range of 0 to 190 °C, Kretschmer [1951] from 30 to 75 °C, and Ling and Van Winkle [1958] from 0 to 95 °C. Most of the other density data have been obtained in the vicinity of room temperature. The density data for methanol, ethanol, and 1-propanol, reported by Costello and Bowden [1958] in the range of 0 to 200 °C, are not based on new measurements but on the published values of Ramsay and Young [1889]. They have compared the density data on a series of alcohols to the Vershaffelt equation, $d(\text{liq})-d(\text{gas})=d_0(1-T/T_c)^m$. Martin, Campbell, and Seidel [1963] have expressed the density values of Ramsay and Young in the form of an equation which is a sum of terms containing powers of $(1-T/T_c)$.

Vapor Pressure and Boiling Points

The Antoine constants were calculated from experimental measurements of vapor pressure and heats of vaporization, as previously explained. The results are summarized in table 34. The best vapor pressure data in the range from 65 to 105 °C are given by Biddiscombe, Collerson, Handley, Herrington, Martin, and Sprake [1963], and the calculated values fall in the range of 0 to 1 mm above theirs. Richardson [1886] reported numerous values from 1 to 98 °C, and his values scatter in a random fashion about the calculated ones, except at the higher temperatures where his measurements are 10 to 15 mmHg too high. The data of Ramsay and Young [1889] are 1 to 5 mmHg higher than the calculated ones in the range of 0 to 110 °C, while those of Schmidt, G. C. [1891] are 0 to 16 mmHg low in the range from 29 to 116 °C. The data reported by Schmidt, G. C. [1926] are within about 4 mmHg of the accepted values, from 0 to 70 °C. Mundel [1913] has measured vapor pressures in the range of −43 to −13 °C. These were outside the temperature range covered in the calculation of the Antoine constants. Ambrose and Townsend [1963] made careful measurements from 133 to 263 °C and fitted the data to a six parameter equation. Martin, Campbell, and Seidel [1963] have fitted the vapor pressure data of Ramsay and Young [1889], Mathews and McKetta [1961], and other tabulations to a seven parameter equation. The calculated and observed heats of vaporization all agree to within about 150 cal, except for that of Bartoszewiczowna, which was higher by 822 cal and of McCurdy and Laidler [1963] which was higher by 387 cal.

Critical Properties

Critical Temperature

Ambrose and Townsend [1963] used a very carefully purified sample in their measurements. They estimated a purity of 99.94 mole percent, based on gas chromatography and freezing point. Values published by Grunberg and Nissan [1948] and Costello and Bowden [1958] shown in table 38 are not the result of experimental measurements. Thus there are only three independent measurements other than that of Ambrose and Townsend and this value was selected. It agrees closely to the value obtained by Ramsay and Young [1889].

Critical Pressure and Density

There are only two sets of independent measurements, those of Ambrose and Townsend and of Ramsay and Young. The critical pressure of Ambrose and Townsend is appreciably higher than that of the older work; but since Ambrose and Townsend undoubtedly used a much purer sample, their measurements of critical density and pressure were selected.

Solid-Liquid Phase Equilibria

Normal Melting Point

Only a few determinations of melting point have been made. The four most recent of these are listed in table 37. The melting point of Parks and Huffman [1926] was measured in a calorimeter and was selected as the best value.

Heat Capacity of the Solid and Liquid at the Melting Point

The only reported heat capacity data of crystalline solid 1-propanol are those of Parks and Huffman [1926]. Gibson, Parks, and Latimer [1920] and Parks and Huffman [1926] report the heat capacity of the liquid and of the glass state down to temperatures around 80 K.

Heat of Fusion

The only experimental measurement is that of Parks and Huffman [1926] so their value was selected.

Properties of the Liquid at 25 °C

Heat Capacity

All available data are summarized in table 40. The selected value was read from a smooth curve drawn through the experimental points in the vicinity of 25 °C.

Absolute Entropy

The value shown in table 40 is based on the heat capacity data of Parks and Huffman [1926] as revised by Parks, Kelley, and Huffman [1929]. A value slightly higher than this was selected to attain internal consistency with other data.

Heat of Combustion

Snelson and Skinner [1961] and Chao and Rossini [1965] have made the most recent measurements. The selected value was an average of these two values, with somewhat more weight given to that of Chao and Rossini.

Properties of Real Gas

Equation of State

Ingle and Cady [1938] measured the gas density from 100 to 118° and calculated the apparent molecular weight. These data indicate some degree of association in the vapor phase. Ramsay and Young [1889] (later revised by Young, S. [1910]) and Ambrose and Townsend [1963] have measured orthobaric volumes of liquid and vapor up to the critical temperature. Ambrose and Townsend fitted their data to empirical equations. Martin, Campbell, and Seidel [1963] fitted the *P-V-T* data of Ramsay and Young to an equation containing 13 parameters. Foz Gazulla, Morcillo, Perez Masia, and Mendez [1954] and Foz Gazulla, Morcillo, and Mendez [1954] reported measurements of pressure, volume and temperature at low pressure. Cox, J. D. [1961] calculates the second virial coefficient from *P-V-T* measurements in the range 340 to 623 mmHg and 105 to 150 °C. He found that the second virial coefficient can be represented by the equation,

$$\log(-B_p') = 12.491 - 3.7 \log T$$

Mathews and McKetta [1961] used the type of equation of state proposed by Weltner and Pitzer [1951] and found that the second and fourth virial coefficients as derived from the *P-V-T* data of Foz Gazulla et al., and their vapor heat capacity measurements could be expressed by,

$$B_p' = 130 - 0.0353\,T \exp\left(\frac{1711}{\mathrm{T}}\right) \text{ ml mol}^{-1}$$

$$D_p' = -4.168 \times 10^{-16}\,T \exp\left(\frac{12669}{T}\right) \text{ ml atm}^{-2}\text{ mol}^{-1}.$$

This gives the change of enthalpy and entropy for formation of dimers as $\Delta H_2 = -3.40$ kcal mol^{-1} and $\Delta S_2 = -15.4$ cal deg^{-1} mol^{-1} and for formation of tetramers

TABLE 34. 1-Propanol. Selected values. Physical and thermodynamic properties

Temp. °C	Refractive Index, n_D	Density g cm^{-3}	Vapor Pressure, mmHg
−20		0.8344	
−10		.8269	
0		.8193	
+10		.8116	
14.3			10
15	1.3873		10.5
20	1.38556	.80375	14.9
25	1.38370	.79975	20.9
30	1.3818	.7957	28.7
35			39.0
40	1.3778	.7875	52.4
45			69.5
50	1.3735	.7790	91.2
51.73			100
55			118.4
60		.7704	152.2
65			193.9
65.65			200
70		.7614	244.8
75			306.5
80		.7522	380.7
81.16			400
85			469.4
90		.7426	574.6
95			698.7
97.20			760
100		* .7326	844.2
105			1013.7
110		* .7222	1182.6
120		* .7112	

Data For Phase Transitions

Initial	Final	Temp. °C	dt/dP deg mm^{-1}	Pressure mmHg	ΔH kcal mol^{-1}	$d\Delta H/dt$	ΔS	ΔC_p
						cal deg^{-1} mol^{-1}		
c	liq	−126.2±0.5		760	1.242±.005	15.6±0.6	8.45±0.03	7.1±0.6
liq	g	25	0.733	20.85±0.2	11.36±.04	−13.6±.6	38.10±0.1	−12.4±0.4
liq	g	97.20	.03473	760	9.982±0.01	−26.3±0.8	−26.95±0.04	−17.2±0.7

Condensed Phase Heat Capacity

State	Temp. °C	C_p
		cal deg^{-1} mol^{-1}
c	−126.2	18.3±0.5
liq	−126.2	25.4±0.3
liq	97.20	46.1±0.5

Properties of the Saturated Real Gas

Temp. °C	H^r-H^0	S^r-S^0	$C_p{}^r-C_p{}^0$
	kcal mol^{-1}	cal deg^{-1} mol^{-1}	
25	−0.016±0.004	−0.05±0.01	0.60±0.2
97.20	−0.170±0.01	0.36±0.02	4.5±0.5

Data for the Standard States at 25 °C

State	Heat of Combustion $\Delta H_c{}^0$ kcal mol^{-1}	Heat of Formation $\Delta H_f{}^0$ kcal mol^{-1}	Entropy S^0 cal deg^{-1} mol^{-1}	Gibbs Energy of Formation $\Delta G_f{}^0$ kcal mol^{-1}	Heat Capacity, C_p cal deg^{-1} mol^{-1}
liq	−482.75±0.05	−72.66±0.05	46.5±0.2	−40.78±0.06	33.7±0.3
g	−494.13±0.06	−61.28±0.06	77.61±0.03	−38.67±0.07	20.82±0.1

Critical Constants

Temp. 263.56 °C, 536.71 K	Pressure 51.02 atm	Density 0.275 g cm^{-3}

			Constants in Vapor Pressure and Density Equation								
			Antoine Equation				Francis Equation				
			Temp. Range	*A*	*B*	*C*	Temp. Range	*A*	$B \times 10^3$	*C*	*E*
			2 to 120 °C	7.84767	1499.21	204.64	−21 to 180 °C	0.88813	0.5448	21.536	313.09

* At saturated vapor pressure

TABLE 35. 1-Propanol. Selected values. Thermodynamic functions of the ideal gas at one atmosphere

Temperature K	Entropy S^0 cal deg^{-1} mol^{-1}	Heat Capacity C_p^0 cal deg^{-1} mol^{-1}	Enthalpy Function $(H^0-H_0^0)/T$ cal deg^{-1} mol^{-1}	Gibbs Energy Function $(G^0-H_0^0)/T$ cal deg^{-1} mol^{-1}	Heat of Formation ΔH_f^0 kcal mol^{-1}	Gibbs Energy of Formation ΔG_f^0 kcal mol^{-1}
0	0	0	0	0	−55.71	−55.71
273.15	75.86	19.67	13.95	−61.95	−60.87	−40.55
298.15	77.61	20.82	14.48	−63.11	−61.28	−38.67
300	77.71	20.91	14.52	−63.19	−61.31	−38.52
400	84.31	25.86	16.74	−67.57	−62.84	−30.64
500	90.54	30.51	19.04	−71.50	−64.14	−22.42
600	96.44	34.56	21.29	−75.15	−65.19	−13.95
700	102.01	38.03	23.43	−78.58	−66.03	−5.33
800	107.29	41.04	25.46	−81.83	−66.67	+3.40
900	112.26	43.65	27.32	−84.94	−67.16	12.18
1000	116.99	45.93	29.08	−87.91	−67.47	21.03

from the monomer as $\Delta H_4 = -25.18$ kcal mol^{-1} and $\Delta S_4 = -75.4$ cal deg^{-1} mol^{-1}. Zhuravlev and Kasavchinskii [1963] have given an 18-equation of state parameter based on published data, which they claim is valid in the range O−360 °C and at reduced densities of 0 to 1.6.

Heat Capacity

Experimental measurements have been made by Bennewitz and Rossner [1938] at 137 °C and 748 mmHg, by Sinke and De Vries [1953] at 100 to 164 °C and 750 mm, and by Mathews and McKetta [1961] at 98 to 178 °C and 250 to 1265 mmHg. Jatkar and Lakshimarayan [1946] and Jatkar [1939] have calculated the vapor heat capacity from measurements of the speed of sound. All these data are summarized and compared by Mathews and McKetta. Eubank and Smith [1962] report relative enthalpy data, measured calorimetrically, in the range 149 to 282 °C and 3.5 to 61 atm pressure.

Corrections to the Ideal Gas State

Values calculated from the equations of state of Cox, and Mathews and McKetta, are given in table 43. The value estimated from the graph of Eubank and Smith cannot be considered reliable since a considerable extrapolation from higher temperatures and pressures is involved.

Vapor-Liquid Equilibrium at 25 °C

Vapor Pressure

The value listed was calculated from the Antoine constants.

TABLE 36. 1-Propanol. Selected values. Refractive index at various temperatures and wavelengths

Symbol	Wavelength,	Refractive Index, n	
		15 °C	20 °C
$\mathrm{He_{red}}$	6678.2	1.3853	1.3833
$\mathrm{H_c}$	6562.8	1.3857	1.3837
$\mathrm{Na_D}$	5892.6	1.3873	1.38556
$\mathrm{He_{blue}}$	5015.7	1.3914	1.3898
$\mathrm{H_F}$	4861.3	1.3923	1.3902
$\mathrm{H_{G'}}$	4340.5	1.3960	1.3918

Heat of Vaporization

Most of the recent values listed in table 39 are in fairly good agreement. The value of McCurdy and Laidler [1963] seems definitely low. The selected value was based on the results of Mathews and McKetta and of Wadso [1966], and was adjusted for internal consistency.

Temperature Derivative of the Heat of Vaporization

The value of $d\Delta H/dT - \Delta C_p$ calculated by means of equation (32) of appendix C, with the selected value of H_r and the equation of state of Cox, is −0.43 cal deg^{-1} mol^{-1}. The equation of state of Mathews and McKetta gives −1.24 cal deg^{-1} mol^{-1} for this quantity. The corresponding values of $d\Delta H/dT$ obtained by substituting the selected heat capacities of liquid and vapor are −12.7 and −13.6 cal deg^{-1} mol^{-1}, respectively. The equation for heat of vaporization obtained by Mathews and McKetta gives −15.7 cal deg^{-1} mol^{-1} at 25 °C. Since all of these calculations use equations at temperatures outside the range of the original experimental measurements, there is an uncertainty of about 1 cal deg^{-1} mol^{-1} connected with each of them.

Vapor-Liquid Equilibrium at the Normal Boiling Point

Normal Boiling Point

The boiling point at one atmosphere was calculated from the Antoine constants.

Heat of Vaporization

The selected value was a compromise among the various values reported in table 39 and the requirements of internal consistency. It agrees closely with the value selected by Martin, Campbell, and Seidel [1963] from an analysis of the available data.

Heat Capacity of the Liquid

The selected value was interpolated from the values of Eucken and Eigen [1951] who measured the heat capacity from 20 to 130 °C.

Temperature Derivative of the Heat of Vaporization

$d\Delta H/dT - \Delta C_p$ calculated from the equation of state of Mathews and McKetta [1961] was −9.08, which gives $d\Delta H/dT$ of −26.3 when combined with ΔC_p. A value of −26.0 is obtained from the equation of heat of vaporization as a function of temperature given by Mathews and McKetta.

Properties of the Ideal Gas State

Molecular Parameters

The list of references ot the molecular vibration spectra of 1-propanol which are given in the Index probably includes all those which are suitable for use in determining the fundamental vibration frequencies. They

TABLE 37. 1-Propanol. Reported values. Simple physical properties

Investigators		Vapor Pressures and Boiling Points		Freezing Point	Density, *d* g cm^{-3}		Refractive Index, n_D	
		°C	mmHg	t_m, °C	20 °C	25 °C	20 °C	25 °C
1-Propanol, C_3H_8O, mol wt. 60.097, state at 25 °C liq.								
Naccari and Pagliani	[1881]					0.8004		
Perkin	[1884]					.80034		
Traube	[1886]				0.8051			
Ramsay and Young	[1889]	97.5	760		.8035			
Jahn	[1891]				.80419			
Schutt	[1892]				.80507		1.38549	
Loomis	[1900]	97.2	760		.80406			
Young and Fortey	[1902]	97.18	760		.80410			
Doroshevskii and Dvorzhanchik	[1908]	97.2	760				1.38547	
Doroshevskii and Rozhdestvenskii	[1908]	97.2–97.3	760					
Doroshevskii	[1909]	97.20	760					
Holmes and Sageman	[1909]	97.2–97.4	760			.79971		
Young	[1910]				.8032			
Doroshevskii and Polyanskii	[1910a]	97.26						
Timmermans	[1910]				.80358			
Wrewski	[1912]	96.83–96.93	760				1.38499	
Wroth and Reid	[1916]					.80715		
Richards and Davis	[1920]	96.6–96.8	760					
Brunel, Crenshaw, and Tobin	[1921]	97.19	760			.79975		1.3833
Brunel	[1923]	97.175	760			.7998		1.3834
Grimm and Patrick	[1923]	97.19	760					
Norris and Ashdown	[1925]	97.2–97.3	760			.79969		
Parks and Huffman	[1926]			−126.2		.8005		
Lloyd, Brown, Bonnell, and Jones	[1928]					.79970		
Berner	[1929]				.80355		1.38533	
Lund and Bjerrum	[1931]				.80335	.79934		
Butler, Thomson, and Maclennan	[1933]	97.19	760			.7999		
Cady and Jones	[1933]			−127.1				
Trew and Watkins	[1933]	96.1	760			.80001		1.38343
Vosburgh, Connell, and Butler	[1933]					.79982		
Timmermans and Delcourt	[1934]	97.15	760					
Webb and Lindsley	[1934]	97.25	760					
Coull and Hope	[1935]					.8016		1.3481
Tomanari	[1936]				.8041		1.38644	
Wojciechowski	[1936]	97.209	760					
Zepalova-Mikhailova	[1937]	97.15			.80357		1.3856	
Venkataraman	[1939]							1.38379
Washburn, Brockway, Graham, and Deming	[1942]							1.3838
Fischer and Reichel	[1943]						1.38534	
Vogel	[1948]	96.4	760		0.8043		1.38556	
Carley and Bertelsen	[1949]	97.19	760				1.3860	
Tschamler, Richter, and Wettig	[1949b]	96.4	760	−126.5		0.7983		
Sackmann and Sauerwald	[1950]			−127.6				
Dimming and Lange	[1951]	95.4	760			.80087		1.38511
Kretschmer	[1951]					.79950		
Ballard and Van Winkle	[1952]	97.44	760				1.38575	
Cook	[1952]	97.2	760		.8042		1.3849	
Hill and Van Winkle	[1952]	97.0	760				1.38581	
Staveley and Spice	[1952]	97.15	760		.8035			
Anisimov	[1953b]					.80001		1.38343
McKenna, Tartar, and Lingafelter	[1953]	97.2	760					1.3837
Purnell and Bowden	[1954]	97.2				.79988		1.3840
Mathers and Pro	[1954]							1.3840
Baker	[1955]					.7999		1.3854
Costello and Bowden	[1958]	97.4	760		.8035			
Ling and Van Winkle	[1958]	97.19	760				1.38572	1.38391
Mathews and McKetta	[1961]	97.19	760					
Brown and Smith	[1962b]	97.08	760			.79959		1.38314
Chu and Thomson	[1962]					.7998	1.3854	1.3833

TABLE 37. 1-Propanol. Reported values. Simple physical properties—Continued

Investigators	Vapor Pressures and Boiling Points		Freezing Point	Density, d g cm^{-3}		Refractive Index, n_D	
	°C	mmHg	t_m, °C	20 °C	25 °C	20 °C	25 °C
1-Propanol, C_3H_8O, mol wt. 60.097, state at 25 °C liq.							
Paraskevopoulos and Missen [1962]					.79984		
Ambrose and Townsend [1963]	97.15	760		.8035			
Biddiscombe, Collerson, Handley, Herington, Martin, and Sprake [1963]	97.151	760					
Selected value [1967]	97.20±0.01 14.30±0.1	760 10	−126.2 ±0.5	.80375 ±0.0001	.79975 ±0.0001	1.38556 ±0.0001	1.38370 ±0.0001

Antoine constants: A 7.84767, B 1499.21, C 204.64 dt/dp at 760 mmHg, 0.03473 °C/mmHg

TABLE 38. 1-Propanol. Reported values. Critical properties

Investigator	t_c, °C	P_c, atm	d_c, g cm^{-3}
Ramsay and Young [1889]	263.7	50.16	0.28
Young [1910]	263.7	50.16	0.2734
Khalivov [1939]	264.1		
Fischer and Reichel [1943]	264.1		
Grunberg and Nissan [1948]	263.7		
Costello and Bowden [1958]	263.7		
Ambrose and Townsend [1963]	263.56	51.02	0.2754
Efremov [1966]	264.	51.0	0.273

include infrared and Raman spectra in the gaseous and liquid states and in solution. This indicates fairly extensive literature on the subject. Plyler [1952] published a partial assignment and selection of fundamental vibrations, and Dyatkina [1954] used a more complete assignment in the calculation of tables of thermodynamic functions. Green [1961] and Mathews and McKetta [1961] reexamined the available information and used improved assignments to calculate the thermodynamic functions, but Green did not publish the frequencies which he used. The complete unambiguous assignment of fundamental vibration frequencies is a difficult task; not only because of the relative complexity of the molecule (30 normal modes), but also because the molecular spectra of the liquid phases, and to some extent of the gas phase, are complicated by the presence of associated species.

Dr. Kunio Fukushima recently examined all of the available spectroscopic and auxiliary data on 1-propanol and made a tentative assignment of the fundamental vibration frequencies. These are listed in table 45 under the heading "Recommended." Assignments given by Plyer and by Mathews and McKetta are also listed in table 45 for comparison. Although a complete discussion of the procedure used in arriving at the "Recommended" values would be quite lengthy, the following observations will give some indication of the basis of selection of the more important vibrations.

TABLE 39. 1-Propanol. Reported values. Heats of vaporization

Investigator	ΔH_v at 25 °C	ΔH_v at t_b	Method and Remarks
Ramsay and Young [1889]		9.90	Calculated from vapor pressure.
Louguinine [1898]		9.83	Calorimetric
Brown, J. C. [1903]			
Bartoszewiczowna [1931]	10.7		Calorimetric, corrected to 25 °C
Bennewitz and Rossner [1938]		9.98	Calorimetric.
Plewes, Jarding and Butler [1954]		10.01	Calorimetric.
Williamson and Harrison [1957]		9.98	Calorimetric, extrapolated.
Williamson and Harrison [1957]	11.31–11.41		Corrected to 25 °C by McCurdy and Laidler.
Green [1906]	11.35		Analysis of published vapor pressure data.
Cosner, Gagliardo, and Storvick [1961]		9.85	Analysis of published data.
Mathews and McKetta [1961]	11.41	9.85	Calorimetric, extrapolated to 25 °C by equation.
Martin, Campbell, and Seidel [1963]	11.55	9.98	Analysis of published data.
Biddiscombe, Collerson, Handley, Herrington, and Sprake [1963]		9.950	Calculated from vapor pressure.
McCurdy and Laidler [1963]	11.13		Calorimetric.
Wadso [1966]	11.31		Calorimetric.
Selected Antoine constants	11.51	9.77	Calculated.

Vapor State. According to the electron diffraction studies of Aziz and Rogowski [1961 and 1964], molecules of 1-propanol in the vapor are predominately in the *trans* conformation with respect to rotation about the CH_2-CH_2 axis. Thus the infrared spectra of the vapor apply to the *trans* rotational isomer, and assignments of the CH_2 vibrations can be made by analogy with those for *trans-n*-butane, which are well known. The assignment of the OH in-plane bending vibration is supported by the work of Stuart and Sutherland [1956] and by the frequency shift observed in C_3H_7OD by Tarte and Depontniere [1957]. The frequencies associated with torsion about the three axes of internal rotation are considerably important in calculating thermodynamic functions. Mathews and McKetta [1961] did not assign frequencies to these modes but did adopt the following barriers to internal rotation: 800 cal mol^{-1} for the rotation of the -OH group and 3100 cal mol^{-1} for the rotation of the -CH_3 group. An unsymmetrical function was used for the rotational potential about the C-C axis in the ethyl group to represent the difference in energy between the *trans* and *gauche* forms. Potential energies of 2310 and 850 cal mol^{-1} were selected. The recommended assignment of 160 cm^{-1} to the CH_2-CH_2 rotation was made because this frequency is expected to be lower than the frequency for rotation of the methyl group, and the only Raman absorption below 240 cm^1 is the one at 160 cm^{-1}. The recommended assignment for the methyl rotation was based on analogy with other CH_3CH_2X compounds and on the weak intensity of the corresponding Raman line. The frequency for the -OH rotation is uncertain, because about half the infrared band is obscured by other bands. However, it agrees well with the frequency calculated using the force constants of methanol.

Liquid State. The vibrational spectrum of the liquid is primarily that of associated molecules. The fact that the Raman line at 463 cm^{-1} is the same in the liquid as in the vapor shows that the most abundant rotational isomer in the liquid is the *trans* isomer, as it is the vapor. The spectrum of the liquid may then be interpreted as that of an equilibrium mixture of *trans* and *gauche* isomers. On the basis of the effect of temperature on the relative intensities of lines for the *trans* and *gauche* isomers, Bertholet, C. [1950] has deduced that the difference in energy between the two isomers is 820±120 cal mol^{-1}. The effect of association is most pronounced on the frequencies of vibrations associated with the -OH group.

Table 45 gives recommended values for all thirty normal frequencies of the monomer of 1-propanol in the *trans* conformation. In addition some of the frequencies which arise from the associated molecules in both the *trans* and the *gauche* conformation are given. These are all derived from the spectra of the liquid. There are four notable discrepancies between the assignments recommended here and those of Mathews and McKetta: The assignment of 760 cm^{-1} to the skeletal deformation (C—C—C—bend) is obviously an error; furthermore, the frequencies of 1103, 1341, and 1393 cm^{-1} which they list belong to an associated molecule rather than to the monomer.

TABLE 40. 1-Propanol. Reported values. Heat capacity and entropy of the liquid at 25 °C

Investigator	C_p^0(1)	Remarks	S^0(1), Third law
Bose and Mueller [1907]	34.3	From equation, calorimetric	
Gibson, Parks and Latimer [1920] and Parks and Huffman [1926]	34.0	Graphical extrapolation from lower temperatures	
Parks, Kelley, and Huffman [1929] (revision of Parks and Huffman)			46.1
Eucken [1948]	34.2	Interpolated	
Eucken and Eigen [1951]	32.7	Extrapolated from higher temperatures	

TABLE 41. 1-Propanol. Reported values. Heat capacity and entropy of the ideal gas at 25 °C

Investigator	$C\mathrm{r}^0$(g)	Remarks	S^0(g) from molecular parameters
Kobe, Harrison, and Pennington [1951]	20.6	Statistical calculation	
Dyatkina [1954]			77.33
Green [1961]	20.82	Statistical calculation	77.59
Mathews and McKetta [1961]	21.0	Derived from calorimetric measurement	77.63
Martin, Campbell and Seidel [1963]	20.45	Analysis of published data	

TABLE 42. 1-Propanol. Reported values. Heat of combustion of the liquid at 25 °C

Investigator	$-\Delta H_c^0$(1) kcal mol^{-1}
Louguinine [1880]	480.1
Thomsen [1886]	*487.2
Zubov [1898] (recalculated by Swietoslawski [1920])	480.9
Richards and Davis [1920]	483.3
Verkade and Coops [1927] (recalculated by Green [1960])	482.23
Snelson and Skinner [1961]	483.12
Chao and Rossini [1965]	482.64

* ΔH_c of gas reported. Value corrected to the liquid.

TABLE 43. 1-Propanol. Differences in properties between real gas and ideal gas

Sources	at 25 °C and 20.85 mmHg			at 97.54 °C and 760 mmHg		
	H^r-H^0	$C_p{}^r-C_p{}^0$	S^r-S^0	H^r-H^0	$C_p{}^r-C_p{}^0$	S^r-S^0
Calculated from equation of state of Cox, J. D. [1961]	−0.007	0.09	−0.019	−0.11	1.10	−0.235
Calculated from equation of state of Mathews and McKetta [1961]	−.015	.57	−0.042	−.176	4.68	−0.394
Estimated from graph given by Eubank and Smith [1962]				−.83		

TABLE 44. 1-Propanol. Comparison of virial coefficients and compressibility factor, Z, derived from experimental measurements

	Virial coefficients			Pressure, atmospheres						
	B_p' cm^3	C_p' cm^3 atm^{-1}	D_p' cm^3 atm^{-2}	0.05	0.1	0.25	1	2	5	10
				Values of $(1-Z)\times100$						
Temperature = 50 °C										
Cox, J. D. [1961]	(−1608)			(0.303)	(0.606)					
Mathews and McKetta [1961]	(−2143)		(−14370)	(.411)	(.862)					
Temperature = 100 °C										
Foz Gazulla, Morcillo, Masia, and Mendes [1954]	−1128			0.184	0.368	0.921	3.68			
Cox, J. D. [1961]	−964			(.154)	(.308)	(.771)	(3.08)			
Mathews and McKetta	−1161		−86.8	.190	.379	.952	4.08			
Temperature = 150 °C										
Cox, J. D. [1961]	−593			(0.085)	(0.171)	(0.427)	(1.708)	(3.42)	(8.54)	
Mathews and McKetta [1961]	−722		−1.78	.104	.208	.520	2.085	(4.20)	(11.04)	
Temperature = 200 °C										
Cox, J. D. [1961]	(−392)			(0.050)	(0.100)	(0.252)	(1.010)	(2.02)	(5.05)	(10.10)
Mathews and McKetta [1961]	(−491)		(−0.0842)	(.063)	(.126)	(.316)	(1.265)	(2.53)	(6.35)	(12.86)

Values in parenthesis have been extrapolated outside the experimental range of temperature or pressure

TABLE 45. 1-Propanol. Summary of published and newly selected values of fundamental vibration frequencies in the gaseous state

Type of Vibrational Mode	Species	Frequencies, in cm^{-1} Recommended	Plyler [1952]	Mathews and McKetta [1961]
/CH_2—CH_2/ internal rotation	*t*	160		
CH_3—CH_2 internal rotation	*t, ta, ga*	240		
/CH_2—OH internal rotation	*t*	286	267	
skeletal deformation	*t, ta*	332		760
skeletal deformation	*t, ta*	463	427	463
OH out of plane bending	*ta*	670		
—CH_2 rock	*t, ta*	758		730
—CH_2 rock	*ga*	821		
	t, ta	858	877	860
C—C stretch	*t, ta*	898		890
CH_2 rock	*ga*	928		
CO stretch	*t, ta*	971		971
CH_3 rock	*t, ta*	1013		1103
	t, ta	1047		1052
	t, ta	1066	1067	1066
CO stretch (bonded)	*ta*	1100		
OH in plane bending	*t*	1218		1393
CH_2 wag	*t, ta*	1237	1242	1272
CH_2 wag	*ga*	1251		
CH_2 twist	*t, ta*	1276		1220
CH_2 wag	*t, ta*	1300		1299
CH_2 twist	*t, ta*	1300		1341
CH_3 symmetrical deformation	*t, ta*	1393	1391	1381
CH_3 asymmetric deformation	*t, ta*	1451(2)	1456	1450(2)
CH_2 bending	*t, ta*	1451		1463
CH_2 bending	*t, ta*	1467		1478
CH_2 symmetric stretch	*t, ta*	2892(2)		2940(2)
CH_3 symmetric stretch	*t, ta*	2892		2940
CH_2 antisymmetric stretch	*t, ta*	2929	2994	2940
CH_2 antisymmetric stretch	*t, ta*	2946		2940
CH_3 asymmetric stretch	*t, ta*	2978(2)		2940(2)
OH stretch (bonded)	*ta*	3360		
OH stretch	*t*	3687	3689	3680

(2) following the frequency indicates doubly degenerate vibration. Species are designated as: *t*—trans isomer, monomer; *ta*—trans isomer, associated; *ga*—gauche isomer, associated.

Entropy at 25 °C

The third law entropy is 0.2 cal deg^{-1} mol^{-1} lower than the one calculated from statistical mechanics at 298.15 K. However, since the uncertainty in the third law value is estimated as 0.6 cal deg^{-1} mol^{-1}, the statistical value was adopted.

Heat Capacity

Bennewitz and Rossner [1938] corrected their measured value at 137 °C to the ideal gas. Kobe, Harrison, and Pennington [1951] published tables of ideal gas heat capacity which were calculated from vibration frequencies and other molecular parameters. They did not report the values selected for the molecular parameters, however. They did given an equation of the form, $C_p{}^0=a+bT+cT^2+dT^3$. Cosner, Gagliardo, and Storvick [1961] used this equation in their calculations on the thermodynamic properties of the gas phase. Mathews and McKetta [1961] extrapolated their measured values of the vapor heat capacity to zero pressure, using their equation of state, and obtained the following equation for the ideal gas heat capacity.

$$C_p{}^0=7.365+4.400\times10^{-2}T$$
$$+5.507\times10^{-6}T^2 \text{ cal deg}^{-1}\text{ mol}^{-1}$$

This is valid in the range 371.2 to 451.2 K. Martin, Campbell, and Seidel [1963] represent all the available data by use of the following equation.

$$C_p{}^0=-2.30593+9.23626\times10^{-2}T\times-5.7999\times10^{-5}T^2$$
$$+1.764816\times10^{-8}T^3 \text{ cal deg}^{-1}\text{ mol}^{-1}.$$

Thermodynamic Functions

Complete tables of thermodynamic functions from 273.15 to 1000 K calculated by statistical procedures have been published by Dyatkina [1954], Chermin [1961], Mathews and McKetta [1961], and Green [1961]. The values of Mathews and McKetta and of Green appear to be identical, except for minor variations in the last figure due to round-off procedures. The values of S^0, $C_p{}^0$, $(G^0-H_0{}^0)/T$ and $H^0-H_0{}^0)/T$ published by Chermin are within a few tenths of a calorie per degree per mol of those of Mathews and McKetta and Green. The data of Dyatkina differ considerably from the others, particularly at the high temperatures. Green pointed out that Dyatkina had made some errors in assignments of fundamental frequencies. The values of Green were adopted.

Chemical Equilibria

No data on chemical equilibria involving 1-propanol in the gas phase were found. This is probably a reflection of the fact that 2-propanol is more stable than 1-propanol at all temperatures, and thus very little 1-propanol can be present at equilibrium. The equilibrium ratio of 2-propanol to 1-propanol is about 100 at 298 and 1.6 at 1000 K.

Tests of Internal Consistency

The consistency of the vapor-liquid equilibria data is indicated by the following cycle, which is similar to that used to check the data of methanol and ethanol.

	ΔH kcal mol^{-1}	ΔS cal deg^{-1} mol^{-1}
liquid (25 °C)→real gas (25 °C, 20.85 mmHg)	11.359±0.02	38.10±0.08
real gas (25 °C)→ideal gas (25 °C)	0.016±0.004	0.05±0.01
ideal gas (25 °C)→ideal gas (97.54 °C)	1.647±0.01	−4.79±0.01
ideal gas (20.85 mmHg)→ideal gas (760 mmHg)	0.0	−7.15±0.01
ideal gas (97.54 °C, 760 mmHg)→real gas (97.54 °C, 760 mmHg)	−.170±0.01	−0.36±0.02
real gas (97.54 °C)→liquid (97.54 °C)	−9.982±0.01	−26.95±0.04
liquid (97.54 °C)→liquid (25 °C)	−2.873±0.02	−8.53±0.05
Sum	−0.003±0.033	−0.05±0.10

Miscellaneous

Dannhauser and Bahe [1964] measured the dielectric constant of the liquid from 25 to 250 °C and calculated the thermodynamics of hydrogen bond formation in the liquid. Nemeth and Reed [1964] calculated a collision diameter of 7.06 Å from values of the viscosity of the vapor. Cosner, Gagliardo, and Storvick [1961], Martin, Campbell, and Seidel [1963], and Eubank and Smith [1962] published tables and graphs of the thermodynamic properties of the liquid and vapor up to high temperatures and pressures. Eubank and Smith included some calorimetric measurements of relative enthalpy. The other two reports are based on previous data available at the time of publication. According to Martin, Campbell, and Seidel, an error was made in calculating the entropy reported by Cosner, Gagliardo, and Storvick.

Recommendations for Future Work

Although a fairly complete set of thermodynamic data can be found for 1-propanol, some additional confirmation is desirable. A more precise third law entropy based on modern heat capacity data is needed. This should also include a check on the heat of fusion and an accurate measurement of the triple point. Additional accurate measurements of pressure-volume-temperature relations and heat capacity in the vapor phase will help to determine the kind of association which occurs in the gas.

Index to the Bibliography

Numbers refer to the Bibliography, page 1–389.

References to data used in the selection of refractive index, density, boiling point, vapor pressure, and melting point are in boldface type.

Numbers in parentheses refer to sources of reviews, or theoretical calculations only.

Reference numbers under each property are listed in the order of date of publication.

Refractive Index

234, **840**, **990**, 1585, 511, **439**, **1991**, **509**, 354, 239, **238**, 1333, 1227, 1855, **135**, **126**, 1080, **1803**, **1779**, 1891, **351**, **1792**, 2021, **1843**, 926, **1885**, **532**, 6, 1404, **1819**, **1856**, **1893**, 269, 1519, 201, 1171, 1224, 1377, 180, 423, 1388, **76**, **338**, **760**, 35, 36, 1145, **1152**, 1906, **1437**, **1139**, 70, 630, 1292, **1069**, 231, **293**, 1279

Density, 20–30 °C Only

1801, 989, **840**, 1564, 1481, 771, 1771, 488, 1087, **1992**, **239**, 1959, 1333, 1350, **1272**, 1227, 1322, **1075**, **135**, 148, **1803**, **254**, 351, 1792, 997, 1222, 1885, 6, 853, 1893, **1807**, 1810, 835, 723, 721, 1377, 1224, 1744, 1682, **338**, 1145, **36**, **1437**, **70**, **1313**, **231**

Density at all Temperatures

1503, 1072, 234, **1236**, 2011, 1561, 1559, **1349**, 1560, 2012, 576, 1556, **1585**, 990, 511, **1455**, **1081**, 2002, **2000**, 439, **443**, **534**, 441, 440, 1999, **436**, 1991, **1591**, **55**, **838**, 509, 1471, **1770**, **238**, 1308, 1569, **42**, **1096**, **904**, **1867**, **1779**, 739, **1667**, **2021**, 1371, **1856**, 1527, **961**, **423**, **35**, 1145, **1069**, (347), **1154**, 1743, **293**, 1131, **23**, 1147, 876

Normal Boiling Point

989, 1503, 1072, 234, 1561, 2011, 1559, 868, 1349, 1560, 1572, 1556, 990, 1585, 1765, 1564, 119, 1083, 2033, 1081, 1257, **2002**, 272, 439, 771, 443, 435, 440, 441, 1768, 1991, 211, 55, 1230, 1960, 838, 509, 1480, 595, 239, 1471, **238**, 1959, 642, 1409, 1746, 1333, 1272, 1308, 1994, 1009, 1227, 573, 42, 1726, 1075, 148, 143, 1080, 242, 870, **254**, 921, 1794, 1803, 1779, 1891, 880, **1977**, **2021**, 820, 351, 125, 591, 902, 926, 1162, 1396, 6, 1554, 1006, 1856, 269, 721, 1807 ,1519, 1377, 1744, 1224, 1745, 1437, 1388, 180, 423, 1902, 1682, 760, 76, 338, 1906, 1152, 630, 1292, 1594, 1964, **1069**, 347, 696, **231**

Vapor Pressure and Boiling Points at Other Pressures

935, 1236, **866**, **1483**, **1455**, **1571**, **1481**, **1999**, 441, 1230, **1569**, **1446**, **1818**, **1819**, **1964**, 1142, 1313, 346, **145**, (1131), 23, 910

Critical Temperature

1453, 1999, 899, 532, (649), (347), (915), 23, 2025

Critical Pressure

1453, 1999, 23, (915), (2025)

Critical Volume and Density

1455, 1999. 23, (915), (2025), 481

Heat Capacity of the Solid
1322

Normal Melting Point
272, 1322, 259, 1807, 1527

Heat of Fusion
1322

Heat Capacity of the Liquid
1083, 183, 595, 1322, 501, 502, 499

Heat Capacity of the Real Gas
125, 845, (846), 1627, 1142, (1129), 499

P-V-T- Data and Equation of State of the Real Gas
1455, 820, 554, 553, (1131), 1142, 356, 23, 2025

Calorimetric Heat of Vaporization at 25 °C
1147, (1131), 1870

Calorimetric Heats of Vaporization at Other Temperatures
(1455), 1083, 219, 1140, 97, 125, 1398, 1964, (626), 1142, (145), (1131), 499

Thermodynamic Functions of the Liquid and Real Gas at Various Temperatures and Pressures
499, (1131), (346)

Heat of Combustion
1084, 1762, 2033, (1721), 1480, (1507), (1848), (626), 1648, 287, 288

Third Law Entropy of the Liquid at 25 °C
1322

Molecular Vibration Frequencies and Spectra
1399, (474), (1440), 1190, 1962, 228, 541, 1740, 1012, 1285, 619, 46, 243, 968, (624), (291), (1142), 1127, 1451, 1846, 1844, 456, 479, 668, 971, 1532

Internal Rotation
137, 1740, 1285, (1142), 479, 971

Molecular Geometry
1142, 59, 60

Thermodynamic Functions of the Ideal Gas
914, 474, 291, (1131), 1142, 624

Association in the Gas Phase
552, 1142, 356, (1258)

Association in the Liquid Phase
842, 78, 1683, (1754), 314, 1048, 1706, 614, 1705, 182, 102, 1451, 570, 1757, 1758, 380

2-Propanol

Properties of the Liquid Phase at Various Temperatures

Refractive Index

A portion of the reported values of the refractive index at the sodium D-line at 20 and 25 °C is given in table 49, and a complete list of sources of data is given in the Index to the Bibliography for 2-propanol. The uncertainty in the selected values is about 0.0001. Values at other temperatures shown in table 46 were taken from a smoothed graph of available data. Most of these were determined by Venkataraman [1939]. Refractive indices at other wavelengths have been reported by Bruhl [1880], Eykman [1919], and Timmermans and Delcourt [1934], along with a few additional scattered values. The data in table 48 were taken from smoothed curves, as described on page 1–21 of the Introduction.

Density

The selected densities in table 46 were calculated from the Francis constants listed there. A total of 63 experimental points, whose sources are identified in the Index, was used to evaluate the constants in the temperature range of −20 to 167 °C. Some experimental values at 20 and 25 °C are shown in table 49. A few values at other temperatures, which may be compared with the calculated densities, are Timmermans and Delcourt [1934], 0.80136 g m^{-1} at 0 °C and 0.77690 g ml^{-1} at 30 °C and Costello and Bowden [1948], 0.8027 g ml^{-1} at 0 °C and 0.7080 g ml^{-1} at 100 °C. Tonomura and Uehara [1931] have measured the density of liquid 2-propanol from 0 down to −106 °C. Their data, however, are not very consistent with other measurements in the −20 to 0 °C range, and they were not included in the evaluation of the Francis constants at temperatures above −20 °C. A separate set of constants was calculated for the temperatures from −54 to 0 °C which included the data of Tonomura and Uehara. These are also given in table 46.

Vapor Pressure and Boiling Points

Accurate vapor pressure measurements, over a range of temperatures, have been made by Parks and Barton [1928] and by Biddiscombe, Collerson, Handley, Herrington, Martin, and Sprake [1963]. The values calculated from the Antoine constants are mostly within 1 mm Hg of the ones reported by Biddiscombe, et al, and mostly within 3 mm of the values of Parks and Barton. The vapor pressures reported by Parks and Barton are generally higher than those listed in table 46, especially at the upper end of the temperature range. The selected normal boiling point is within 0.02 °C of the accurate measurement of Biddiscombe, et al., and within 0.04 °C of the other significant values listed in table 49. Ambrose and Townsend [1963] have determined vapor pressures from 122 °C to the critical temperature.

TABLE 46. 2-Propanol. Selected values. Physical and thermodynamic properties

Temp. °C	Refractive Index, n_D	Density g cm^{-3}	Vapor Pressure, mmHg
−20		0.8168	
−10		.8093	
0		.8016	8.30
2.49			10
5			12.0
10		.7936	17.1
15	1.3792		24.0
20	1.3772	.78545	33.1
25	1.3752	.78126	45.2
30	1.3731	.7770	60.8
35			81.0
38.80			100
40	1.3687	.7683	106.7
45			139.1
50	1.3642	.7593	179.5
52.17			200
55			229.5
60		.7499	290.5
65			365.7
67.01			400
70		.7402	456.0
75			564.5
80		.7300	693.7
82.26			760
85			846.8
90		* .7195	1027.1
100		* .7084	
110		* .6968	
120		* .6846	

Data For Phase Transitions

Initial	Final	Temp. °C	dt/dP deg mm^{-1}	Pressure mmHg	ΔH kcal mol^{-1}	$d\Delta H/dt$ cal deg^{-1} mol^{-1}	ΔS cal deg^{-1} mol^{-1}	ΔC_p cal deg^{-1} mol^{-1}
c	liq	−88.5±0.3		760	1.293±0.03	8.2±1	7.00±0.03	1.2±1
c	liq	−87.9±0.05						
liq	g	25	0.364	45.16±0.2	10.85±0.04	−17.5±1	36.39±0.03	−13.6±0.03
liq	g	82.26±0.03	0.03294	760	9.510±0.005	−29.2±1	26.73±0.02	−14.0±1

Condensed Phase Heat Capacity

State	Temp. °C	C_p cal deg^{-1} mol^{-1}
c	−87.9	24.8±1
liq	−87.9	26.0±0.1
liq	−82.26	48.3±0.2

Properties of the Saturated Real Gas

Temp. °C	H^r-H^0 kcal mol^{-1}	S^r-S^0 cal deg^{-1} mol^{-1}	$C_p^r-C_p^0$ cal deg^{-1} mol^{-1}
25	−0.015±0.005	−0.13±0.01	1.9±0.3
82.26	−.23±0.01	−0.58±0.01	10.0±1

Data for the Standard States at 25 °C

State	Heat of Combustion ΔH_c^0 kcal mol^{-1}	Heat of Formation ΔH_f^0 kcal mol^{-1}	Entropy S^0 cal deg^{-1} mol^{-1}	Gibbs Energy of Formation ΔG_f^0 kcal mol^{-1}	Heat Capacity, C_p cal deg^{-1} mol^{-1}
liq	−479.44±0.05	−75.97±0.05	43.16±0.04	−43.09±0.06	36.06±0.03
g	−490.29±0.06	−65.11±0.06	74.07±0.03	−41.44±0.07	21.21±0.1

Critical Constants

Temp. 235.16 °C, 508.31 K	Pressure 47.02 atm	Density 0.273 g cm^{-3}

				Constants in Vapor Pressure and Density Equation								
				Antoine Equation				Francis Equation				
				Temp. Range	*A*	*B*	*C*	Temp. Range	*A*	$B \times 10^3$	*C*	*E*
				0 to 101 °C	8.11778	1580.92	219.61	−20 to 167 °C	0.96262	0.3632	61.725	383.28
								−54 to 20 °C	1.21666	.2849	291.13	704.16

* At saturated vapor pressure.

TABLE 47. 2-Propanol. Selected values. Thermodynamic functions of the ideal gas at one atmosphere

Temperature K	Entropy S^0 cal deg^{-1} mol^{-1}	Heat Capacity $C_p{}^0$ cal deg^{-1} mol^{-1}	Enthalpy Function $(H^0-H_0{}^0)/T$ cal deg^{-1} mol^{-1}	Gibbs Energy Function $(G^0-H_0{}^0)/T$ cal deg^{-1} mol^{-1}	Heat of Formation $\Delta H_f{}^0$ kcal mol^{-1}	Gibbs Energy of Formation $\Delta G_f{}^0$ kcal mol^{-1}
0	0	0	0	0	−59.33	−59.33
273.15	72.28	19.86	13.16	−59.12	−64.70	−43.40
298.15	74.07	21.21	13.77	−60.30	−65.11	−41.44
300	74.31	21.31	13.92	−60.39	−65.11	−41.30
400	81.25	26.78	16.56	−64.70	−66.53	−33.11
500	87.71	31.89	19.05	−68.66	−67.75	−24.61
600	93.75	35.76	21.44	−72.32	−68.72	−15.87
700	99.51	39.21	23.73	−75.79	−69.44	−6.99
800	104.97	42.13	25.86	−79.11	−69.96	+1.96
900	110.07	44.63	27.80	−82.27	−70.34	10.97
1000	114.82	46.82	29.56	−85.29	−70.61	20.03

Critical Properties

Critical Temperature

The measurements of Ambrose and Townsend [1963] and Kreglewski [1954] are the most carefully done of those shown in table 50 and show excellent agreement. Both of these were determined by observing the disappearance of the meniscus.

Critical Pressure and Density

Ambrose and Townsend [1963] have made the only accurate measurements in recent years, and their values are adopted.

Solid-Liquid Phase Equilibria

Normal Melting Point

Several values of the melting point are listed in table 49. The measurements of Parks and Kelley [1925b and 1928] and of Kelley [1929c] were carried out in a calorimeter. Although the original articles were not clear on this point, apparently the alcohol was sealed in the calorimeter in the presence of some air so that the fusion occurred under conditions approximating equilibration with air at one atmosphere. Cady and Jones [1933] measured the temperature at which the liquid was in equilibrium with a small quantity of solid in a sealed melting point tube. Here again, it was not clearly stated whether or not air was present. There is no obvious reason for the much higher value which they obtained. The selected value was based primarily on the result of Parks and Kelley.

Triple Point

Andon, Counsell, and Martin [1963] found a fusion temperature of −87.95 °C by extrapolating the melting curve obtained in an adiabatic calorimeter containing helium at a pressure of 3 cm Hg. Ross, Dixon, Frolen, and Termini [1963] obtained a triple point of −87.87 °C for a very carefully purified sample in an evacuated freezing point cell. Thus the triple point seems to be considerably higher than the freezing point measured in the presence of air. This is similar to the behavior of 1-butanol and 2-methyl-2-propanol. It cannot be determined at present whether this is a real phenomenon or whether it reflects the experimental errors in the older data. Ross et al., also found a metastable form of 2-propanol which melts at −90.50 °C.

Heat Capacity of the Solid and Liquid at the Melting Point

The data reported in table 46 were obtained by a graphical extrapolation of the experimental values of Andon, Counsell, and Martin [1963].

Heat of Fusion

Parks and Kelley [1925b and 1928] measured the heat of fusion of 1.267 kcal mol^{-1} in their calorimeter, and Kelley [1929c] obtained 1.284 kcal mol^{-1}. The selected value for the stable form was taken from the calorimetric data of Andon, Counsell, and Martin [1963]. From the slope of the cooling curve, Ross, Dixon, Frolen, and Termini [1963] estimated the heat of fusion of the metastable form to be 1.055 kcal mol^{-1}.

Properties of the Liquid at 25 °C

Heat Capacity

A weighted average of the measured values of Ginnings and Corruccini [1948] and Andon, Counsell, and Martin [1963] was selected.

Absolute Entropy

The value obtained by Andon, Counsell, and Martin [1963] is the best available one and is consistent with the other thermodynamic properties.

Heat of Combustion

The average of the values reported by Snelson and Skinner [1961] and by Chao and Rossini [1965] was selected.

Properties of the Real Gas

Equation of State

Ingle and Cady [1938] calculated the molecular weight from gas density in the range of 84 to 102 °C. Kretschmer and Wieb [1954] measured pressure, volume, and temperature for gaseous 2-propanol in the range of 60 to 120° C and at pressures from 1 atm, or one half the vapor pressure, down to about one half the maximum pressure. Using the model of Weltner and Pitzer [1951], they calculated the second and fourth virial coefficients in the equation

$$PV = RT + B_p' + D_p' P^2$$

and expressed them as functions of temperature by,

$$B_p' = -300 - 0.755 \exp\left(\frac{2483}{T}\right) \text{ ml mol}^{-1}$$

$$D_p' = 15.6 - 1.83\times10^{-9} \exp\left(\frac{9215}{T}\right) \text{ ml atm}^{-2} \text{ mol}^{-1}.$$

J. D. Cox [1961] fits the second virial coefficient obtained from $P-V-T$ measurements in the range of 357 to 755 mm Hg and 105 to 150 °C to the equation,

$$\log(-B_p') = 14.012 - 4.3 \log T.$$

Hales, Cox, and Lees [1963] report the following equations for the virial coefficients as giving the best overall fit to both their heat capacity measurements and the $P-V-T$ data of Kretschmer and Wiebe.

$$B_p' = -150 - 4.509 \times 10^{-3} T \exp\left(\frac{2265}{T}\right) \text{ ml mol}^{-1}$$

$$D_p' = -8.536 \times 10^{-15} T \exp\left(\frac{11524}{T}\right) \text{ ml atm}^{-2} \text{ mol}^{-1}.$$

Berman, Larkan, and McKetta [1964] state that the following equations fit their heat capacity and heat of vaporization measurements,

$$B_p' = -450 - 1.085 \times 10^{-3} T \exp\left(\frac{2673}{T}\right) \text{ ml mol}^{-1}$$

$$D_p' = -1.604 \times 10^{-14} T \exp\left(\frac{11230}{T}\right) \text{ ml atm}^{-2} \text{ mol}^{-1}.$$

However, they do not satisfactorily fit the data of Kretschmer and Wiebe, Cox, and Hales, Cox, and Lees. It appears that a single equation of this form for B_p' and D_p' cannot be adjusted to fit all of these data.

Ambrose and Townsend [1963] measured orthobaric densities of liquid and vapor from 134 °C to the critical temperature and expressed the experimental values in terms of a series of powers of $(t_c - t)$.

Heat Capacity

Early direct measurements of vapor heat capacity have been reported by Bennewitz and Rossner [1938] at 137 °C and 748 mm Hg by Parks and Shomate at 1 atm and 155, 185, and 207 °C; and by Sinke and De Vries [1953] at 750 mmHg and a series of temperatures from 86 to 164 °C. Jatkar [1939] and Jatkar and Lakshimarayan [1946] have calculated the heat capacity at 134 °C with the aid of experimental measurements on the velocity of sound through the vapor.

Hales, Cox, and Lees [1963] measured the heat capacity in a flow calorimeter in the range 85 to 200 °C and 190 to 760 mmHg. They expressed these data in an equation of the form,

$$C_p = C_p{}^0 + aP + cP^3$$

where,

$$C_p{}^0 = 0.702 + 7.9342 \times 10^{-2} T$$
$$- 3.25 \times 10^{-5} T^2 \text{ cal deg}^{-1} \text{ mol}^{-1}$$

$$a = \frac{560}{T^2} \exp\left(\frac{2265}{T}\right) \text{ cal deg}^{-1} \text{ atm}^{-1} \text{ mol}^{-1}$$

$$c = \frac{9.151 \times 10^{-9}}{T^2} \exp\left(\frac{11524}{T}\right) \text{ cal deg}^{-1} \text{ atm}^{-3} \text{ mol}^{-1}.$$

TABLE 48. 2-Propanol. Selected values. Refractive index at various temperatures and wavelengths

Symbol	Wave-length, Å	Refractive Index, n		
		15 °C	20 °C	25 °C
He_{red}	6678.2	1.3770	1.3751	1.3731
H_{c}	6562.8	1.3773	1.3754	1.3734
Na_{D}	5892.6	1.3792	1.3772	1.3752
Hg_{e}	5460.7	1.3808	1.3788	1.3768
He_{blue}	5015.7	1.3830	1.3810	1.3790
H_{F}	4861.3	1.3839	1.3819	1.3799
Hg_{g}	4358.3	1.3877	1.3856	1.3836
$\text{H}_{\text{G}'}$	4340.5	1.3878	1.3857	1.3837

Berman, Larkan, and McKetta [1964] also measured the heat capacity with a vapor flow calorimeter in the range of 98 to 178 °C and 253 to 1013 mmHg. They used the same function to express these data, where,

$$C_p{}^0 = 3.9558 + 6.275 \times 10^{-2} T$$
$$- 1.429 \times 10^{-5} T^2 \text{ cal deg}^{-1} \text{ mol}^{-1}$$

$$a = \frac{188.1}{T^2} \exp\left(\frac{2673}{T}\right) \text{ cal deg}^{-1} \text{ atm}^{-1} \text{ mol}^{-1}$$

$$b = \frac{16.33 \times 10^{-9}}{T^2} \exp\left(\frac{11230}{T}\right) \text{ cal deg}^{-1} \text{ atm}^{-3} \text{ mol}^{-1}.$$

Corrections to the Ideal Gas State

The values of $H^r - H^\circ$ and $S^r - S^\circ$ were based on the equations of state of Kretschmer and Wiebe [1954] and Hales, Cox, and Lees [1963]. The values of $C_p{}^r - C_p{}^\circ$ were based on the heat capacity equations of Hales, Cox, and Lees and of Berman, Larkan, and McKetta [1964].

Vapor-Liquid Equilibrium at 25 °C

Vapor Pressure

The vapor pressure was calculated from the selected Antoine constants.

Heat of Vaporization

The only significant direct calorimetric measurements of heat of vaporization at 25° are those of McCurdy and Laidler [1963] and Wadso [1966]. The careful work of Wadso agrees quite well with the values calculated from the equations of Hales, Cox, and Lees [1963] and Berman, Larkan, and McKetta [1964] which represented experimental measurements at higher temperatures. A value was selected which was consistent with these measurements and with other thermodynamic properties.

TABLE 49. 2-Propanol. Reported values. Simple physical properties

Investigators		Vapor Pressures and Boiling Points		Freezing Point	Density, d g cm^{-3}		Refractive Index, n_D	
		°C	mmHg	t_m, °C	20 °C	25 °C	20 °C	25 °C
2-Propanol, C_3H_8O, mol wt. 60.097, state at 25 °C liq								
Gartenmeister	[1890]				0.7854			
Louguinine	[1898]	82.04	760					
Young and Fortey	[1902]	82.44	760					
Doroshevski and Dvorzhanchik	[1908]	82.2–82.3	760				1.37733	
Brunel, Crenshaw, and Tobin	[1921]	82.28	760					
Lebo	[1921]	82.4	760		.7855			
Brunel	[1923]	82.58	760			0.7808		1.3748
Williams and Daniels	[1924]	81.95–82.05	760					1.37709
Parks and Kelley	[1925a]					.78086		1.3750
Parks and Kelley	[1925b]			−88.6		.78086		
Norris and Ashdown	[1925]	82.4	760			.78071		
Mathews	[1926]	82.16–82.26	760					1.37592
Parks and Chaffee	[1927]					.78130		1.3743
Timmermans	[1927]	82.0	760	−89.5				
Parks and Barton	[1928]					.78091		
Parks and Kelley	[1928]			−88.6		.78093		
Parks and Nelson	[1928]					.78108		
Berner	[1929]				.78505			
Kelley	[1929c]			−88.43		.78905		
Cady and Jones	[1933]			−86.6				
Trew and Watkins	[1933]	82.1	760					1.37538
Swietoslawski	[1934]	82.29	760					
Timmermans and Delcourt	[1934]	82.40	760	−89.5				
Butler, Ramchandani, and Thomson	[1935]	82.39	760			.78126	1.36886	
Olsen and Washburn	[1935]					.78087		
Venkataraman	[1939]							1.37516
Washburn, Graham, Arnold, and Transue	[1940]					.7809		1.37487
Kretschmer, Nowakowska, and Wiebe	[1946]	82.24	760			.7801		
Vogel	[1948]	82.3	760		.7864		1.37711	
Cook	[1952]	82.3	760	−88	.7855		1.3772	
Wilson and Simons	[1952]	82.23–82.28	760			.78091		
Anisimov	[1953a]					.7813		1.3743
Anisimov	[1953b]					.7811		1.37538
Ballard and Van Winkle	[1953]	82.33	760				1.37716	
Wetzel, Miller, and Day	[1953]	82.0–82.6	760				1.3776	
Purnell and Bowden	[1954]	82.1	760			.78088		1.3764
Kretschmer and Wiebe	[1954]					.78083		
Williamson and Harrison	[1957]	82.4						
Union Carbide Corporation	[1958]			−87.8				
Costello and Bowden	[1958]	82.0	760		0.7862			
Brown and Smith	[1962b]	82.33	760			0.78100		1.37497
Chu and Thompson	[1962]					.7807	1.3772	1.3749
Ambrose and Townsend	[1963]				.7854			
Biddiscombe, Collerson, Handley, Herington, Martin, and Sprake	[1963]	82.241	760					
Selected value	[1967]	82.26±0.03	760	−88.5	0.78545	.78126	1.3772	1.3752
		2.49±0.1	10	±0.3	±.00005	±.00005	±0.0001	±0.0001

Antoine constants: *A* 8.11778, *B* 1580.92, *C* 219.61

dt/*dp* at 760 mmHg, 0.03294 °C/mmHg

◆

Temperature Derivative of the Heat of Vaporization

The value of $d\Delta H/dT-\Delta C_p$ calculated from the equation of state of Kretschmer and Wiebe is −3.12 cal deg^{-1} mol^{-1}, and from that of Hales, Cox, and Lees is −3.69 cal deg^{-1} mol^{-1}. Using the selected value of ΔC_p gives −16.67 and −17.24 cal deg^{-1} mol^{-1}, respectively for $d\Delta H/dT$. The equations of Berman, Larkan, and McKetta and of Hales, Cox, and Lees for the heat of vaporization as a function of temperature, yield −18.55 and −1846 cal deg^{-1} mol^{-1} respectively, for $d\Delta H/dT$. All of these calculations utilize equations which are outside the range of the experimental data used to derive them. The value obtained from the equation of state of Hales, Cox, and Lees and the heat capacities of the liquid was considered to be the most reliable.

TABLE 50. 2-Propanol. Reported values. Critical properties

Investigator	t_c, °C	P_c, atm	d_c, g cm^{-3}
Nadezhdin [1883] and [1882]	235.0	53.1	
Mathias			0.274
Brown, J. C. [1906]	243.47		
Fischer and Reichel [1943]	235.6		
Stull [1947]	235.0	53.0	
Kreglewski [1954]	235.25		
Ravikovich and Solomko [1958]	238.0		
Ambrose and Townsend [1963]	235.25	47.02	0.2727

Vapor-Liquid Equilibrium at the Normal Boiling Point

Normal Boiling Point

The value calculated from the selected Antoine constants was used.

Heat of Vaporization

As shown in table 51 many values, both calorimetric and those calculated from vapor pressure have been reported. However, the results of Hales, Cox, and Lees [1963] and Berman, Larkan, and McKetta [1964] agree very well and are the best values. The selected value was obtained by adjusting their values slightly for internal consistency with other properties. Hales, Cox, and Lees represented their three measured results in the range of 51 to 82 °C by,

$$\Delta H_v = 11{,}279 - 13.787t - 0.093573t^2 \text{ cal mol}^{-1}.$$

Berman, Karkan, and McKetta represented their measurements in the range of 57 to 89.5 °C by,

$$\Delta H_v = 11{,}293 - 13.857t - 0.09382t^2 \text{ cal mol}^{-1}$$

Heat Capacity of the Liquid

The heat capacity at the boiling point was calculated from the equation of Ginnings and Corruccini [1947]. They list heat capacities and related properties for 0 to 200 °C.

Temperature Derivative of the Heat of Vaporization

The equations of heat of vaporization as a function of temperature, given above, based on the calorimetric measurements of Hales, Cox, and Lees and of Berman, Larkan, and McKetta, yield −29.18 and −29.29 cal deg^{-1} mol^{-1}, respectively, for $d\Delta H/dT$ at the boiling point. An average value was selected. For comparison, the equation of state of Kretschmer and Wiebe in combination with the heat capacity of the liquid gives −26.1 cal deg^{-1} mol^{-1}, and that of Hales, Cox, and Lees with the heat capacity of the liquid gives −31.1 cal deg^{-1} mol^{-1}.

TABLE 51. 2-Propanol. Reported values. Heats of vaporization

Investigator	ΔH_v at 25 °C	ΔH_v at t_b	Method and Remarks
Louguinine [1898]		9.48	Calorimetric.
Brown, J. C. [1903]		9.73	Calorimetric.
Mathews [1926]		9.54	Calorimetric.
Mathews [1926], extrapolated by McCurdy and Laidler [1963]	10.70–	10.77	Calculated.
Parks and Barton [1928]	10.62	9.60	For ideal gas, calculated from vapor pressure.
Parks and Nelson [1928]		9.71	Calorimetric.
Bartoszewiczowna [1931]	10.47		Calorimetric, corrected to 25 °C
Bennewitz and Rossner [1938]		9.67	Calorimetric, corrected to t_b.
Williamson and Harrison [1957]		9.56	Calorimetric, extrapolated.
McCurdy and Laidler [1963]	10.52		Calorimetric.
Hales, Cox and Lees [1963]	10.88	9.512	Calorimetric, value at 25 °C by extrapolation.
Berman, Larkan and McKetta [1964]	10.89	9.519	Calorimetric, value at 25 °C by extrapolation.
Biddiscombe, Collerson, Handley, Herington, Martin and Sprake [1963]		9.65	Calculated from vapor pressure.
Wadso [1966]	10.81		Calorimetric.
Selected Antoine constants	10.65	9.51	Calculated.

TABLE 52. 2-Propanol. Reported values. Heat capacity and entropy of the liquid at 25 °C

Investigator	$C_p{}^0(1)$	Remarks	$S^0(1)$, Third law
Williams and Daniels [1924]	39.5	From equation	
Parks and Kelley [1925]	37.9	Graphical extrapolation	43.1 (revised 1929)
Kelley [1929]	36.7	Graphical extrapolation	43.0
Ginnings and Corruccini [1948]	36.84		
Andon, Counsell and Martin [1963]	36.94	Interpolated	43.16

Properties of the Ideal Gas State

Molecular Parameters

References to information on vibrational frequencies will be found in the index. Tanaka [1962b,c,d] has published a vibrational assignment based on his studies of the infrared and Raman spectra. Green [1963] has selected the following frequencies for calculation of thermodynamic functions: 3650, 2940(6), 2875, 1475(2), 1460(2), 1387, 1367, 1340, 1256(2), 1153, 1130, 1072, 955(2), 940, 818, 488, 427, and 373 cm^{-1}, along with an assignment of 4000 cal mol^{-1} to the internal rotation of the methyl groups, and 800 cal mol^{-1} for the hydroxyl group. More recently Blanks and Prausnitz [1963] and Durocher and Sandorfy [1965] have studied the infrared spectra of solutions of 2-propanol in carbon tetrachloride and have determined the -OH stretching frequencies in the monomer and in several polymeric species. Durocher and Sandorfy also determined anharmonic contributions.

TABLE 53. 2-Propanol. Reported values. Heat capacity of the ideal gas at several temperatures

	Temperature, K			
	298.15	300	400	500
	C_p^0, cal deg^{-1} mol^{-1}			
Parks and Shomate [1940]*			25.04	33.63
Kobe, Harrison, and Pennington [1951]	21.90	22.00	27.50	32.31
Hales, Cox, and Lees [1963]	21.47	21.58	27.24	32.25
Green, J. H. S. [1963]	21.21	21.31	26.78	31.89
Berman, Larkan, and McKetta [1964]	21.39	21.50	26.77	31.76

* Corrected to zero pressure.

TABLE 54. 2-Propanol. Reported values. Heat of combustion of the liquid at 25 °C

Investigator	$-\Delta H_c^0(1)$ kcal mol^{-1}
Louguinine [1880]	478.1
Thomsen [1886]	*484.4
Zubov [1898] (recalculated by Swietoslawski [1920])	475.2
Parks and Moore [1939]	478.9
Parks, Mosley and Peterson [1950]	479.26
Snelson and Skinner [1961]	479.39
Chao and Rossini [1965]	479.66

* ΔH_c of gas measured. Value corrected to the liquid.

Entropy at 25 °C

There have been surprisingly few statistical calculations of the ideal gas thermodynamic properties of 2-propanol. Schumann and Aston [1938] calculated the entropy at temperatures from 355.5 to 500 K, assuming both free internal rotation and restricted rotation with barrier heights of 3400 cal mol^{-1} and 5000 cal mol^{-1}, respectively, for the methyl and hydroxyl groups. They compared these results with the entropy obtained from experimental equilibrium constants on the dehydrogenation reaction and concluded that the calculation based on restricted rotation gave better agreement than the one based on free rotation. The selected value in table 46 was calculated by Green [1963] from the molecular parameters. These were adjusted to give close agreement with the third law value.

Heat Capacity

Bennewitz and Rossner [1938] measured the vapor heat capacity at 137 °C and converted the result to zero pressure. Parks and Shomate [1940] obtained three measurements with a flow calorimeter at 1 atm from 428 to 480 K and expressed these as a linear function of temperature. Kobe, Pennington, and Harrison [1951] calculated the ideal gas heat capacity from molecular parameters adjusted to fit the experimental data available at that time. They also gave the constants in the equation expressing C_p^0 as a polynomial function of temperature. Equations expressing C_p^0 as quadratic functions of temperature derived by Hales, Cox, and Lees [1963] and Berman, Larkan, and McKetta [1964] from their calorimetric measurements have been given on page 1–81. Table 53 summarizes the ideal gas heat capacity at several comparable temperatures from these sources, as well as from the statistical calculations of Green [1963]. Parks and Shomate's data have been corrected to zero pressure. Since Green's calculations agree well with the two recent sets of measurements within the observed temperature range, they have been selected for the extended temperature range.

Thermodynamic Functions

The selected values were taken from Green [1963]. The only other recent published calculations are those of Zhuravlev and Rabinovich [1959]. They also include data on some deuterated derivatives.

Chemical Equilibria

Equilibrium constants for the gas phase reaction,

$$CH_3CHOHCH_3(g) \rightarrow CH_3COCH_3(g) + H_2(g)$$

have been experimentally determined by Rideal [1921], Parks and Kelley [1928], Kolb and Burwell, Jr. [1945],

TABLE 55. 2-Propanol. Differences in properties between real and ideal gas

Sources	at 25 °C and 45.2 mmHg			at 82.26 °C and 760 mmHg		
	H^r-H^0	$C_p^r-C_p^0$	S^r-S^0	H^r-H^0	$C_p^r-C_p^0$	S^r-S^0
Calculated from equation of state of Kretschmer and Wiebe [1954]	−0.01	1.57	−0.13	−0.052	8.96	−0.58
Calculated from equation of state of Cox, J. D. [1961]	−0.02	0.26	−0.06	−0.142	1.72	−0.40
Calculated from equation of state of Hales, Cox and Lees [1963]	−0.028	2.07	−0.16	−0.244	11.36	−0.61
Calculated from equation of state of Berman, Larkan and McKetta [1964]	−0.040	1.87	−0.12	−0.217	9.57	−0.52

TABLE 56. 2-Propanol. Comparison of virial coefficients and compressibility factor, *Z*, derived from experimental measurements

	Virial coefficients			Pressure, atmospheres					
	B_p'	C_p'	D_p'	0.25	1	2	5	10	20
	cm^3	cm^3 atm^{-1}	cm^3 atm^{-1}	Values of $(1-Z)\times100$					
Temperature = 50 °C									
Kretschmer and Wiebe [1954]	−1940		−4419	2.089					
Cox, J. D. [1961]	(−1666)			(1.571)					
Hales, Cox, and Lees [1963]	(−1763)		(−8476)	(2.162)					
Berman, Larkan, and McKetta [1964]	(−1821)		(−6413)	(2.095)					
Temperature = 100 °C									
Foz Gazulla, Morcillo, Masia, and Mendes [1954]	−927			0.757	3.027	(6.06)			
Kretschmer and Wiebe [1954]	−885		−81.5	0.727	3.156	(7.91)			
Cox, J. D. [1961]	−897			(.732)	(2.930)	(5.86)			
Hales, Cox, and Lees [1963]	−873		−82.3	.721	3.136	(7.89)			
Berman, Larkan, and McKetta [1964]	−973		−73.0	.798	3.407	(8.19)			
Moreland, McKetta, and Silberberg [1967]	−889	−48.02		.736	3.072	6.54			
Temperature = 150 °C									
Kretschmer and Wiebe [1954]	(−459)		(+14.0)	(0.330)	(1.282)	(2.32)	(1.57)		
Cox, J. D. [1961]	−523			(.377)	(1.506)	(3.01)	(7.53)		
Hales, Cox, and Lees [1963]	−553		−2.38	.398	1.599	(3.24)	(8.82)		
Berman, Larkan, and McKetta [1964]	−704		−2.28	.507	2.034	(4.11)	(10.96)		
Moreland, McKetta, and Silberberg [1967]	−557	−11.30		.407	1.702	3.621	11.19		
Temperature = 200 °C									
Kretschmer and Wiebe [1954]	(−390)		(+15.1)	(0.251)	(0.968)	(1.703)	(0.174)		
Cox, J. D. [1961]	(−323)			(.207)	(.832)	(1.664)	(4.16)	(8.32)	(16.64)
Hales, Cox, and Lees [1963]	−406		−0.15	.326	1.303	(2.609)	(6.56)	(13.42)	(29.21)
Berman, Larkan, and McKetta [1964]	(−596)		−0.15	(.834)	(1.535)	(3.073)	(7.73)	(15.75)	(33.88)
Moreland, McKetta, and Silberberg [1967]	−388	−3.208		.250	1.007	2.032	5.22	11.01	25.62

Values in parenthesis have been extrapolated outside the experimental range of temperature or pressure.

and Buckley and Herington [1965]. By plotting log K versus $1/T$ in the range of 105 to 275 °C, Rideal calculated a heat of reaction of 20.1 kcal per mol. The other three pairs of workers fitted their experimental data to an equation whose constants are given in table 58. The constants shown for the data of Kolb and Burwell, Jr. have been recalculated from their data by Cubberley and Mueller [1946]. Also shown in this table are the experimental temperature range and values of ΔH^0 and ΔG^0 calculated from the corresponding equation. The values at 150° fall in the experimental range for all the investigations, while the values at 25 °C were extrapolated. Taking $\Delta H_f{}^0(g) = -51.80$ kcal per mol and $\Delta G_f{}^0(g) = -36.37$ kcal per mol as the most consistent with the data for propanone and using the corresponding properties for 2-propanol from the summary sheet gives $\Delta H^0 = 13.31$ kcal per mol and $\Delta G^0 = 5.07$ kcal per mol for this reaction at 25 °C.

Stanley, Youell, and Dymock [1934] have studied the equilibrium constant in the reaction,

$$CH_2{=}CHCH_3(g) + H_2O(g) \rightarrow CH_3CHOHCH_3(g)$$

in the temperature range of 140–250 °C. Their equation gives $\Delta H = -8.92$ kcal per mol in this range and $\Delta G = -0.66$ kcal per mol when extrapolated to 25 °C. These are considerably different than the values calculated with data on propene from the API Research Project 44 Tables. These are −12.19 kcal per mol and −1.79 kcal per mol, respectively, at 25 °C. Uhlir, Uhlirova, Kolinsky, Ruzicka, and Pasek [1964] have published calculated values for the equilibrium constant of this reaction.

Tests of Internal Consistency

Intercomparison of thermodynamic properties of 2-propanol in the liquid, liquid-vapor equilibrium, and gas phase between 25 °C and the boiling point are shown below.

TABLE 57. 2-Propanol. Enthalpies and entropies of formation of dimers and tetramers from the monomer in the ideal gas state

Investigator	Dimer (kcal per mol)		Tetramer (kcal per mol)	
	ΔH_2	ΔS_2	ΔH_4	ΔS_4
Foz Gazulla, Garcia de la Banda and Perez Masia [1952], thermal conductivity	−7.4	−27.0		
Kretschmer and Wiebe [1954], *PVT* data	−4.93	−21.0	−18.3	−62.6
Hales, Cox, and Lees [1963], heat capacity	−4.50	−19.5	−22.9	−75.3
Berman, Larkan and McKetta [1964] heat capacity	−5.30	−22.4	−22.3	−74.2

TABLE 58. 2-Propanol. Enthalpy and Gibbs energy change for the dehydrogenation to propanone and hydrogen in the gas phase and constants in the equation:

$$\Delta H^0 = \Delta H_0{}^0 + AT + \tfrac{1}{2}BT^2 + \tfrac{1}{3}CT^3$$
and
$$\Delta G^0 = \Delta H_0{}^0 - AT \ln T + IT - \tfrac{1}{2}BT^2 - \tfrac{1}{6}CT^3$$

	Parks and Kelley [1928]	Kolb and Burwell, Jr. [1945] Cubberley and Mueller [1946]	Buckley and Herington [1965]
$\Delta H_0{}^0$, cal mol^{-1}	13,310	11,585	11,010
A	4.0	6.571	12.125
B	—	−0.0078	−0.03924
C	—	—	3.57×10^{-5}
I	−2.6	14.28	43.88
Experimental Temperature Range °C	184–202	144–219	124–200
ΔH^0(150 °C), kcal mol^{-1}	15.00	13.667	13.529
ΔG^0(150 °C), kcal mol^{-1}	1.97	1.510	1.611
ΔH^0(25 °C), kcal mol^{-1}	14.50	13.197	13.196
ΔG^0(25 °C), kcal mol^{-1}	5.75	5.035	5.082

	ΔH kcal mol^{-1}	ΔS cal deg^{-1} mol^{-1}
liquid (25 °C)→real gas (25 °C, 45. 2mmHg)	10.85 ±0.01	36.30 ±0.03
real gas (25 °C)→ideal gas (25 °C)	0.015±0.005	0.13 ±0.01
ideal gas (25 °C)→ideal gas (82.26 °C)	1.357±0.01	4.085±0.01
ideal gas (45.2 mmHg)→ideal gas (760 mmHg)	0.0	−5.610±0.005
ideal gas (82.26 °C, 760 mmHg)→real gas (82.26 °C, 760 mmHg)	−.23 ±0.01	−0.58 ±0.01
real gas (82.26 °C)→liquid (82.26 °C)	−9.510±0.005	−26.73 ±0.02
liquid (82.26 °C)→liquid (25 °C)	−2.648±0.01	−7.525±0.02
Sum	0.004±0.02	0.08 ±0.05

Miscellaneous

Nemeth and Reed [1964] calculated a collision diameter of 6.93 Å for 2-propanol molecules from measured values of gas viscosity. Katti and Shil [1966] reported values of the compressibility of the liquid, $-(1/V)(\partial V/\partial P)_T$ which ranges from 120.2×10^{-6} atm^{-1} at 30.25 °C to 206.6×10^{-6} atm^{-1} at 70.0 °C. Dannhauser and Bahe [1964] measured the dielectric constant of the liquid from 25 to 230 °C.

Index to the Bibliography

Numbers refer to the Bibliography, page 1–389.

References to data used in the selection of refractive index, density, boiling point, vapor pressure, and melting point are in boldface type.

Numbers in parentheses refer to sources of reviews, or theoretical calculations only.

Reference numbers under each property are listed in the order of date of publication.

Refractive Index
235, **439**, 1838, 500, **509**, **1307**, 354, **238**, **1961**, **1324**, **1140**, 1227, **1320**, 8, **135**, **1718**, **1779**, **1803**, 1891, 253, 1112, **1843**, 71, 1884, **1886**, 1885, 532, 1404, **1856**, **1893**, 721, 201, 834, 1171, 1316, 1377, 180, 423, 1367, **76**, 264, **338**, **35**, **36**, **77**, 1152, **1906**, 2016, 208, 1437, 1651, 1824, 610, 1208, 1292, 48, **231**, **293**, 1279

Density at 20–30 °C Only
239, 311, **238**, **1326**, **1324**, **1448**, 1272, 1183, 1140, 1320, **1319**, **1325**, 1331, **887**, **135**, 1795, 1112, 253, 1290, 2021, 997, 1184, 1189, 1886, 1885, **963**, 1893, 723, 835, 1316, 1377, 338, **1968**, 1338, 35, 1823, 208, **1437**, **965**, 610, 48, 231, 293, 23, 1147

Density at all Temperatures
1072, 235, 1424, 2011, 1561, 1559, 1560, 1349, **576**, **1763**, **2002**, **439**, 55, 1838, 509, **1005**, 1308, **42**, 1718, **1795**, **739**, 1371, **992**, 471, 241, 1856, 721, 423, **264**, 35, 36, **1797**, **347**, **380**, 876

Normal Boiling Point
1072, 235, 1424, 2011, 1561, 1560, 1349, 1765, 1763, 2033, 1083, 2002, 272, 1395, 439, 435, 655, 656, 55, 1838, 1960, 509, 1896, 1307, **239**, 1005, 311, **238**, 1961, 1308, 1272, 1009, 1227, **1140**, 42, 1772, 8, **1319**, 1718, 143, 1795, 870, 1794, 1803, **1720**, **1779**, **253**, 2021, 820, 125, 1189, 71, 1884, 1134, 1162, 241, 471, 1404, 1006, **963**, **1856**, 600, **721**, 834, 1377, 1316, 1899, 423, 180, 1388, **338**, 264, 1902, 76, **1968**, 1906, 1152, 77, 1906, 2016, 1825, 208, 1437, 1824, 719, 1208, 610, 1292, **1964**, 48, 1823, **231**

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1320, **1319**, **1968**, **1823**, **1964**, **347**, 89, 23, **145**, 1205, 1192, 1206

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Heat of Fusion
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Heat Capacity of the Liquid
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P-V-T Data and Equation of State of the Real Gas
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Calorimetric Heats of Vaporization at Other Temperatures
(1455) 219, 1140, 1331, 1964, 683, 1823, 132, 125

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Third Law Entropy of the Liquid at 25 °C
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Molecular Vibration Frequencies and Spectra
(1584), 725, 2016, 1190, 1048, 91, 1705, 528, 1109, 1740, 1742, 821, 530, 1012, 1451, 1640, 1844, 1731, 1732, 1733, 65, (627), 1127, 456, 668, 669, 470

Internal Rotation
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Association in the Gas Phase
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Association in the Liquid Phase
769, 1754, 1048, 1705, 528, 530, 1109, 392, 1451, 1757, 159, 1758, 461, 380, 470

1-Butanol

Properties of the Liquid Phase at Various Temperatures

Refractive Index

Eighty-one references to published values of the refractive index of 1-butanol are listed in the index. A few of the more reliable values are given in table 62 Most of these lie within about 0.0002 of the selected values reported in the summary sheet. Venkataraman [1939] reported values at the Na_D line from 26 to 45 °C. A few other measurements have been reported at 15 and 30 °C. The values in table 61 were taken from graphs of refractive indices at various temperatures and wavelengths in the same manner as was done for the lower alcohols. The values at 25 °C at wavelengths other than the Na_D line were obtained by extrapolation of experimental data from lower temperatures. Refractive indices at 4000 Å and below were calculated from a quadratic equation in $1/(\lambda-1000)^{1.6}$ obtained by a least squares fit to the values of Stephens and Evans [1930], after correcting them to 15 °C. The uncertainty in these results is about 0.0005.

Density

Numerous values of the density of 1-butanol have been reported in the literature. Representative data at 20 and 25 °C are listed in table 62. The selected densities in table 59 have been calculated from the Francis equation. Almost all of the data used in evaluating the constants in the Francis equation fall within $\pm$ 0.001 g m^{-1} of the calculated values. These sources are identified in the Index to the Bibliography. The density values of Dannhauser and Bahe [1964] in the range from 60 to 150 °C run 0,002 to 0.004 g ml^{-1} below the ones calculated from the Francis equation.

Vapor Pressures and Boiling Points

Despite the voluminous literature on the boiling point in the vicinity of 1 atm, there are relatively few accurate measurements of vapor pressure over an extended range of temperatures. The principal data used to calculate the Antoine constants given in tables 59 and 62 are those of Kahlbaum [1898] from 15 to 115 °C; Butler, Ramchandani, and Thomson [1935], from 25 to 110 °C; Allen, Lingo, and Felsing [1939] at 25 and 117.3 °C; and Biddiscombe, Collerson, Handley, Herington, Martin, and Sprake [1963], from 89 to 125 °C. The data of Biddiscombe et al. were given a high weight in the calculations, and the calculated vapor pressures were within about 1 mm Hg of their experimental values except near 125°, where the calculated values were about 2 mm Hg high. Kay and Donham [1955], Shemilt, Esplen, and Mann [1959], and Ambrose and Townsend [1963] have measured the vapor pressure from near the boiling point or above to the critical temperature. The measurements of Ambrose and Townsend are done with special care. Some of the more accurate determinations of the normal boiling point have been collected in table 62.

Critical Properties

Critical Temperature

Three accurate measurements, Kay and Donham [1955], Singh and Shemilt [1955], and Ambrose and Townsend [1963], are available. All of these were made with pure compounds and accurate thermometry. However, the critical temperature obtained by Singh and Shemilt was decidedly lower than the other two and lower than most of the others shown on table 63. The average of the values obtained by Kay and Donham and Ambrose and Townsend was adopted.

Critical Pressure

The situation is similar to that for the critical temperature. The value obtained by Singh and Shemilt is appreciably higher than that of the other two recent measurements. The result of Ambrose and Townsend [1963] was adopted.

Critical Density

Here the result of Singh and Shemilt [1955] was very close to that of Ambrose and Townsend [1963]. The value of Ambrose and Townsend was selected, since it was the most carefully measured one.

Solid-Liquid Phase Equilibria

Normal Melting Point

The more significant melting point values listed in table 62 scatter over a temperature range of about one degree. The selected melting point is near the upper end of this range.

Triple Point

Counsell, Hales, and Martin [1965] measured a melting point of -88.64 °C in their calorimeter in the presence of a low pressure of helium exchange gas. Therefore it should correspond closely to the solid-liquid-gas triple point. The uncertainty is about 0.05 °C. It is about 0.7 °C higher than the selected value of the normal melting point in the presence of air at 1 atm. Although part of this difference may be due to the errors in the measurement of the normal melting point, it is still unexpectedly large. This is similar to the situation found for 1-propanol.

Heat Capacity of the Solid and Liquid at the Melting Point

The selected values are taken from the measurements published by Counsell, Hales, and Martin [1965].

Heat of Fusion

Parks [1965] obtained a calorimetric measurement of 2.218 kcal mol^{-1} and Counsell, Hales, and Martin [1965] obtained 2.240 kcal mol^{-1}. The more recent result was selected for table 59.

Properties of the Liquid at 25 °C

Heat Capacity

The three values in table 65 are in good agreement, but the more accurate measurements of Counsell, Hales, and Martin [1965] were adopted.

Absolute Entropy

The value listed in table 65 for Parks [1925] is the revised value of Parks, Kelley, and Huffman [1929]. It is within the experimental uncertainty of the value obtained by Counsell, Hales, and Martin [1965] from their heat capacity measurements. A value slightly higher than this was selected in order to give better agreement with the entropy of the ideal gas in the tables of Green [1961].

Heat of Combustion

Four recent measurements of heat of combustion have been made. The result of Tjebbes [1960 and 1961] is low compared to both the recent and the older values. The selected value was an average of those of Skinner and Snelson [1960], Chao and Rossini [1965], and Gundry, Head, and Lewis [1962].

Properties of the Real Gas

Equation of State

Ingle and Cady [1938] calculated a molecular weight from measured values of gas density from 120 to 136 °C. This showed some degree of association. Ambrose and Townsend [1963] measured the orthobaric densities of liquid and gas from 166 °C to the critical temperature and fitted these data to an equation containing powers of (t_c-t). Shemilt, Esplen, and Mann [1959] evaluated the constants in the Beattie-Bridgman equation of state from available data for the range of 250 to 300 °C. J. D. Cox [1961] expressed the second virial coefficient, derived from his measurements of P-V-T data in the range 120 to 166 °C, as

$$\log(-B_p')=14.711-4.5\log T.$$

Counsell, Hales, and Martin [1965] obtained the following equations for the second and fourth virial coefficients, using the usual model of dimers and tetramers, by fitting the P-V-T data of Cox and their vapor heat capacity data to the constants.

$$B_p'=50-0.02595T\exp\left(\frac{1862.1}{T}\right)\text{ ml mol}^{-1}$$

$$D_p'=-1.743\times10^{-13}T\exp\left(\frac{10820.3}{T}\right)\text{ ml atm}^{-1}\text{ mol}^{-1}.$$

This gives the enthalpy and entropy change for the formation of dimers and tetramers from the monomers of $\Delta H_2=-3700$ cal mol^{-1}, $\Delta S_2=-16.01$ cal deg^{-1} mol^{-1}, $\Delta H_4=-21{,}500$ cal mol^{-1}, and $\Delta S_4=-69$ cal deg^{-1} mol^{-1}.

Corrections to the Ideal Gas State

Ideal gas corrections based on these three equations of state are shown in table 69. The values shown for 25 °C do not have much significance, since this is well below the range of temperature of the data used to establish the original equations. However, these corrections are negligible for most thermodynamic calculations at 25°C and at the equilibrium vapor pressure. The values calculated from the equations of J. D. Cox [1961] and Counsell, Hales, and Martin [1965] are similar, but this is not surprising since both were formulated to be consistent with the same experimental P-V-T data.

Vapor-Liquid Equilibrium at 25 °C

Vapor Pressure

At 25 °C the selected Antoine constants give a vapor pressure of 6.18 mmHg. However, this is below the range of data used to evaluate these constants, and the selected value was calculated from the vapor pressure equation of Counsell, Hales, and Martin [1965].

Heat of Vaporization

The selected value was essentially that of Wadso [1966] with slight adjustment for better internal consistency. This is also quite close to the value calculated from the equation of Counsell, Hales, and Martin [1965] which was derived from measurements at higher temperature. The heat of vaporization calculated from the selected Antoine constants is much higher; but since 25 °C is at the lower end of the region of applicability, a reliable value would not be expected when calculated this way.

Temperature Derivative of the Heat of Vaporization

At the low equilibrium pressure at 25 °C, the gas

TABLE 59. 1-Butanol. Selected values. Physical and thermodynamic properties

Temp. °C	Refractive Index, n_D	Density g cm^{-3}	Vapor mmHg
−20		0.8381	
−10		.8312	
0		.8242	
10		.8170	
15	1.4012		
20	1.3993	.8097	
25	1.3971	.8060	6.18
30	1.3950	.8022	8.93
31.58			10
35			12.7
40	1.3908	.7946	17.8
45			24.5
50	1.3865	.7867	33.2
55			44.6
60		.7786	59.0
65			77.3
69.99			100
70		.7703	100.1
75			128.3
80		.7616	162.9
84.45			200
85			205.0
90		.7526	255.8
95			316.5
100		.7431	388.7
100.71			400
105			474
110		.7332	574
115			690.6
117.66			760
120		* .723	825.7

Data For Phase Transitions

Initial	Final	Temp. °C	dt/dP deg mm^{-1}	Pressure mmHg	ΔH kcal mol^{-1}	$d\Delta H/dt$	ΔS	ΔC_p
						cal deg^{-1} mol^{-1}		
c	liq	−89.3±0.2		760	2.24±0.01	21.27±0.1	12.18±0.05	9.09±0.1
c	liq	−88.64±0.05						
liq	g	−88.64±0.05			14.2±0.2		77.0±1	
liq	g	25	1.960	6.75±0.2	12.52±0.4		41.99±0.1	−15.9±0.2
liq	g	117.66±0.05	0.03686	760	10.31±0.04		26.38±0.1	−24.8±1

Condensed Phase Heat Capacity

State	Temp. °C	C_p
		cal deg^{-1} mol^{-1}
c	−88.64	23.23±0.1
liq	−88.64	32.32±0.1
liq	117.66	60.5±1

Properties of the Saturated Real Gas

Temp. °C	H^r-H^0	S^r-S^0	$C_p^r-C_p^0$
	kcal mol^{-1}	cal deg^{-1} mol^{-1}	
25	−0.005±0.002	−0.01±0.005	0.12±0.02
117.66	−0.146±0.005	−0.32±0.01	2.81±0.1

Data for the Standard States at 25 °C

State	Heat of Combustion ΔH_c^0 kcal mol^{-1}	Heat of Formation ΔH_f^0 kcal mol^{-1}	Entropy S^0 cal deg^{-1} mol^{-1}	Gibbs Energy of Formation ΔG_f^0 kcal mol^{-1}	Heat Capacity, C_p cal deg^{-1} mol^{-1}
liq	−639.6±0.2	−78.18±0.2	54.1±0.1	−38.84±0.2	42.31±0.05
g	−652.1±0.2	−65.65±0.2	86.7±0.1	−36.04±0.2	26.29±0.2

Critical Constants

Temp. 289.78 °C, 562.93 K	Pressure 43.55 atm	Density 0.270 g cm^{-3}

			Constants in Vapor Pressure and Density Equation								
			Antoine Equation				Francis Equation				
			Temp. Range	*A*	*B*	*C*	Temp. Range	*A*	$B \times 10^3$	*C*	*E*
			15 to 131 °C	7.47680	1362.39	178.77	−33 to 147 °C	0.87172	0.5363	13.026	273.80

* At saturated vapor pressure.

TABLE 60. 1-Butanol. Selected values. Thermodynamic functions of the ideal gas at one atmosphere

Temperature K	Entropy S^0 cal deg^{-1} mol^{-1}	Heat Capacity C_p^0 cal deg^{-1} mol^{-1}	Enthalpy Function $(H^0-H_0^0)/T$ cal deg^{-1} mol^{-1}	Gibbs Energy Function $(G^0-H_0^0)/T$ cal deg^{-1} mol^{-1}	Heat of Formation ΔH_f^0 kcal mol^{-1}	Gibbs Energy of Formation ΔG_f^0 kcal mol^{-1}
0	0	0	0	0	−58.80	−58.80
273.15	84.51	24.78	17.10	−67.41	−65.15	−38.50
298.15	86.70	26.29	17.81	−68.89	−65.65	−36.04
300	86.85	26.40	17.86	−68.99	−65.69	−35.85
400	95.23	32.80	20.80	−74.43	−67.54	−25.57
500	103.16	38.76	23.81	−79.34	−69.09	−14.87
600	110.65	43.90	26.73	−83.92	−70.34	−3.89
700	117.73	48.31	29.49	−88.24	−71.33	+7.28
800	124.44	52.11	32.10	−92.34	−72.06	18.57
900	130.75	55.40	34.50	−96.26	−72.60	29.93
1000	136.75	58.26	36.74	−100.01	−72.94	41.36

phase of 1-butanol is nearly ideal. The equations of state given above predict that $d\Delta H/dT$ is only about 0.3 to 0.4 cal deg^{-1} mol^{-1} lower than ΔC_p. Thus a value of $d\Delta H/dT$ of -16.3 cal deg^{-1} mol^{-1} is predicted. The equation of Counsell, Hales, and Martin [1965] based on data at higher temperature gives -18.5 cal deg^{-1} mol^{-1}. The selected value was slightly higher than the one calculated from heat capacity and volume of the gas phase.

Vapor-Liquid Equilibrium at the Normal Boiling Point

Normal Boiling Point

The selected value, listed in tables 59 and 62, was calculated from the Antoine constants also given there. This is slightly lower than the accurate measurements of Biddiscombe, Collerson, Handley, Herington, Martin, and Sprake [1963] but is within the experimental uncertainties in the best available data.

Heat of Vaporization

The selected value was calculated from the equation of Counsell, Hales, and Martin [1965],

$$\Delta H_v = 12347.7 + 20.159T - 0.06491T^2 \text{ cal mol}^{-1}$$

which was derived from calorimetric measurements at 390.88, 372.62, and 356.40 K. This is within about 0.1 kcal mol^{-1} of all the values shown in table 64.

TABLE 61. 1-Butanol. Selected values. Refractive index at various temperatures and wavelengths

Symbol	Wave-length, Å	Refractive Index, n		
		15 °C	20 °C	25 °C
$\mathrm{He}_{\mathrm{red}}$	6678.2	1.3989	1.3970	1.3950
H_{c}	6562.8	1.3991	1.3973	1.3952
Na_{D}	5892.6	1.4012	1.3993	1.3971
Hg_{e}	5460.7	1.4029	1.4009	1.3988
$\mathrm{He}_{\mathrm{blue}}$	5015.7	1.4054	1.4034	1.4014
H_{F}	4861.3	1.4061	1.4041	1.4021
Hg_{g}	4358.3	1.4101	1.4080	1.4060
$\mathrm{H}_{\mathrm{G'}}$	4340.5	1.4102	1.4081	1.4061
	4000	1.4134		
	3500	1.4208		
	3000	1.4328		
	2700	1.4436		

Temperature Derivative of the Heat of Vaporization

This was calculated from the equation of Counsell, Hales, and Martin [1965] for the heat of vaporization shown above. The heat capacities of the liquid and vapor, along with the equations of state of J. D. Cox [1961] and of Counsell, Hales, and Martin, give $d\Delta H/dT$ of -30.0 and -31.3 cal deg^{-1} mol^{-1} respectively.

Properties of the Ideal Gas State

Molecular Parameters

Although a number of studies of various features of the infrared spectra listed in the Index to the Bibliography has been made, there have been only a few attempts to make a complete vibrational assignment. A very approximate assignment was made by Dyatkina [1954] for use in calculating the thermodynamic functions, and this was also used with minor alterations by Chermin [1961]. These are not satisfactory for reliable calculation of thermodynamic functions however.

Entropy at 25 °C

Three calculated values are shown in table 66. They were taken from the corresponding tables of thermodynamic functions. The third law entropy of the liquid, in combination with the heat of vaporization and other auxiliary data, gives an entropy for the ideal gas of 86.71 cal deg^{-1} mol^{-1}. This falls between the two most recently calculated values and is the selected one.

Heat Capacity

Three values of heat capacity are also shown in table 66; two are calculated, and one is based on an extrapolation of experimental data to zero pressure. The heat capacity and entropy relative to the ideal gas at 400 K from two sources are compared in table 70 for the temperature range of 298.15 to 500 K. The values from Counsell, Hales, and Martin [1965] were calculated from their equation, which in turn was based on experimental measurements of vapor heat capacity in the range of 363 to 453 K. Within this range the entropy is quite close to that predicted by Green [1961], and the heat capacity is within about 0.2 cal deg^{-1} mol^{-1}. The value given by Green is considered to be more reliable at 25 °C.

Thermodynamic Functions

Three sets of ideal gas thermodynamic functions have been published: Dyatkina [1954], Chermin [1961], and Green [1961]. The first two were calculated by the usual methods of statistical mechanics, while the values of Green were obtained by the incremental method of extrapolating the trends found in the first three normal alcohols. Because of the large uncertainties in the vibrational frequencies and barriers to internal rotation, the selected values were obtained by subtracting 0.2 cal deg^{-1} mol^{-1} from the entropies tabulated by Green. This correction gives agreement with the third law value at 25 °C.

TABLE 62. 1-Butanol. Reported values. Simple physical properties

Investigators		Vapor Pressures and Boiling Points		Freezing Point	Density, d g cm^{-3}		Refractive Index, n_D	
		°C	mmHg	t_m, °C	20 °C	25 °C	20 °C	25 °C
1-Butanol, $C_4H_{10}O$, mol wt. 74.124, state at 25 °C liq								
Louguinine	[1898]	117.02	760					
Kahlbaum	[1898]				0.80978		1.39931	
Doroshevskii and Dvorzhanchik	[1908]	117.1	760				1.39933	
Richards and Mathews	[1908]	117	760		.8094			
Reilly and Ralph	[1919]	117.5	760		.80974			
Brunel, Crenshaw, and Tobin	[1921]	117.71				0.8057		1.3974
Cox	[1921]	116.1–116.6	760				1.3992	
Timmermans	[1921]	117.1	760	−89.8				
Grimm and Patrick	[1923]	117.71						
Williams and Daniels	[1924]	117.6–117.7	760					1.39753
Norris and Ashdown	[1925]	117.8–117.9	760			.8055		
Parks	[1925]	116–118	760	−89.3				
Mathews	[1926]	117.7–117.9	760		.8099	.8061		
Clarke, Robinson, and Smith	[1927]	117.6	760		.8094	.8056		
Lloyd, Brown, Bonnell, and Jones	[1928]					.80569		
Timmermans and Martin	[1928]	118.0		−90.2			1.3993	
Berner	[1929]				.80978		1.39949	
Smyth and Stoops	[1929]	117.2–117.4	760		.8098		1.39921	
Smyth and Engel	[1929]	117.1–117.2	760				1.39942	
Smyth and Walls	[1931]	117.2–117.4	760			.80605	1.39922	1.39727
Ellis and Reid	[1932]	117.3	760			.80563		
Ernst, Litkenhous, and Spanyer	[1932]	117.69	760			.8056		1.3981
Cady and Jones	[1933]			−90.4				
Butler, Thomson, and Maclennan	[1933]	117.71	760			.8055		
Trew and Watkins	[1933]	117.25	760			.80612		1.39748
Butler, Ramchandani, and Thomson	[1935]	117.71	760			.80593	1.39982	
Tomanari	[1936]				.8118		1.39964	
Wojciechowski	[1936]	117.726	760					
Jones and Christian	[1939]	117.70	760			.8057		
Allen, Lingo, and Felsing	[1939]	117.3	760			.8057		1.3974
Venkataraman	[1939]							1.39630
Bridgman	[1941]			−89.8				
Brunjes and Bogart	[1943]	117.8	760			.80567		1.3970
Kretschmer, Nowakowska, and Wiebe	[1946]	117.67	760			.80573		
Vogel	[1948]	117.2	760		.8104		1.39929	
Dreisbach and Martin	[1949]			−89.53				
Dreisbach and Shrader	[1949]	117.40	760					
Tschamler, Richter, and Wettig	[1949b]	118.1		−80.6		.8073		
Pichler, Ziesecke, and Traeger	[1950]	117.8	760		0.8098		1.3993	
Mumford and Phillips	[1950]	117.9	760		.8102	0.8066	1.3992	
Sackmann and Sauerwald	[1950]			−84				
Cook	[1952]	117.6	760	−87	.8101		1.3992	
Dunning and Washburn	[1952]					.8058		1.3974
Hill and Van Winkle		117.0	760				1.39911	
Stavely and Spice	[1952]	117.61	760		.8098			
Anisimov	[1953b]					.8062		1.39748
Hellwig and Van Winkle	[1953]	117.1	760				1.39905	
McKenna, Tartar, and Lingafelter	[1953]	117.7	760					1.3973
Purnell and Bowden	[1954]	117.7	760			.80574		1.3970
Singh and Shemilt	[1955]	117.5	760					1.3973
Dannhauser and Cole	[1955]					.8056		1.3994
Kuss	[1955]				.8099			
Toropov	[1956b]				.8096			
Costello and Bowder	[1958]	117.0	760		.8086			
Lin and Tuan	[1958]	117.0–117.7	760			.80590		1.3969
Ling and Van Winkle	[1958]	117.8	760				1.39919	1.39739
Union Carbide Corporation	[1958]	117.7	760	−89.3	.8094			
Shemilt, Esplen, and Mann	[1959]	117.67	760					
Tjebbes	[1960]				.8099	.8059		
Brown and Smith	[1962b]	117.52				.80578		1.39731
Paraskevopoulos and Missen	[1962]					.80590		
Biddiscombe, Collerson, Handley, Herington, Martin, and Sprake	[1963]	117.726						

TABLE 62. 1-Butanol. Reported values. Simple physical properties—Continued

Investigators	Vapor Pressures and Boiling Points		Freezing Point	Density, d g cm^{-3}		Refractive Index, n_D	
	°C	mmHg	t_m, °C	20 °C	25 °C	20 °C	25 °C
1-Butanol, $C_4H_{10}O$, mol wt. 74.124, state at 25 °C liq							
Ambrose and Townsend [1963]				.8096			
Selected value [1967]	117.66±0.05 31.58±0.1	760 10	−89.3 ±0.2	0.8097 ±0.001	.8060 ±0.002	1.3993 ±0.001	1.3971 ±0.002

Antoine constants: *A* 7.47680, *B* 1362.39, *C* 178.77

dt/*dp* at 760 mmHg, 0.03686 °C/mmHg

TABLE 63. 1-Butanol. Reported values. Critical properties

Investigator	t_c, °C	P_c, atm	d_c, g cm^{-3}
Pawlewski [1883]	287.1		
Herz and Neukirch [1923]		48.4	
Fischer and Reichel [1943]	288.0		
Stull [1947]	287.0	48.4	
Kay and Donham [1955]	289.74	43.6	0.267
Singh and Shemilt [1955]	286.95	48.60	0.2700
Ravikovich and Solomko [1958]	291.0		
Ambrose and Townsend [1963]	289.83	43.55	0.2699
Efremov [1966]	288.0	42.4	0.271

TABLE 64. 1-Butanol. Reported values. Heats of vaporization

Investigator	ΔH_v at 25 °C	ΔH_v at t_b	Method and Remarks
Louguinine [1898]		10.22	Calorimetric.
Brown, J. C. [1903]		10.67	Calorimetric.
Mathews [1926]		10.44	Calorimetric.
Mathews [1926], extrapolated by McCurdy and Laidler [1963]	12.12–12.34		Calculated.
Bartoszewiczowna [1931]	11.0		Calorimetric.
Bennewitz and Rossner [1938]		10.48	Calorimetric, corrected to t_b
Shemilt, Esplen and Mann [1959]	12.34	10.47	Calculated from vapor pressure and *PVT* data
Green [1960]	12.62		Calculated from vapor pressure.
Biddiscombe, Collerson, Handley, Herington, Martin and Sprake [1963]		10.35	Calculated from vapor pressure.
McCurdy and Laidler [1963]	12.19		Calorimetric.
Counsell, Hales and Martin [1965]	12.59	10.31	Calorimetric, value at 25° extrapolated by equation.
Wadso [1966]	12.50		Calorimetric.
Selected Antoine constants	13.33	10.42	Calculated.

TABLE 65. 1-Butanol. Reported values. Heat capacity and entropy of the liquid at 25 °C

Investigator	$C_p^0(l)$	Remarks	$S^0(l)$, Third law
Williams and Daniels [1924]	42.0	Extrapolated from higher temperatures by equation	
Parks [1925]	42.5	Graphical extrapolation from lower temperatures	54.5
Counsell, Hales and Martin [1965]	42.31	From table of smoothed values	53.95

TABLE 66. 1-Butanol. Reported values. Heat capacity and entropy of the ideal gas at 25 °C

Investigator	$C_p^0(g)$	Remarks	$S^0(g)$ from molec-param-eters
Dyatkina [1954]			89.06
Green [1961]	26.29	Incremental rule	86.90
Chermin [1961]	26.19	Statistical calculation	86.48
Counsell, Hales and Martin [1965]	25.84	Equation based on calorimetric measurements	

TABLE 67. 1-Butanol. Reported values. Heat of combustion of the liquid at 25 °C

Investigator	$-\Delta H_c^0(l)$ kcal mol^{-1}
Zubov [1898] (recalculated by Swietoslawski [1920])	639.2
Richards and Davis [1920]	639.0
Verkade and Coops [1927] (recalculated)	639.25
Tjebbes [1960] and [1961]	638.2
Skinner and Snelson [1960]	639.31
Chao and Rossini [1965]	639.92
Gundry, Head and Lewis [1962]	639.69

TABLE 68. 1-Butanol. Comparison of virial coefficients and compressibility factor, Z, derived from experimental measurements

	Virial coefficients		Pressure, atmospheres							
	B_p' cm^3	D_p' cm^3 atm^{-2}	0.05	0.1	0.25	0.5	1	2	5	10
				Values of $(1-Z)\times100$						
			Temperature = 50 °C							
Cox, J. D. [1961]	(−2622)		(0.494)							
Counsell, Hales, and Martin [1965]	(−2617)	(−19610)	(.503)							
			Temperature = 100 °C							
Foz Gazulla, Morcillo, Masia, and Mendes [1954]	−1314		0.215	0.429	1.073	2.146				
Cox, J. D. [1961]	(−1372)		.224	.448	1.120	2.240				
Counsell, Hales, and Martin [1965]	−1373	−255	.224	.449	1.134	2.346				
			Temperature = 150 °C							
Cox, J. D. [1961]	−780		0.112	0.225	0.562	1.123	2.246	(4.49)		
Counsell, Hales, and Martin [1965]	−845	−9.40	.122	.243	.609	1.220	2.461	(5.08)		
			Temperature = 200 °C							
Shemilt, Esplen, and Mann [195]					(0.398)		(1.606)	(3.25)	(8.49)	(18.58)
Cox, J. D. [1961]	(−472)		0.061	0.122	.304	0.608	1.216	(2.43)	(6.08)	(12.15)
Counsell, Hales, and Martin [1965]	−578	−0.70	.074	.149	.372	0.745	1.491	(2.99)	(7.67)	(16.70)

Values in parenthesis have been extrapolated outside the experimental range of temperature and pressure.

TABLE 69. 1-Butanol. Differences in properties between real gas and ideal gas

Sources	at 25 °C and 6.75 mmHg			at 117.66 °C and 760 mmHg		
	H^r-H^0	$C_p^r-C_p^0$	S^r-S^0	H^r-H^0	$C_p^r-C_p^0$	S^r-S^0
Calculated from equation of state of Esplen and Mann [1959]	−0.001	0.005	−0.001	−0.118	0.43	−0.086
Calculated from equation of state of Cox, J. D. [1961]	−.004	.067	−.012	−.149	1.71	−0.31
Calculated from equation of state of Counsell, Hales and Martin [1965]	−.005	.12	−.015	−.146	2.81	−0.32

TABLE 70. 1-Butanol. Comparison of heat capacity and entropy of ideal gas reported by Green [1961] with that calculated from equation of Counsell, Hales, and Martin [1965]

T K	Heat Capacity, C_p^0(g)		Relative Entropy, S^0(g, T) − S^0(g, 400)	
	Green	Counsell, Hales, and Martin	Green	Counsell, Hales, and Martin
298.15	26.29	25.84	−8.53	−8.56
300	26.40	25.98	−8.38	−8.40
400	32.80	33.08	0.00	0.00
500	38.76	39.27	7.93	8.27

Chemical Equilibria

No data on chemical equilibria in the gas phase were located.

Tests of Internal Consistency

The internal consistency of the thermodynamic properties of the liquid and gas and of liquid-gas equilibria is shown by the following cycle between 25 °C and the normal boiling point.

	ΔH kcal mol^{-1}	ΔS cal deg^{-1} mol^{-1}
liquid (25 °C)→real gas (25 °C, 6.75 mmHg)	12.52±0.04	41.99±0.1
real gas (25 °C)→ideal gas (25 °C)	0.0005±0.002	0.01±0.005
ideal gas (25 °C)→ideal gas (117.66 °C)	2.71±0.05	7.78±0.1
ideal gas (6.75 mmHg)→ideal gas (760 mmHg)	0.0	−9.386±0.005
ideal gas (117.66 °C, 760 mmHg)→real gas (117.66 °C, 760 mmHg)	−0.146±0.005	−0.32±0.01
real gas (117.66 °C)→liquid (117.66 °C)	−10.31±0.04	−26.38±0.1
liquid (117.66 °C)→liquid (25 °C)	−4.77±0.05	−13.82±0.1
Sum	0.01±0.09	−0.13±0.2

Miscellaneous

Harris, Haycock, and Alder [1953] have studied the effect of pressure on the dielectric properties of 1-butanol in the range of 14 to 50 °C and up to 200 atm. These data were interpreted in terms of liquid structure. Malecki [1962a and 1962b] measured dielectric polarization at high electric field strength and used these data to determine the type of intermolecular interactions present.

Recommendations for Future Work

The investigations of Counsell, Hales, and Martin [1965], along with other recent studies of heat of combustion and vapor pressure, have established the properties of the liquid in the vicinity of room temperature with considerable confidence. Properties which concern vapor-liquid equilibria are also well determined. The principal deficiency at present is in the thermodynamic functions of the ideal gas. A detailed statistical calculation based on a complete vibrational analysis is needed, supplemented by experimental data on vapor heat capacity over a wider range of temperature than is now available.

Index to the Bibliography

Numbers refer to the Bibliography, page 1–389.

References to data used in the selection of refractive index, density, boiling point, vapor pressure, and melting point are in boldface type.

Numbers in parentheses refer to sources of reviews, or theoretica calculations only.

Reference numbers under each property are listed in the order of date of publication.

Refractive Index

235, 511, **865**, **439**, 1345, **509**, **239**, **354**, **1961**, **1140**, **1227**, 1274, 1855, **1784**, **135**, 1113, **1645**, **1646**, **1647**, 1687, 494, **1803**, **1262**, 1891, **253**, **1792**, 632, 1910, 1939, 21, **1843**, 799, 926, 1649, **241**, 532, 6, 783, 1404, 1615, 335, **1856**, **1893**, 282, 1420, 1637, 13, 201, 960, 1224, 1240, **1377**, 180, 1388, **338**, **462**, **760**, 1865, **35**, **737**, 1145, **1152**, 856, **1437**, 1632, 1834, 381, **1626**, 1292, 1521, **1459**, **1067**, **1069**, 1188, **231**, 1746, 851, 367

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989, 235, 1801, **865**, 1081, 1481, 1087, 1345, **1472**, 1294, **239**, 750, 1959, 1272, 1227, **1140**, **308**, **1075**, **1646**, **135**, 1113, 147, 1696, 494, **254**, **1803**, **1867**, **253**, 1792, 21, 997, 799, 1222, 1649, 241, **963**,, 6, 1615, (853), 335, 1810, 1807, 1377, **1224**, 1745, 1682, 1865, 462, 1338, 1521, 1232, 1459, **338**, **462**, 1823, 36, 1145, 858, 1632, **1436**, **104**, **381**, **1067**, **1789**, **231**, **1313**, **23**, 1147

Density at all Temperatures

1060, 1424, **1559**, 2012, 511, 273, 439, **55**, 509, 1471, 1409, 1746, 1308, 1350, 1848, **1784**, 851, **1795**, **1647**, **486**, 1262, 739, 880, 854, 1371, **962**, 1856, 1893, 1145, **978**, 1626, **1797**, **347**, **1069**, **1154**, **380**, 481

Normal Boiling Point

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865, 750, 1262, **253**, **21**, 453, **1848**, **1823**, 878, 1313, 23, **145**, **1603**

Critical Temperature
748, 1433, 532, 649, 1626, 878, 1461, 23, 1344

Critical Pressure
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Critical Volume and Density
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Normal Melting Point
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Association in the Liquid Phase
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2-Butanol

Properties of the Liquid Phase at Various Temperatures

2-Butanol is optically active. However, there is no evidence of any difference in physical properties other than specific rotation between either of the resolved *d*- or *l*-isomers and the racemic mixture in the liquid or gaseous states.

Refractive Index

The more significant values of the refractive index at the sodium D-line at 20 and 25 °C are given in table 74. The selected values at these temperatures are uncertain by about 0.001. A few scattered values at other temperatures from 15 to 30 °C have been published by Faillebin [1925a], Timmermans and Martin [1928], Nevgi and Jatkar [1934], Mahanti [1935], Weissler [1948], and Thomas and Meatyard [1963]. The selected values in table 71 were taken from a smooth curve drawn through these points. Values at other wavelengths, given in table 73, are based on the data of Eykman [1919] and of Timmermans and Martin [1928], along with the temperature coefficient from table 71.

Density

There are fewer accurate measurements for 2-butanol than there are for 1-butanol and for the lower alcohols. Some values at 20 and 25 °C are given in table 74. Timmermans and Martin [1928] reported 0.82273 gms ml^{-1} at 0 °C, 0.81089 g ml^{-1} at 15 °C, and 0.79898 g ml^{-1} at 30 °C, and Weissler [1948] reported 0.7983 g ml^{-1} at 30 °C. The only data above 80 °C are those of Costello and Bowden [1958], from −60 to 180 °C, and of Dannhauser and Bahe [1964], which are reported to only 3 figures after the decimal point. Densities calculated from the Francis equation are listed in table 71. Most of the observed values lie within about 0.001 g ml^{-1} of the calculated ones.

TABLE 71. 2-Butanol. Selected values. Physical and thermodynamic properties

Temp. °C	Refractive Index, n_D	Density g cm^{-3}	Vapor Pressure, mmHg
−20		0.8394	
−10		.8315	
0		.8234	
10		.8152	
15	1.3995		
16.4			10
20	1.3972	.8069	12.9
25	1.3949	.8026	18.3
30	1.3926	.7984	25.4
35			34.9
40		.7897	47.1
45			62.9
50		.7809	82.9
53.5			100
55			108.1
60		.7720	139.3
65			177.8
67.5			200
70		.7628	224.8
75			281.6
80		.7536	349.9
83.2			400
85			431.2
90		.7441	527.5
95			640.6
99.55			760
100		* .7345	772.8
105			926.2
110		* .7247	1103.4
120		* .7147	

Data For Phase Transitions

Initial	Final	Temp. °C	dt/dP deg mm^{-1}	Pressure mmHg	ΔH kcal mol^{-1}	$d\Delta H/dt$ cal deg^{-1} mol^{-1}	ΔS cal deg^{-1} mol^{-1}	ΔC_p cal deg^{-1} mol^{-1}
c	liq	−114.7±2		760				
liq	g	25	0.808	18.29±0.2	11.87±0.02	−20.5±0.5	39.81±0.0	−19.8±0.5
liq	g	99.55±0.04	.03559	760	9.75±0.02	−35.1±0.2	26.16±0.07	−26.6±0.5

Condensed Phase Heat Capacity

State	Temp. °C	C_p cal deg^{-1} mol^{-1}
liq	99.55	63.5±0.6

Properties of the Saturated Real Gas

Temp. °C	$H^r - H^0$ kcal mol^{-1}	$S^r - S^0$ cal deg^{-1} mol^{-1}	$C_p^r - C_p^0$ cal deg^{-1} mol^{-1}
25	−0.02±0.01	−0.06±0.02	0.6±0.1
99.55	−0.0168±.005	−0.37±.01	

Data for the Standard States at 25 °C

State	Heat of Combustion ΔH_c^0 kcal mol^{-1}	Heat of Formation ΔH_f^0 kcal mol^{-1}	Entropy S^0 cal deg^{-1} mol^{-1}	Gibbs Energy of Formation ΔG_f^0 kcal mol^{-1}	Heat Capacity, C_p cal deg^{-1} mol^{-1}
liq	−635.90±0.05	−81.88±0.05	53.3±0.2	−42.31±0.07	47.5±0.5
g	−647.84±0.05	−69.94±0.05	85.8±0.2	−40.06±0.07	27.08±0.05

Critical Constants

Temp. 262.80 °C, 535.95 K	Pressure 41.39 atm	Density 0.276 g cm^{-3}

			Constants in Vapor Pressure and Density Equation								
			Antoine Equation				Francis Equation				
			Temp. Range	A	B	C	Temp. Range	A	$B \times 10^3$	C	E
			25 to 120 °C	7.47431	1314.19	186.55	−20 to 140 °C	2.25464	−0.1898	2041.65	1426.50

* At saturated vapor pressure.

Table 72. 2-Butanol. Selected values. Thermodynamic functions of the ideal gas at one atmosphere

Temperature K	Entropy S^0 cal deg^{-1} mol^{-1}	Heat Capacity $C_p{}^0$ cal deg^{-1} mol^{-1}	Enthalpy Function $(H^0-H_0{}^0)/T$ cal deg^{-1} mol^{-1}	Gibbs Energy Function $(G^0-H_0{}^0)/T$ cal deg^{-1} mol^{-1}	Heat of Formation $\Delta H_f{}^0$ kcal mol^{-1}	Gibbs Energy of Formation $\Delta G_f{}^0$ kcal mol^{-1}
0	0	0	0	0	−62.96	−62.96
273.15	83.66	24.46	16.57	−67.03	−69.46	−42.56
298.15	85.81	27.08	17.39	−68.42	−69.94	−40.06
300	85.98	27.20	17.44	−68.53	−69.98	−39.87
400	94.78	33.70	20.71	−74.07	−71.74	−29.59
500	103.01	39.70	23.92	−79.09	−73.20	−18.91
600	110.74	44.72	26.97	−83.76	−74.36	−7.96
700	117.99	49.02	29.82	−88.17	−75.27	+3.16
800	124.80	52.68	32.46	−92.34	−75.94	14.39
900	131.20	55.88	34.90	−96.33	−76.41	25.71
1000	137.26	58.62	37.14	−100.14	−76.70	37.06

TABLE 73. 2-Butanol. Selected values. Refractive index at various temperatures and wavelengths

Symbol	Wavelength, Å	Refractive Index, n	
		15 °C	20 °C
He_{red}	6678.2	1.3972	1.3950
H_c	6562.8	1.3975	1.3952
Na_D	5892.6	1.3995	1.3972
Hg_e	5460.7	1.4012	1.3998
He_{blue}	5015.7	1.4034	1.4010
H_F	4861.3	1.4044	1.4019
Hg_g	4358.3	1.4082	1.4056
$H_{G'}$	4340.5	1.4084	1.4058

Vapor Pressures and Boiling Points

The vapor pressure data used to calculate the Antoine constants in table 71 were taken from the publications of Butler, Ramchandani, and Thomson [1935], from 25 to 91 °C; Berman and McKetta [1962], from 66 to 105 °C; Thomas and Meatyard [1963], 17 to 99 °C; and Biddiscombe, Collerson, Handley, Herington, Martin, and Sprake [1963], from 72 to 107 °C. The data of Biddiscombe et al. were given the highest weight. The calculated values are within 2 mmHg of their observed vapor pressures in the range of 83 to 107 °C. The calculated values are 2 to 3 mmHg high from 72 to 80 °C. Ambrose and Townsend [1963] have measured the vapor pressure from 149 °C to the critical point. Values of some of the more carefully determined normal boiling points are listed in table 74. The selected boiling point, as calculated from the Antoine constants, is probably within 0.04 °C of the true value.

Critical Properties

Critical Temperature, Pressure and Density

Since Ambrose and Townsend [1963] report the only modern measurements of high accuracy, their values are adopted.

Solid-Liquid Phase Equilibria

Melting Point

Cady and Jones [1933] report the only value of the melting point, which is the one selected in table 71. Both Cook [1952] and Parks, Thomas, and Light [1936] found that 2-butanol did not crystallize when cooled but set to a glass instead. Additional studies are needed to determine whether the value found by Cady and Jones is a true equilibrium melting point.

Heat Capacity of the Solid and Liquid

Parks, Thomas, and Light [1936] have measured the heat capacity of the glass and liquid forms from −171 to 9 °C.

Properties of the Liquid at 25 °C

Heat Capacity

The value shown in table 71 was obtained by extrapolating the data of Parks, Thomas, and Light [1936] from 9 to 25 °C.

Absolute Entropy

Since Parks, Thomas, and Light [1936] found that 2-butanol formed a glass in their calorimeter, rather than a crystalline solid, their data cannot be used to calculate the absolute entropy by means of the third law. The selected value was calculated from the entropy of the vapor phase, the entropy of vaporization, and other auxiliary data.

Heat of Combustion

Only three values, shown in table 77, have been reported. However, the data of Skinner and Snelson [1960] and Chao and Rossini [1965] are in good agreement; and, since both sets of measurements were carefully done, the value selected, which is an average of these two, should be quite reliable.

Properties of Real Gas

Equation of State

J. D. Cox [1961] expressed the second virial coefficient as obtained from P-V-T measurements from 105 to 150 °C as,

$$\log(-B_p') = 14.678 - 4.5 \log T.$$

Berman and McKetta [1962] used an equation based on the model of monomers, dimers, and tetramers, as has been done for the other alcohols. They evaluated the constants in the following equations for the second and fourth virial coefficients,

$$B_p' = -480 - 1.690 \times 10^{-3} T \exp\left(\frac{2625}{T}\right) \text{ ml mol}^{-1}$$

$$D_p' = -1.1738 \times 10^{-14} T \exp\left(\frac{11559}{T}\right) \text{ ml atm}^{-2} \text{ mol}^{-1}$$

TABLE 74. 2-Butanol. Reported values. Simple physical properties

Investigators		Vapor Pressures and Boiling Points		Freezing Point	Density, d g cm^{-3}		Refractive Index, n_D	
		°C	mmHg	t_m, °C	20 °C	25 °C	20 °C	25 °C
2-Butanol. $C_4H_{10}O$, mol wt. 74.124. state at 25 °C liq								
Pickard and Kenyon	[1911]	99	760		0.8020		1.3954	
Timmermans	[1911]	99.5	760					
Wilcox and Brunel	[1916]	98.4–99.0	760			0.8034		
Brunel, Crenshaw, and Tobin	[1921]	99.53	760			.80229		1.39495
Reilly and Hickinbotton	[1921]	99.4–99.5	760					
Brunel	[1923]	99.529	760			.80235		1.39495
Clough and Johns	[1923]	99.40	760		.8063	.8027		
Norris and Ashdown	[1925]	99.47–99.57	760			.8022		
Munch	[1926]	98.0	760			.8095		1.3942
Pahlavouni	[1927]						1.39780	
Roland	[1928]	99.5	760					
Timmermans and Martin	[1928]	99.50	760					
Berner	[1929]				.80652		1.39738	
Cady and Jones	[1933]			−114.7				
Webb and Lindsley	[1934]	99.6	760				1.3970	
Butler, Ramchandani, and Thomson	[1935]	99.95	760			.80299	1.39846	
Parks, Thomas, and Light	[1936]	99.52–99.55	760					
Allen, Lingo, and Felsing	[1939]	99.6	760			.8022		1.3946
Pichler, Ziesecke, and Traeger	[1950]	99.5	760		.8064			
Braun, Spooner, and Fenske	[1950]						1.3973	
Bothner-By	[1951]	99.5–100.0	760					1.3974
Leroux and Lucas	[1951]					.8042	1.3970	1.3949
Cook	[1952]	99.4	760		.8072		1.3972	
Dunning and Washburn	[1952]					.8024		1.3950
McKenna, Tartar, and Lingafelter	[1953]	99.4	760					1.3950
Hellwig and Van Winkle	[1953]	99.3	760				1.39713	
Kuss	[1955]				.8073	.8033		
Costello and Bowden	[1953]	99.3	760		.8060			
Brown and Smith	[1962b]	99.41	760			.80251		1.39525
Berman, Neil, and McKetta	[1962]	99.63	760					
Ambrose and Townsend	[1963]				.8129			
Biddiscombe, Collerson, Handley, Herington, Martin, and Sprake	[1963]	99.513	760					
Selected value	[1967]	99.55±0.04 16.4±0.1	760 10	−114.7 ±2	.8069 ±0.002	.8026 ±0.002	1.3972 ±0.001	1.3949 ±0.001

Antoine constants: A 7.47431, B 1314.19, C 186.55

dt/dp at 760 mmHg, 0.03559 °C/mmHg

by fitting them to their experimental heat capacity measurements from 92 to 182 °C and to the calorimetric heats of vaporization and vapor pressure data. This gives, for the enthalpy and entropy of formation of dimers and tetramers, $\Delta H_2 = -5.25$ kcal mol^{-1}, $\Delta S_2 = -21.4$ cal deg^{-1} mol^{-1}, $\Delta H_4 = -23.118$ kcal mol^{-1}, and $\Delta S_4 = -74.7$ cal deg^{-1} mol^{-1}.

Ambrose and Townsend [1963] measured orthobaric densities of liquid and vapor from 134 °C to the critical point.

TABLE 75. 2-Butanol. Reported values. Critical properties

Investigator	t_c, °C	P_c, atm	d_c, g cm^{-3}
Brown, J. C. [1906]	265.19		
Stull [1947]	265.0	48.0	
Ambrose and Townsend [1963]	262.80	41.39	0.2755

Heat Capacity

Direct vapor phase heat capacity measurements have been made by Reynolds and De Vries [1950], Sinke and De Vries [1953], and Berman and McKetta [1962]. Jatkar and Lakshimarayan [1946] have derived the heat capacity from the observed velocity of sound. Berman and McKetta have expressed the heat capacity as a function of pressure using the same model as for the equation of state. They have also compared their measurements with the earlier ones. As for the other alcohols, pressure has a marked effect on the vapor heat capacity, and it increases very rapidly near saturation with the liquid.

Corrections to the Ideal Gas State

These data for the saturated vapor at 25 °C and at the normal boiling point are shown in table 79 and were calculated from the equations of state of J. D. Cox [1961] and Berman and McKetta [1962]. The agreement at 25 °C is poor, but this temperature is considerably below the experimental range for both sets of data. The agreement at the boiling point is better, except for the heat capacity. Since heat capacity data were used to derive the equation of Berman and McKetta, but not of Cox, the former should give a more accurate value for the heat capacity correction.

Vapor-Liquid Equilibrium at 25 °C

Vapor Pressure

This was calculated from the selected Antoine constants.

Heat of Vaporization

The only directly measured values are those of McCurdy and Laidler [1963] and of Wadso [1966], as shown in table 76. The value listed for Berman and McKetta was calculated from the equation derived from measurements at higher temperatures. The carefully measured value of Wadso [1966] was selected. This was quite close to the value calculated from the selected Antoine constants.

Temperature Derivative of the Heat of Vaporization

The equation for heat of vaporization of Berman and McKetta [1962] gave -27.22 cal deg^{-1} mol^{-1}, while both the equations of state of J. D. Cox [1961] and Berman and McKetta, in combination with the heat capacities of the liquid and the gas, gave -20.5 cal deg^{-1} mol^{-1}. Although the corrections for deviations from ideal behavior were rather uncertain, they were small at the saturation pressure at 25 °C. The value calculated from the heat capacities was considered more reliable and was adopted.

Vapor-Liquid Equilibrium at the Normal Boiling Point

Normal Boiling Point

The boiling point at 1 atm was calculated from the selected Antoine constants. It is within a few hundredths of a degree of most of the data in table 74.

Heat of Vaporization

The selected value was calculated from the equation,

$$\Delta H_v = 1092.15(225.30-t)^{0.45282} \text{ cal mol}^{-1}$$

where t is the temperature in degrees C. This was derived by Berman and McKetta [1962] to reproduce their calorimetrically measured data from 66 to 99.5 °C. It agrees fairly well with the other recent data listed in table 76.

TABLE 76. 2-Butanol. Reported values. Heats of vaporization

Investigator	ΔH_v at 25 °C	ΔH_v at t_b	Method and Remarks
Brown, J. C. [1903]		10.15	Calorimetric.
Mathews [1926]		9.91	Calorimetric.
Mathews [1926], extrapolated by McCurdy and Laidler [1963]	11.29–11.50		
Mathews [1926], extrapolated by Skinner and Snelson [1960]	11.82		
Berman and McKetta [1962]	12.04	9.75	Calorimetric, extrapolated to 25 °C by equation.
Biddiscombe, Collerson, Handley, Herington, Martin and Sparke [1963]		9.80	Calculated from Antoine constants.
McCurdy and Laidler [1963]	11.59		Calorimetric.
Wadso [1966]	11.87		Calorimetric.
Selected Antoine constants	11.90	9.73	Calculated.

Heat Capacity of the Liquid

Since there is no directly measured value, the heat capacity was calculated from $d\Delta H/dT$, the heat capacity of the gas and equation of state. Since the result is strongly influenced by experimental errors, it cannot be considered as very accurate.

Temperature Derivative of the Heat of Vaporization

This was calculated from the heat of vaporization equation of Berman and McKetta [1962].

TABLE 77. 2-Butanol. Reported values. Heat of combustion of the liquid at 25 °C

Investigator	$-\Delta H_c^0$ kcal mol^{-1}
Richards and Davis [1920]	638.2
Skinner and Snelson [1960]	635.91
Chao and Rossini [1965]	635.89

TABLE 78. 2-Butanol. Comparison of virial coefficients and compressibility factor, Z, derived from experimental measurements

	Virial coefficients			Pressure, atmospheres						
				0.05	0.1	0.25	0.5	1	2	5
	B_p' cm^3	C_p' cm^3 atm^{-1}	D_p' cm^3 atm^{-2}	Values of $(1-Z)\times100$						
Temperature = 50 °C										
Cox, J. D. [1961]	(−2431)			(0.458)	(0.917)					
Berman and McKetta [1962]	(−2321)		(−12990)	(.444)	(.924)					
Temperature = 100 °C										
Cox, J. D. [1961]	−1272			(0.208)	(0.415)	(1.038)	2.08	(4.15)		
Berman and McKetta [1962]	−1195		−124	(.195)	(.391)	0.982	2.00	(4.31)		
Temperature = 150 °C										
Cox, J. D. [1961]	−723			(0.104)	(0.208)	(0.521)	1.041	(2.08)	(4.16)	(10.41)
Berman and McKetta [1962]	−834		−3.63	(.106)	(.211)	.529	1.058	2.12	(4.31)	(11.88)
Temperature = 200 °C										
Cox, J. D. [1961]	(−437)			(0.056)	(0.113)	(0.281)	(0.563)	(1.13)	(2.25)	(5.63)
Berman and McKetta [1962]	(−685)		(−0.226)	(.088)	(.176)	(.441)	(.882)	(1.77)	(3.53)	(8.89)

Values in parenthesis have been extrapolated outside the experimental range of temperature or pressure.

Properties of the Ideal Gas State

Molecular Parameters

Some reference to molecular spectra and related properties are given in the Index to the Bibliography. However, the only attempt of a complete vibrational assignment suitable for calculation of thermodynamic functions has been given by Berman and McKetta [1962]. The vibrational assignments and nature of rotational isomers were based on available infrared and Raman spectra and by analogy with 2-butanethiol propane, and ethanol. Potential barriers to internal rotation were taken as 3100 and 4000 cal mol^{-1} for the methyl groups, and 800 cal mol^{-1} for the hydroxyl group. A value of 2150 cal mol^{-1} was taken for rotation about the central C—C bond. Because of the complexity of the situation and the scarcity of appropriate data, these assignments can be considered only as tentative at present.

Entropy at 25 °C

The only value available is the one calculated by Berman and McKetta [1962] from molecular parameters.

TABLE 79. 2-Butanol. Differences in properties between real gas and ideal gas

Sources	at 25 °C and 18.3 mmHg			at 99.55 °C and 760 mmHg		
	H^r-H^0	$C_p{}^r-C_p{}^0$	S^r-S^0	H^r-H^0	$C_p{}^r-C_p{}^0$	S^r-S^0
Calculated from equation of state of Cox, J. D. [1961]	−0.006	0.09	−0.016	−0.171	2.06	−0.37
Calculated from equation of state of Berman and McKetta [1962]	−0.019	.64	−.055	−.167	5.02	−0.37

TABLE 80. 2-Butanol. Enthalpy and Gibbs energy change for the dehydrogenation to butanone and hydrogen in the gas phase and constants in the equation:

$$\Delta H^0 = \Delta H_0^0 + AT + \tfrac{1}{2}BT^2 + \tfrac{1}{3}CT^3 \quad \text{and} \quad \Delta G^0 = \Delta H_0^0 - AT\ln T + IT - \tfrac{1}{2}BT^2 - \tfrac{1}{6}CT^3$$

	Kolb and Burwell, Jr. [1945]	Kolb and Burwell, Jr. [1945], recalculated by Cubberley and Mueller [1946]	Cubberley and Mueller [1946]	Buckley and Herington [1965]
ΔH_0^0, cal mol^{-1}	12,700	11,338	11,338	11,430
A	3.00	6.610	6.610	5.417
B		-7.8×10^{-3}	-7.8×10^{-3}	1.63×10^{-3}
C				-1.85×10^{-5}
I	−8.535	15.01	14.57	9.62
Experimental Temperature Range °C	147–199	147–199	172–246	113–216
ΔH^0 (200 °C), kcal mol^{-1}	14.12	13.59	13.59	13.54
ΔG^0 (200 °C), kcal mol^{-1}	−0.08	−0.06	−0.12	0.34
ΔH^0 (150 °C), kcal mol^{-1}	13.97	13.44	13.44	13.41
ΔG^0 (150 °C), kcal mol^{-1}	1.41	1.48	1.29	1.72
ΔH^0 (25 °C), kcal mol^{-1}	13.59	12.96	12.96	12.96
ΔG^0 (25 °C), kcal mol^{-1}	5.06	4.94	4.80	5.11

Heat Capacity

Extrapolation of the data of Berman and McKetta [1962] to zero pressure gives the equation,

$$C_p^0 = 5.533 + 0.07687T - 1.598\times10^{-5}T^2 \text{ cal deg}^{-1}\text{ mol}^{-1}$$

which is valid in the range of 92 to 182 °C. This gives 27.03 cal deg^{-1} mol^{-1} at 298.15 K and 33.72 cal deg^{-1} mol^{-1} at 400 K. The corresponding values which they calculate by statistical methods from the molecular parameters are 27.08 and 33.70 cal deg^{-1} mol^{-1}, respectively.

Thermodynamic Functions

The data given in table 72 were taken from the calculations of Berman and McKetta [1962], except for ΔH_f^0 and ΔG_f^0, which were recalculated so as to be consistent with the other selected data. There is little with which to compare these data and to judge their accuracy. As shown in the previous paragraph, the heat capacity does agree well with the experimentally derived values. The values which they list for ΔG_f^0 and log K_f^0 are incorrect, apparently as a result of an arithmetic error.

Chemical Equilibria

Three sets of experimental studies of the equilibrium constant have been made on the gas phase dehydrogenation of 2-butanol.

$$CH_3CH_2CHOHCH_3(g) \rightarrow CH_3CH_2COCH_3(g) + H_2(g).$$

The results have been summarized in table 80. Cubberley and Mueller [1946] expressed both their equilibrium constant data and those of Kolb and Burwell, Jr. [1945] in the form of equations which had the same ΔH_0^0 and heat capacity values. The more recent measurements of Buckley and Herington [1965] are probably the most accurate and were also conducted over a wider temperature range than the older ones. The values of ΔH^0 and ΔG^0 obtained at 25 °C from the four sets of equations show good agreement, considering that this is well below the temperature of the experimental measurements. Stanley, Youell, and Dymock [1934] have measured the equilibrium constant of the reaction,

$$C_4H_8(g) + H_2O(g) \rightarrow CH_3CH_2CHOHCH_3(g)$$

in the range from 150 to 250 °C. This is similar to the corresponding reaction for 2-propanol which they also studied. They could distinguish no difference between 1-butene and 2-butene. The discrepancy between the ΔH and ΔG for this reaction obtained by extrapolating their data to 25 °C and the ΔH and ΔG calculated from accepted enthalpies and Gibbs energies of formation of the components of the reaction is even greater than it was for the formation of 2-propanol from propene.

Tests of Internal Consistency

The usual test for internal consistency of the thermodynamic data concerning liquid-vapor equilibria is not so effective for 2-butanol as for most of the other alcohols because of the uncertainty in the heat capacity of the liquid between 25 °C and the boiling point. A linear function was assumed to exist between the values at these two temperatures shown on the summary sheet. However, the ΔH and ΔS for this cycle is zero within the experimental uncertainties.

	ΔH kcal mol^{-1}	ΔS cal deg^{-1} mol^{-1}
liquid (25 °C)→real gas (25 °C, 18.3 mmHg)	11.87±0.02	39.81±0.07
real gas (25 °C)→ideal gas (25 °C)	0.02±0.01	0.06±0.02
ideal gas (25 °C)→ideal gas (99.55 °C)	2.20±0.02	6.63±0.05
ideal gas (18.3 mmHg)→ideal gas (760 mmHg)	0.0	−7.407±0.01
ideal gas (99.55 °C, 760 mmHg)→real gas (99.55 °C, 760 mmHg)	−0.168±0.005	−0.37±0.01
real gas (99.55 °C)→liquid (99.55 °C)	−9.75±0.02	−26.16±0.07
liquid (99.55 °C)→liquid (25 °C)	−4.14±0.07	−12.29±0.2
Sum	0.03±0.08	0.27±0.24

Miscellaneous

Nemeth and Reed [1964] calculated a collision diameter of 7.66 Å from measurements of the viscosity of the vapor.

Recommendations for Future Work

The most significant gap in the thermodynamic properties of 2-butanol is the lack of a third-law value of the absolute entropy. This probably results from the difficulty in crystallizing 2-butanol. Data on the heat capacity of the liquid at room temperature and at higher temperatures are also needed. The heat of combustion seems to be well established, and recent studies, especially those of Berman and McKetta [1962] and Wadso [1966], have furnished reliable values for the heat of vaporization. In addition, Berman and McKetta have made a good start in calculating the thermodynamic functions of the ideal gas, but refinements in this should be introduced, particularly if it turns out that a third law entropy value is not accessible. This should include a more careful study of the molecular vibrations and geometry and more detailed information about barriers to internal rotation and the energy differences among the conformational isomers.

Index to the Bibliography

Numbers refer to the Bibliography, page 1–389.

References to data used in the selection of refractive index, density, boiling point, vapor pressure, and melting point are in boldface type.

Numbers in parentheses refer to sources of reviews, or theoretical calculations only.

Reference numbers under each property are listed in the order of date of publication.

Refractive Index
1378, 1379, 1838, 123, 509, **239**, **238**, **512**, **1227**, 1302, **1784**, **135**, 793, 782, **1262**, **1891**, 253, 1112, **21**, **1930**, **1203**, 783, **1893**, 282, 13, **201**, 960, **1377**, 28, 184, **1015**, 1388, **338**, **462**, 737, **1152**, 2016, 1824, 226, 1521, 901, 1594, 505, 1193, **231**, **1758**

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Properties of the Liquid Phase at Various Temperatures

Refractive Index

Some reported values of the refractive index at the sodium D-line at 20 and 25 °C are listed in table 83. Schwers [1912b and 1915] and Venkataraman [1939] have measured the refractive index from 8 to 86 °C. The data for refractive index in table 82 for temperatures other than 20 and 25 °C were based on these measurements and a few other scattered values. Landolt and Jahn [1892], Schwers [1915], Eykman [1919], Timmermans and Martin [1928], and Vogel [1948] have reported values for wavelengths other than the sodium D-line. Most of the selected values in table 82 were taken from smooth curves drawn through their data. Refractive indices above 25 °C were obtained primarily from the measurements of Schwers. Below 4000 Å refractive indices were calculated from a quadratic equation in the variable $1/(\lambda-1000)^{1.6}$ obtained from a least squares fit of the data of Stephens and Evans [1930] corrected to 15 °C. The uncertainty in these results is about 0.0005.

Density

Although a fairly large number of density measurements have been published in the literature, the agreement among different investigators is poor. Some values at 20 and 25 °C are summarized in table 83. The selected values listed in table 81 have been calculated from the Francis equation. Above 60 °C selections are based on the data of Costello and Bowden [1958], Naccari and Pagliani [1881], and Dannhauser and Bahe [1958]. Most of the reported values are within 0.003 g ml^{-1} of the calculated ones, although some deviate as much as 0.007 g ml^{-1}. Uncertainties in the selected values are about 0.002 g ml^{-1} up to 80 °C and are somewhat larger at higher temperatures.

Vapor Pressures and Boiling Points

A large amount of vapor pressure data, extending back many years, has been published. The measurements of Biddiscombe, Collerson, Handley, Herington, Martin, and Sprake [1963] are the most accurate, but they range only from 80 to 115 °C. Older data must be used to establish the lower end of the vapor pressure curve. The final nonlinear calculation of the Antoine constants in table 81 was based principally on the data of Biddiscombe et al., Richardson [1886], from 25 to 106 °C; Butler, Ramchandani, and Thomson [1935], from 25 to 105 °C; Allen, Lingo, and Felsing [1939], at 25 and 107 °C; Union Carbide and Carbon Chemicals Company [1956], and a few other scattered points, as well as three heats of vaporization measurements. Most of the vapor pressure data of Biddiscombe et al. were about 0.5 mmHg lower than the ones calculated from the final set of constants. Richardson's values scattered within about 5 mmHg of the calculated curve. The calculated boiling point at one atmosphere is slightly lower than most of the values shown in table 83, but it is probably within the range of uncertainty which they represent. Kay and Donham [1955] and Ambrose and Townsend [1963] have measured the vapor pressure up to the critical point.

Critical Properties

Critical Temperature

The selected value is an average of the values of Kay and Donham [1955] and Ambrose and Townsend [1963]. Both sets of measurements were made on samples of high purity. There is no obvious explanation for the considerably higher value of Kreglewski [1954].

TABLE 81. 2-Methyl-1-Propanol. Selected values. Physical and thermodynamic properties

Temp. °C	Refractive Index, n_D	Density g cm^{-3}	Vapor Pressure, mmHg
−20		0.8309	
−10		.8238	
0		.8166	
+10	1.3994	.8092	
15	1.3976		
20	1.3958	.8016	7.2
24.4			10
25	1.3938	.7978	10.4
30	1.3918	.7938	14.9
35			21.
40	1.3875	.7858	29.1
45			39.6
50	1.3830	.7776	53.3
55			70.7
60	1.3785	.7691	92.7
61.44			100
65			120.1
70	1.3740	.7602	154.
75			195.5
75.48			200
80	1.3695	.7511	245.9
85			306.5
90	1.3651	.7415	378.9
91.31			400
95		.7316	464.7
100			565.6
105			683.6
107.87			760
110		* .7212	820.7
115			979.1
120		* .7102	

Data For Phase Transitions

Initial	Final	Temp. °C	dt/dP deg mm^{-1}	Pressure mmHg	ΔH kcal mol^{-1}	$d\Delta H/dt$	ΔS	ΔC_p
						cal deg^{-1} mol^{-1}		
liq	g	25	1.31	10.4±0.5	12.14±.03	−16.8±1	40.72±0.1	−16.3±1
liq	g	107.87±0.05	0.03609	760	10.05±0.1	−36.±1.5	26.38±0.3	−28.7±1

Condensed Phase Heat Capacity

State	Temp. °C	C_p
		cal deg^{-1} mol^{-1}
liq	107.87	65.3±0.8

Properties of the Saturated Real Gas

Temp. °C	$H^r - H^0$	$S^r - S^0$	$C_p^r - C_p^0$
	kcal mol^{-1}	cal deg^{-1} mol^{-1}	
25	−0.007±0.002	−0.02±0.01	−0.15±0.05
107.87	−0.18±0.01	−0.39±0.03	−1.5±1.0

Data for the Standard States at 25 °C

State	Heat of Combustion ΔH_c^0 kcal mol^{-1}	Heat of Formation ΔH_f^0 kcal mol^{-1}	Entropy S^0 cal deg^{-1} mol^{-1}	Gibbs Energy of Formation ΔG_f^0 kcal mol^{-1}	Heat Capacity, C_p cal deg^{-1} mol^{-1}
liq	−637.93±0.08	−79.85±0.08			43.1±0.5
g	−650.09	−67.69±0.09			26.6±1

Critical Constants

Temp. 274.58 °C, 547.73 K	Pressure 42.39 atm	Density 0.272 g cm^{-3}

Constants in Vapor Pressure and Density Equation

Antoine Equation				Francis Equation				
Temp. Range	A	B	C	Temp. Range	A	$B \times 10^3$	C	E
20 to 115 °C	7.32705	1248.48	172.92	−20 to 147 °C	0.91253	0.4480	2041.65	1426.50

* Undercooled liquid.

TABLE 82. 2-Methyl-1-propanol. Selected values. Refractive index at various temperatures and wavelengths

Symbol	Wavelength, Å	Refractive Index, *n*							
		10 °C	15 °C	20 °C	25 °C	30 °C	40 °C	50 °C	60 °C
He_{red}	6678.2	1.3971	1.3954	1.3936	1.3917	1.3896	1.3852	1.3807	1.3763
H_c	6562.8	1.3974	1.3956	1.3939	1.3919	1.3899	1.3855	1.3810	1.3766
Na_D	5892.6	1.3994	1.3976	1.3958	1.3938	1.3918	1.3875	1.3830	1.3785
Hg_e	5460.7	1.4013	1.3994	1.3974	1.3934	1.3935	1.3892	1.3849	1.3802
He_{blue}	5015.7	1.4037	1.4017	1.3997	1.3977	1.3957	1.3916	1.3873	1.3825
H_F	4861.3	1.4047	1.4026	1.4006	1.3986	1.3966	1.3926	1.3883	1.3835
Hg_g	4358.3	1.4082	1.4066	1.4044	1.4024	1.4000	1.3964	1.3921	1.3871
$H_{G'}$	4340.5	1.4084	1.4068	1.4046	1.4026	1.4002	1.3966	1.3923	1.3873
	4000		1.4101						
	3500		1.4175						
	3000		1.4295						
	2700		1.4410						

Critical Pressure and Density

The values of Ambrose and Townsend [1963] were selected. The pressure is also close to the value obtained by Kay and Donham [1955].

Solid-Liquid Phase Equilibria

Normal Melting Point

Carrara and Coppadoro [1903] report that 2-methyl-1-propanol forms a glass at −108 °C, and Cook [1952] found that it sets to a glass between −120 and −105 °C. Hagemeyer and DeCroes [1953] report a melting point of −108 °C, but this probably refers to the temperature of glass formation reported by Carrara and Coppadoro. Thus, no value can be assigned to the equilibrium melting point of the crystalline solid at this time.

Heat Capacity of the Liquid and Solid at the Melting Point and Heat of Fusion

No measurements of these properties have been made.

Properties of the Liquid at 25 °C

Heat Capacity

The only data on the heat capacity of the liquid, other than the questionable value of Louguinine [1898], are those of Williams and Daniels [1924] between 30 and 80 °C. The value shown on the summary sheet was obtained by extrapolation to 25 °C through the use of their equation of specific heat as a function of temperature.

Absolute Entropy

There are no data which can be used to calculate the absolute entropy, either by the third law or by statistical thermodynamics of the gas phase.

Heat of Combustion

Several experimental values are listed in table 86. The selected value was the average of the ones reported by Skinner and Snelson [1960] and Chao and Rossini [1965].

Properties of the real gas

Equation of State

The only direct *P-V-T* measurements which have been reported are those of J. D. Cox [1961]. He found that the second virial coefficient obtained in the range from 120 to 166 °C could be fit to the same function of temperature which applied to 1-butanol. Ambrose and Townsend [1963] measured the orthobaric densities of liquid and vapor from 148 °C to the critical temperature.

Heat Capacity

Bennewitz and Rossner [1938] measured the vapor heat capacity at 137 °C and 748 mmHg, and Sinke and De Vries [1953] measured it over the range of 110 to 164 °C at 750 mmHg pressure. The value of Bennewitz and Rossner was about two cal deg^{-1} mol^{-1} lower than the value interpolated from Sinke and De Vries at the same temperature. There have been no studies of the effect of pressure on the heat capacity.

Corrections to the Ideal Gas State

The corrections calculated from the equation of state of J. D. Cox [1961] are shown in table 87. These can be considered only as highly approximate, especially the heat capacity correction, because terms higher than the second virial coefficient have been neglected. It is difficult to obtain an accurate temperature derivative of the second virial coefficient from *P-V-T* data alone. Cox

TABLE 83. 2-Methyl-1-propanol. Reported values. Simple physical properties

Investigators		Vapor Pressures and Boiling Points		Freezing Point	Density, *d* g cm^{-3}		Refractive Index, n_D	
		°C	mmHg	t_m, °C	20 °C	25 °C	20 °C	25 °C
2-Methyl-1-propanol, $C_4H_{10}O$, mol wt. 74.124, state at 25 °C liq								
Naccari and Pagliani	[1881]	108.1	760		0.8010			
Perkin	[1884]	107.6–107.3	760		.8024			
Kahlbaum	[1884]	106.4	760					
Jahn	[1891]				.8021			
Schall and Kossakowsky	[1891]				.9016			
Landolt and Jahn	[1892]	107.25	760		.8027		1.3959	
Louguinine	[1898]	107.53	760					
Zubov	[1898]	107.63–107.71	760					
Young and Fortey	[1902]	108.06	760		.8018			
Doroshevskii and Dvorzhanchik	[1908]	107.9	760				1.39583	
Doroshevskii	[1911a]	107.3–107.7	760					
Bridgman	[1913]	107.0–107.2	760					
Schwers	[1915]				.80377			1.39332
Peacock	[1915]					0.7994		1.3944
Willcox and Brunel	[1916]	107.85–107.95	760					
Wroth and Reid	[1916]					.79949		
Brunel, Crenshaw, and Tobin	[1921]	107.89	760			.7963		1.3939
Reilly and Hickinbotton	[1921]	107.9	760		.8020			
Willard and Smith	[1923]					.79807		
Williams and Daniels	[1924]	107.7–107.8	760					
Norris and Ashdown	[1925]	107.65–107.75	760			.79798		
Palmer and Constable	[1925]	107.7–107.8	760					
Mathews	[1926]	107.6–107.7	760		.8027			1.39436
Munch	[1926]	105.9	760			.8016		1.3936
Timmermans and Martin	[1928]	108.10	760			.79817	1.39573	
Longinov and Pryanishnikov	[1931]						1.3959	
Bylewski	[1932]	107.894			.80196			
Trew and Watkins	[1933]	107.8	760			.79806		1.39387
Vosburgh, Connell, and Butler	[1933]					.79837		
Rutler, Ramchandani, and Thomson	[1935]	107.85	760			.79833	1.39603	
Greenwood, Whitmore, and Crooks	[1938]						1.3950	
Allen, Lingo, and Felsing	[1939]	108.3	760			.7982		1.3936
Alberty and Washburn	[1945]					.79811	1.39615	
Pollack, Collett, and Lazzell	[1946]	107.0	760				1.3960	
Shostakovskii and Prilezhaeva	[1947]	108.6–108.7	760			0.8020	1.3980	
Vogel	[1948]	107.8	760		.8021		1.39549	
Mumford and Phillips	[1950]	108.0	760		.8030	0.7994	1.3953	
Pichler, Ziesecke, and Traeger	[1950]	107.9	760		.8027		1.3959	
Ballard and Van Winkle	[1952]	108.1	760				1.39614	
Cook	[1952]	108.1	760		0.8024		1.3958	
Dunning and Washburn	[1952]					0.7982		1.3939
Anisimov	[1953b]							1.39387
McKenna, Tartar, and Lingafelter	[1953]	180.0						1.3938
Dannhauser and Cole	[1955]					.7972		1.3939
Kuss	[1955]				.8023			
Rush, Ames, Hoost, and Mackay	[1956]					.7980		1.3939
Toropov	[1953b]				.8016			
Costello and Bowden	[1958]	108.0	760		.8021			
Brown and Smith	[1962b]	107.75	760			.79779		1.39384
Ambrose and Townsend	[1963]				.8020			
Biddiscombe, Collerson, Handley, Herington, Martin, and Sprake	[1963]	107.888	760					
Selected value	[1967]	107.87±0.05	760		.8016	.7978	1.3958	1.3938
		24.4±0.2	10		±0.0002	±0.0002	±0.0002	±0.0002

Antoine constants: *A* 7.32705, *B* 1248.48, *C* 172.92

dt/*dp* at 760 mmHg, 0.03609 °C/mmHg

found that the second virial coefficient of 2-methyl-1-butanol follows the same function of temperature as that of 1-butanol, within the range of his experimental measurements. It has been shown that for the other alcohols, the heat capacity correction calculated from Cox's equation was much smaller than the calculated from other equations based on the monomer-dimer-tetramer equilibria. Since Cox found that the second virial coefficients of 2-methyl-1-propanol were the same as that of 1-butanol at the same temperature, it seems likely that the complete equation of state is similar for the two compounds. For comparison, corrections to the ideal gas state for 2-methyl-1-propanol are shown on table 87 which have been calculated from the equation of state of 1-butanol determined by Counsell, Hales, and Martin (1965). Except for the heat capacity correction, the two sets of values are similar.

TABLE 84. 2-Methyl-1-propanol. Reported values. Critical properties

Investigator	t_c, °C	P_c, atm	d_c, g cm^{-3}
Nadezhdin [1883] and [1882]	265.00	48.0	
Brown, J. C. [1906]	277.63		
Kreglewski [1954]	276.7		
Kay and Donham [1955]	274.59	42.4	0.269
Ambrose and Townsend [1963]	274.56	42.39	0.2722

Vapor-Liquid Equilibrium at 25 °C

Vapor Pressure

The value shown on the summary sheet was calculated from the selected Antoine constants.

Heat of Vaporization

The value of Wadso [1966], obtained by calorimetry, was selected. This was also close to the values obtained by extrapolating the data of Mathews [1926]. The heat of vaporization calculated from the Antoine constants, as shown on table 85, is high. However, this is at the lower end of the range of applicability of these constants, and an accurate heat of vaporization obtained in this way should not be expected.

Temperature Derivative of the Heat of Vaporization

The equation of state of J. D. Cox [1961] predicts that $d\Delta H/dT - \Delta C_p$ is -0.5 cal deg^{-1} mol^{-1} at 25 °C. However, this cannot be considered as reliable for the reasons discussed in the section on Corrections to the Ideal Gas State. Assuming that 2-methyl-1-propanol follows the same equation of state as Counsell, Hales, and Martin [1965] found for 1-butanol, a value of -0.6 cal deg^{-1} mol^{-1} is obtained for $d\Delta H/dT - \Delta C_p$. A value of -0.5 cal deg^{-1} mol^{-1} with an uncertainty of ± 0.3 was selected. The value of $d\Delta H/dT$ shown on the summary sheet was then calculated with the use of the heat capacities of the liquid and vapor.

TABLE 85. 2-Methyl-1-propanol. Reported values. Heats of vaporization

Investigator	ΔH_v at 25 °C	ΔH_v at t_b	Method and Remarks
Louguinine [1898]		9.96	Calorimetric.
Brown, J. C. [1903]		10.31	Calorimetric.
Mathews [1926]		10.17	Calorimetric.
Mathews [1926], extrapolated to 25 °C by McCurdy and Laidler [1963]	12.02		
Mathews [1926], extrapolated to 25 °C by Skinner and Snelson [1960]	12.12		
Bartoszewiczowna [1931]	10.9		Calorimetric.
Bennewitz and Rossner [1938]		10.37	Calorimetric, corrected to t_b.
Biddiscombe, Collerson, Handley, Herington, Martin and Sprake [1963]		10.05	Calculated from Antoine constants.
McCurdy and Laidler [1963]	11.91		Calorimetric.
Wadso [1966]	12.15		Calorimetric.
Selected Antoine constants	13.15	10.00	Calculated.

Vapor-Liquid Equilibrium at the Normal Boiling Point

Normal Boiling Point

The boiling point at one atmosphere was calculated from the Antoine constants.

TABLE 86. 2-Methyl-1-propanol. Reported values. Heat of combustion of the liquid at 25 °C

Investigator	$-\Delta H_c^0(1)$ kcal mol^{-1}
Louguinine [1880]	636.5
Thomsen [1886]	*646.3
Zubov [1898] (recalculated by Swietoslawski [1920]	636.4
Richards and Davis [1920]	637.8
Skinner and Snelson [1960]	637.79
Chao and Rossini [1965]	638.06

* ΔH_c of gas reported. Value corrected to the liquid.

Heats of Vaporization

The values calculated from vapor pressure by Biddiscombe, Collerson, Handley, Herington, Martin, and Sprake [1963], and from the selected Antoine constants listed in table 81, agree fairly well with the calorimetric measurement of Mathews [1926]. An average value was selected.

TABLE 87. 2-Methyl-1-propanol. Differences in properties between real gas and ideal gas

Sources	at 25 °C and 10.4 mmHg			at 107.87 °C and 760 mmHg		
	H^r-H^0	$C_p{}^r-C_p{}^0$	S^r-S^0	H^r-H^0	$C_p{}^r-C_p{}^0$	S^r-S^0
Calculated from equation of state of Cox, J. D. [1961]	−0.007	0.10	−0.019	−0.17	1.96	−0.357
Calculated from equation of state for 1-butanol of Counsell, Hales, and Martin [1965]	−0.008	0.20	−0.023	−0.19	4.43	−0.41

Heat Capacity of the Liquid

This was calculated from the equation of Williams [1924] based on measurements up to 80 °C. The 27-degree extrapolation gives rise to a fairly large uncertainty.

Temperature Derivative of the Heat of Vaporization

In a manner similar to that carried out at 25 °C, the value of $d\Delta H/dT-\Delta C_p$ is −6.1 cal deg^{-1} mol^{-1}, according to the equation of state of J. D. Cox [1961], and −9.4 cal deg^{-1} mol^{-1} assuming that the equation of state is the same as that of 1-butanol found by Counsell, Hales, and Martin [1965]. Since the predictions of Cox's equations are generally too small, a value of −7 cal deg^{-1} mol^{-1} was estimated for this quantity. This, in combination with the heat capacities of the liquid and vapor, gives the result shown in table 81.

Properties of the Ideal Gas State

Molecular Parameters

References to a few spectroscopic studies are listed in the Index to the Bibliography. However, no complete assignment of molecular vibration frequencies was located.

Heat Capacity

The heat capacity data of Sinke and De Vries [1953] from 121 to 164 °C were converted to the ideal gas state by use of the equation of state for 1-butanol of Counsell, Hales, and Martin [1965]. The correction at 110 °C was considered too uncertain to be usable. At 132 °C and above, $C_p{}^r-C_p{}^0$ calculated from Cox's equation was within 0.2 cal deg^{-1} mol^{-1} of that calculated from the equation for 1-butanol. These data can be represented quite closely by,

$$C_p{}^0(\mathrm{g})=6.746+0.06644T \text{ cal deg}^{-1}\text{ mol}^{-1}.$$

On an absolute basis, the overall uncertainty in the heat capacity calculated from this equation is about 0.5 to 1 cal deg^{-1} mol^{-1}.

Thermodynamic Functions

Tables of complete thermodynamic functions have not been prepared.

Chemical Equilibria

No studies of chemical equilibria have been made.

Entropy at 25 °C

No data or calculations for absolute entropy were found.

Tests of Internal Consistency

Because of the rather large uncertainties in some of the properties, especially the heat capacities of the liquid and gas phases, checks for internal consistency of the liquid-vapor equilibrium data are not very helpful. However, the following table shows that these data are consistent within the experimental uncertainties.

	ΔH kcal mol^{-1}	ΔS cal deg^{-1} mol^{-1}
liquid (25 °C) real gas (25 °C), 10.4 mmHg)	12.14±0.03	40.72±0.1
real gas (25 °C) ideal gas (25 °C)	0.007±0.002	0.02±0.01
ideal gas (25 °C) ideal gas (107.87 °C)	2.43±0.1	7.16±0.5
ideal gas (10.4 mmHg) ideal gas (760 mmHg)	0.0	−8.53±0.01
ideal gas (107.97 °C, 760 mmHg) real gas (107.87 °C, 760 mmHg)	−0.18±0.01	−0.39±0.03
real gas (107.87 °C) liquid (107.87 °C)	−10.05±0.1	−26.38±0.3
liquid (107.87 °C) liquid (25 °C)	−4.43±0.2	−12.98±0.5
Sum	−0.08±0.3	−0.38±0.8

Miscellaneous

Nemeth and Reed [1964] obtained a collision diameter of 7.73 Å from the measured viscosity of the gas at 25 °C.

Recommendations for Future Work

Although there have been many measurements of the simple physical properties of 2-methyl-1-propanol, such as refractive index, density, vapor pressure and boiling point, data on many of the basic thermodynamic properties are scarce or lacking altogether. Low temperature heat capacity data, which can be used to calculate the entropy by means of the third law, would be very helpful if this compound can be crystallized. Measurements of vapor heat capacity over a range of pressures which can be used to help establish the equation of state, such as has been done for the other alcohols, are needed. The heat of combustion and heats of vaporization have been satisfactorily measured, but there have been no statistical calculations of the ideal gas thermodynamic functions.

Index to the Bibliography

Numbers refer to the Bibliography, page 1–389.

References to data used in the selection of refractive index, density, boiling point, vapor pressure, and melting point are in boldface type.

Numbers in parentheses refer to sources of reviews, or theoretical calculations only.

Reference numbers under each property are listed in the order of date of publication.

Refractive Index
607, **840**, **990**, 168, **439**, **1589**, 381, **1345**, **1590**, **509**, **239**, 354, **1961**, **1140**, **1227**, **1784**, 1687, **1080**, **793**, **1803**, **1634**, **253**, 1112, 367, **632**, 1910, **21**, **1843**, 843, 1649, **20**, **783**, 1404, **1615**, **1819**, **1856**, 1893, 11, 370, **1224**, 1377, 180, **76**, 338, **462**, 35, **36**, 675, **1152**, **381**, 1292, **1521**, **1594**, **231**, 1279

Density at 20–30 °C Only
1071, 1384, **1236**, **1559**, **1560**, **1349**, **576**, **1556**, **990**, **2002**, **439**, **436**, **1589**, **1590**, **838**, 1471, 1173, 1409, 42, **1784**, 793, **1634**, 176, **20**, **1856**, **35**, **978**, **1797**, **347**, **380**

Normal Boiling Point
1071, 1384, 1228, 917, 1236, 1349, 1559, 866, 1083, 1560, 868, 1562, 1556, 990, 119, 2033, 2002, 1526, 272, 928, 168, 1395, 439, 538, 435, 1336, 1768, 211, 1284, 1479, **1960**, 1020, 838, 509, 355, 1471, **239**, 1173, 1409, 1961, **1272**, 1308, 1140, 1227, 1772, 42, **1784**, 1007, 436, 332, 143, 1080, 1696, 12, 870, 793, **257**, 242, 1794, 1803, 1634, 928, 1891, 253, 1910, 632, 367, 125, 902, 843, 174, 176, 929, 1554, 1404, 1006, 783, 1615, 1856, 1007, 1224, 370, 1377, 804, 725, 1745, 180, 1902, 76, 675, 1152, **338**, 1823, 1292, 1594, 505, 1148, **231**, 1193, **145**

Vapor Pressures and Boiling Points at Other Pressures
1236, 935, 866, 1483, **1571**, **253**, **21**, 1947, **1819**, 1824, 878, **1823**, **347**, **145**, **23**

Critical Temperature
747, 878, 347, 23, 218, 1237, 1238

Critical Pressure
747, 878, 23, 1238

Critical Volume and Density
878, 23

Normal Melting Point
272, 338, 675, 1823

Heat Capacity of the Liquid
1083, 1961, 1823

Heat Capacity of the Real Gas
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P-V-T Data and Equation of State of the Real Gas
356, 23

Calorimetric Heat of Vaporization at 25 °C
97, 1147, (1629), 1870

Calorimetric Heats of Vaporization at Other Temperatures
1083, 1140, 1823, 219, 125

Heat of Combustion
1084, 1762, 2033, (1721), 1480, 1629, 287, 288

Molecular Vibration Frequencies and Spectra
1190, 529, 541, 1196, 379, 1844, 668, 669

Association in the Gas Phase
356, (1258)

Association in the Liquid Phase
1104, 78, (1754), 1705, 529, 489, 1758, 1757

2-Methyl-2-Propanol

Properties of the Liquid at Various Temperatures

Refractive Index

The refractive index data at 20 and 25 °C listed in table 91 refer to the undercooled liquid. There are no data for the crystal form or for the liquid outside the temperature range of 20 to 30 °C. The data at wavelengths other than the sodium D-line in table 90 were based on the results of Bruhl [1880b], Eykman [1919], Swarts [1919], Timmermans and Delcourt [1934], and Marsden and Evans [1937]. Values below 4000 Å were calculated from a quadratic equation in $1/(\lambda-1000)^{1.6}$ fitted to the data of Marsden and Evans (1937).

Density

There are only a few accurate measurements. Those used to establish the Francis constants listed in table 88 are identified in the Index to the Bibliography. The only data above 100° are those of Costello and Bowden [1958] and Dannhauser and Bahe [1964].

Vapor Pressure and Boiling Point

The vapor pressure data used to calculate the Antoine constants in table 88 were taken from the measurements of Parks and Barton [1928], from 20 to 90 °C; Butler, Ramchandani and Thomson [1935], from 30 to 80 °C; Allen, Lingo, and Felsing (1939), at 25 and 82.3 °C; Dreisbach and Shrader [1949], from 43 to 82 C; Beynon and McKetta [1963], from 57 to 90 °C; and Biddiscombe, Collerson, Handley, Herington, Martin, and Sprake [1963], from 61 to 90 °C. The vapor pressure values of Parks and Barton range from 0 to 18 mm below the calculated ones, while that of Biddiscombe *et al.*, and Beynon and McKetta range from 0 to 5 mmHg high. Most of the other values scatter about within 5 mmHg of the calculated vapor pressure. A selection of values of boiling point measurements is given in table 91. Krone and Johnson [1956] have measured the vapor pressure from 93 °C to the critical temperature, and Ambrose and Townsend [1963] have also measured the vapor pressure from 103 °C to the critical temperature.

The vapor pressure of the solid from 15 °C to the triple point shown on the summary sheet was calculated from the appropriate thermodynamic formulas using the heat capacity of the solid given by Oetting [1963], the heat capacity of the undercooled liquid obtained by extrapolating to data from above the triple point, and the vapor pressure of the undercooled liquid as given by the Antoine constants.

Critical Properties

Critical Temperature

Both Krone and Johnson [1956] and Ambrose and Townsend [1963] used samples which were carefully purified and used carefully calibrated thermometers. The reason for the large difference is not obvious. The value obtained by Ambrose and Townsend was selected since they seemed to have made accurate measurements on the other alcohols, and it is more likely that the selected value for 2-methyl-2-propanol is consistent with their values of other alcohols.

Critical Pressure and Density

As a result of the fact that the critical temperature obtained by Krone and Johnson [1956] is higher than that obtained by Ambrose and Townsend [1963], their critical pressure is also higher and their critical density is lower. The selected values were taken from the work of Ambrose and Townsend in order to obtain better internal consistency.

Solid-Solid Phase Equilibria

Transition Temperatures and Heats of Transition

Atkins [1911], Getman [1940], and Simonsen and Washburn [1946] have reported some evidence that 2-methyl-2-propanol exists in two or more crystalline forms, although they did not obtain much specific information about their properties. In a recent calorimetric study Oetting [1963] has definitely identified two enantiotropic forms with the transition temperature and heat of transition shown in table 80. He states that x-ray diffraction patterns have been obtained on powdered samples of crystals I and II, but these data have not yet been interpreted in terms of lattice structures. He has also obtained some evidence for the existence of a third metastable crystalline form. This metastable form changes to crystal II at 8.39 °C, with a heat of transition of 0.198 cal mol^{-1}, and to crystal I at 21.32 °C, with a heat of transition of 0.117 cal mol^{-1}.

Heat Capacity of the Solid Phases

These were taken from the data of Oetting [1963].

Solid-Liquid Phase Equilibria

Normal Melting Point

There have been many determinations of the melting point. A survey of the better values is given in table 91. 2-Methyl-2-propanol has been proposed several times as a convenient solvent for cryoscopic measurements of molecular weight. See Atkins [1911] and Getman [1940], for example. De Vries and Soffer [1951] made a careful

TABLE 88. 2-Methyl-2-Propanol. Selected values. Physical and thermodynamic properties

Temp. °C	Refractive Index, n_D	Density g cm^{-3}	Vapor Pressure, mmHg
15			19.3(c,I)
20	1.3877	*0.7866	28.6(c,I); *30.1(l)
25	1.3852	* .7812	41.7(c,I); *42.0(l)
25.82			44.3(c,I); 44.3(l)
30	1.3823	.7757	57.6
35			77.8
39.36			100
40		.7649	103.7
45			136.4
50		.7540	177.3
52.38			200
55			227.8
60		.7431	289.8
65			364.9
67.06			400
70		.7322	455.2
75			562.9
80		.7214	690.5
82.42			760
85			840.3
90		.7105	1015.2
95			1218.0
100		.6996	1451.8

Data For Phase Transitions

Initial	Final	Temp. °C	dt/dP deg mm^{-1}	Pressure mmHg	ΔH kcal mol^{-1}	$d\Delta H/dt$	ΔS	ΔC_p
						cal deg^{-1} mol^{-1}		
c,I	c,II	12.99±0.05			0.20±0.01	−14.82±0.06	0.70±0.08	−15.52±0.05
c,I	g	25		41.67±0.1	12.73±0.03	−8. ±1.6	42.73±0.1	−5.1±0.5
*liq	g	25	0.368	41.98±0.1	11.14±0.03	−26. ±1.5	37.40±0.1	−22.8±0.5
c,I	liq	25.66±0.03		760	1.60±0.01	23.01±0.06	5.35±0.03	17.66±0.05
c,I	liq	25.82±0.02		44.26±0.1				17.66±0.05
liq	g	25.82±0.02	.352	44.26±0.1	11.12±0.03	−26. ±1.5	37.26±0.1	−22.8±0.5
liq	g	82.42±0.1	.03348	760	9.33±0.05	−36. ±1.5	26.21±0.15	−21.2±0.9

Condensed Phase Heat Capacity

State	Temp. °C	C_p
		cal deg^{-1} mol^{-1}
c,I	25.82	35.04±0.05
liq	25.82	52.66±0.05
liq	82.42	63.6±0.5

Properties of the Saturated Real Gas

Temp. °C	$H^r - H^0$	$S^r - S^0$	$C_p{}^r - C_p{}^0$
	kcal mol^{-1}	cal deg^{-1} mol^{-1}	
25	−0.05±0.01	−0.27±0.04	2.7±0.5
82.42	−0.29±0.02	−0.71±0.03	11.2±0.7

Data for the Standard States at 25 °C

State	Heat of Combustion $\Delta H_c{}^0$ kcal mol^{-1}	Heat of Formation $\Delta H_f{}^0$ kcal mol^{-1}	Entropy S^0 cal deg^{-1} mol^{-1}	Gibbs Energy of Formation $\Delta G_f{}^0$ kcal mol^{-1}	Heat Capacity, C_p cal deg^{-1} mol^{-1}
c,I	−630.32±0.2	−87.45±0.2	40.77±0.05	−44.14±0.2	34.92±0.1
*liq	−631.92±0.2	−85.86±0.2	46.10±0.05	−44.14±0.2	52.61±0.1
g	−643.11±0.2	−74.67±0.2	77.98±0.05	−42.46±0.2	27.10±0.1

Critical Constants

Temp. 233.0 °C, 506.2 K	Pressure 39.20 atm	Density 0.270 g cm^{-3}

Constants in Vapor Pressure and Density Equation								
Antoine Equation				Francis Equation				
Temp. Range	*A*	*B*	*C*	Temp. Range	*A*	$B\times10^3$	*C*	*E*
20 to 103 °C	7.31994	1154.48	177.65	20 to 100 °C	0.87919	1.0881	−4226.2	−59630

* Undercooled liquid.

Table 89. 2-Methyl-2-propanol. Selected values. Thermodynamic functions of the ideal gas at one atmosphere

Temperature K	Entropy S^0 cal deg^{-1} mol^{-1}	Heat Capacity C_p^0 cal deg^{-1} mol^{-1}	Enthalpy Function $(H^0-H_0^0)/T$ cal deg^{-1} mol^{-1}	Gibbs Energy Function $(G^0-H_0^0)/T$ cal deg^{-1} mol^{-1}	Heat of Formation ΔH_f^0 kcal mol^{-1}	Gibbs Energy of Formation ΔG_f^0 kcal mol^{-1}
0	0	0	0	0	−67.43	−67.43
273.15						
298.15	77.98	27.10	16.51	−61.47	−74.67	−42.46
300	78.15	27.23	16.58	−61.57	−74.70	−42.25
400	86.94	34.16	20.11	−66.82	−76.45	−31.16
500	95.24	40.27	23.56	−71.69	−77.85	−19.67
600	103.05	45.37	26.78	−76.27	−78.94	−7.90
700	110.38	49.64	29.74	−80.63	−79.79	+3.98
800	117.25	53.28	32.46	−84.79	−80.41	15.98
900	123.71	56.42	34.85	−88.76	−80.92	28.05
1000	129.79	59.16	37.23	−92.56	−81.08	40.18

study of the melting point for possible use as a thermometric standard. However, difficulties have prevented this alcohol from being widely adopted for these purposes. The melting point is greatly influenced by small quantities of water which are readily absorbed from the atmosphere. The existence of more than one crystalline form sometimes causes difficulty in attaining a stable melting point. Finally, solutions of many organic compounds in 2-methyl-2-propanol deviate strongly from ideal behavior, which is undesirable for cryoscopic determination of molecular weights.

TABLE 90. 2-Methyl-2-propanol. Selected values. Refractive index at various wavelengths at 25 °C

Symbol	Wavelength, Å	Refractive Index, n
He_{red}	6678.2	1.3829
H_c	6562.8	1.3832
Na_D	5892.6	1.3852
Hg_e	5460.7	1.3832
He_{blue}	5015.7	1.3891
H_F	4861.3	1.3901
Hg_g	4358.3	1.3939
$H_{G'}$	4340.5	1.3941
	4000	1.3975
	3500	1.4048
	3000	1.4170
	2700	1.4293

De Vries and Soffer [1951] determined the melting point of carefully dried samples with considerable accuracy. The alcohol was kept in a freezing point cell which was isolated from atmospheric moisture. They did not state that the cell was evacuated, so their value presumably corresponds to the normal melting point in equilibrium with air. They obtained the same value as Simonsen and Washburn [1946], and this was selected as the best value. Simonsen and Washburn also reported 25.0 °C as a melting point of a second crystalline form which apparently corresponds to crystal II of Oetting.

Triple Point

Oetting [1963] determined the melting point in a calorimeter which presumably contained only helium exchange gas, and thus it should represent the triple point. This value is appreciably higher than any of the melting points found in the presence of air which are listed in table 93.

Heat Capacity of Solid and Liquid at the Melting Point

Heat capacities have been reported by de Forcrand [1903] and Parks and Anderson [1928], but the much more accurate measurements of Oetting [1963] were selected.

Heat of Fusion

Five values for the heat of fusion are listed in table 93. Two of these were calculated from observed values of the cryoscopic constant. Oetting [1963] measured the heat of fusion by direct calorimetry, and this value was selected.

Heat of Vaporization at the Triple Point

The heat of vaporization adopted for 25 °C was corrected to 25.82 °C by use of the selected value of $d\Delta H/dT$ shown in table 88. The vapor pressure was calculated from the Antoine constants which represent the vapor pressure of the liquid phase.

Properties of the Undercooled Liquid at 25 °C

Heat Capacity

Three values of heat capacity are shown in table 95. de Forcrand [1903] obtained an average value in the range 25.5 to 44.8 °C. The other two reported values result from a short extrapolation from higher temperatures. The value based on Oetting's [1963] data was the most reliable, and it was selected.

Absolute Entropy

Two values are shown in table 95. The one reported by Parks, Kelley, and Huffman [1929] was calculated from the heat capacity data obtained by Parks and Anderson [1926] down to 90 K. The more recent value reported by Oetting [1963] is based on measurements down to 15 K, and it is much more accurate. It agrees within 0.05 cal deg^{-1} mol^{-1} with the statistical calculation of Beynon and McKetta [1963] for the ideal gas, taking into account the other auxiliary data.

Heat of Combustion

The four older values shown in table 96 scatter over a range of about 3 kcal mol^{-1}. The recent value obtained by Skinner and Snelson [1960] was selected.

Properties at the Solid at 25 °C

Heat Capacity

The stable form of 2-methyl-2-propanol at 25 °C is the crystal I described by Oetting [1963], and his value of the heat capacity was adopted. Heat capacity of the solid phase has also been reported by de Forcrand [1903] and by Parks and Anderson [1926].

TABLE 91. 2-Methyl-2-propanol. Reported values. Simple physical properties

Investigators		Vapor Pressures and Boiling Points		Freezing Point	Density, *d* g cm^{-3}		Refractive Index, n_D	
		°C	mmHg	t_m, °C	20 °C	25 °C	20 °C	25 °C
2-Methyl-2-propanol, $C_4H_{10}O$, mol wt. 74.124, state at 25 °C Crystal								
Bruhl	[1880b]	82.5–83.0	760	29	0.7864		1.38779	
Perkin	[1884]	81.5–82.0	760			0.78126		
Thorpe and Rodger	[1894]	82.25	760					
Zubov	[1898]			24.88				
Young and Fortey	[1902]	82.55	760	25.53	.78553	.78056		
de Forcrand	[1903]	82.8	760	25.45				
Boedtker	[1904]			25				1.38705
Carrara and Ferrari	[1906]	82.94	760			.7822		
Atkins	[1911]	82.35–82.55	760					
Doroshevskii	[1911b]	82.57	760	25		.78062		1.38548
Willcox and Brunel	[1916]	81.7–82.1	760					
Norris and Ashdown	[1925]	82.2–82.3	760	24.3		.7804		
Munch	[1926]	82.0	760			.7859		1.3840
Adkins and Broderick	[1928a]	82.5–82.7	760	25				1.38458
Parks and Barton	[1928]	82.86	760	25.50				
Swarts	[1929]	82.55	760			.7819		
Bhatnagar, Mathur, and Mal	[1930]	82.22	760					
Smyth and Dornte	[1931]	82.6–82.8	760				1.38777	
Cady and Jones	[1933]			25.7				
Ebers and Lucas	[1934]			25.10				
Timmermans and Delcourt	[1934]	82.50	760	25.55	.78670			1.3852
Butler, Ramchandani, and Thomson	[1935]	82.75	760	25.5				
Deffet	[1935]			25.55				
Spells	[1936]					.78462		
Allen, Lingo, and Felsing	[1939]	82.6	760	25.4		.7804		1.3845
Getman	[1939]	81–82	760	25.1				
Owen, Quayle, and Beavers	[1939]					.7785		
Maryott	[1941]			24.85–25.0				
Whitmore, Laughlin, Matuszeski, and Surmatis	[1941]			25.0–25.5				
Lecat	[1946]	82.45	760					
Simonsen and Washburn	[1946]			25.66		.78043		1.38483
Dreisbach and Martin	[1949]	82.41	760	25.00	.78581	.78086	1.38468	1.38231
Pichler, Ziesecke and Traeger	[1950]	82.6	760		.7840		1.3878	
DeVries and Soffer	[1951]			25.663				
Shreve, Heether, Knight, and Swern	[1951]						1.3878	
Dunning and Washburn	[1952]					.7806		1.3851
McKenna, Tartar, and Lingafelter	[1953]	82.6	760					1.3850
Westwater and Audrieth	[1954]	82.8	760		0.7873		1.38695	
Boud, Cleverdon, Collins, and Smith	[1955]	82.4	760	25.54		0.7811		1.3851
Westwater	[1955]	82.8	760		.7873		1.38695	
Kuss	[1955]					.7816		
Rathmann, Curtis, McGreer, and Smyth	[1956]	82.3–82.4	760	25.4				1.38516
Rush, Ames, Hoost, and MacKay	[1956]					.7806		1.3849
Costello and Bowden	[1958]	82.0	760	25.5				
Mikus and Lauder	[1958]	82.8	760				1.3877	
Barnard	[1959]	81.46	760	25.50				
Brown and Smith	[1962b]	82.32	760			.78058		1.38477
Ambrose and Townsend	[1963]					.7803		
Beynon and McKetta	[1963]	82.34	760					
Biddiscombe, Collerson, Handley, Herington, Martin, and Sprake	[1963]	82.347	760					
Selected value	[1967]	82.42±0.1	760	25.66 ±0.03	* .7866 ±0.0004	* .7812 ±0.0003	* 1.3877 ±0.0004	* 1.3852 ±0.0004

Antoine constants: *A* 7.31994, *B* 1154.48, *C* 177.65 *dt*/*dp* at 760 mmHg, 0.03348 °C/mmHg

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* Undercooled liquid.

Absolute Entropy

The value calculated from the low temperature heat capacity measurements of Oetting [1963] was selected. It is consistent with the other thermodynamic properties shown in table 88.

TABLE 92. 2-Methyl-2-propanol. Reported values. Critical properties

Investigator	t_c, °C	P_c, atm	d_c, g cm^{-3}
Pawlewski [1883]	234.9		
Stull [1947]	235.0	49.0	
Krone and Johnson [1956]	235.72	41.8	0.26
Ambrose and Townsend [1963]	233.0	39.20	0.2700

TABLE 93. 2-Methyl-2-propanol. Reported values. Condensed phase transitions

	Transition c, II c, I		Fusion		
Investigator	t_t, °C	ΔH_t	t_{tp}, °C	t_m, °C	ΔH_m
Young and Fortey [1902]				25.53	
de Forcrand [1903]				25.45	1.55
Atkins [1911]				**25.5	*1.39
Parks and Anderson [1926]				25.4	1.622
Parks and Barton [1928]				25.50	
Cady and Jones [1933]				25.7	
Timmermans and Delcourt [1934]				25.55	
Deffet [1935]				25.55	
Getman [1940]				25.1	*1.58
Simonsen and Washburn [1946]				25.66	
Dreisbach and Martin [1949]				25.00	
De Vries and Soffer [1951]				25.66	
Barnard [1959]				25.50	
Oetting [1963]	12.99	0.198	25.82		1.602

* Calculated from observed cryoscopic constant.
** Taken from previously published data.

Heat of Formation

This was calculated from the heat of formation of the undercooled liquid, based on the heat of combustion and the heat of fusion at 25 °C.

TABLE 94. 2-Methyl-2-propanol. Reported values. Heats of vaporization

Investigator	ΔH_v at 25 °C	ΔH_v at t_b	Method and Remarks
Brown, J. C. [1903]		9.74	Calorimetric.
de Forcrand [1903]		9.43	Calorimetric.
Parks and Barton [1928]	10.89	9.48	Calculated from vapor pressure.
Bartoszewiczowna [1931]	10.78		Calorimetric.
Biddiscombe, Collerson, Handley, Herington, Martin and Sprake [1963]		9.40	Calculated from vapor pressure.
McCurdy and Laidler [1963]	10.72		Calorimetric.
Beynon and McKetta [1963]	11.12	9.335	Calorimetric, extrapolated to 25°C by equation.
Wadso [1966]	11.14		Calorimetric.
Selected Antoine constants	11.33	9.32	Calculated.

TABLE 95. 2-Methyl-2-propanol. Reported values. Heat capacity and entropy of the undercooled liquid at 25 °C

Investigator	C_p^0(1)	Remarks	S^0(1), Third Law
de Forcrand [1903]	53.5		
Parks and Anderson [1926]	53.7		
Parks, Kelley and Huffman [1929]			45.3 (Parks and Anderson revised).
Oetting [1963]	52.61		46.15

TABLE 96. 2-Methyl-2-propanol. Reported values. Heat of combustion of the liquid at 25 °C

Investigator	$-\Delta H_c^0$(1), kcal mol^{-1}
Louguinine [1882a]	632.5
Thomsen [1886]	*630.2
Zubov [1898] (recalculated by Swietoslawski [1920])	629.8
Raley, Rust, and Vaughan [1948]	629.4
Skinner and Snelson [1960]	631.92

* ΔH_c of gas measured. Value corrected to the liquid.

Properties of the Real Gas

Equation of State

Krone and Johnson [1956] measured pressure, volume, and temperature of the real gas in the range 93 to 260 °C

TABLE 97. 2-Methyl-2-propanol. Differences in properties between real gas and ideal gas

Sources	at 25 °C and 42.0 mmHg			at 82.42 °C and 760 mmHg		
	H^r-H^0	$C_p{}^r-C_p{}^0$	S^r-S^0	H^r-H^0	$C_p{}^r-C_p{}^0$	S^r-S^0
Calculated from equation of state of Cox, J. D. [1961]	−0.024	0.38	−0.065	−0.183	2.46	−0.426
Calculated from equation of state of Beynon and McKetta [1963]	−0.053	2.73	−0.159	−0.287	11.27	−0.712
Calculated from equation of state of Krone and Johnson [1956]	−0.004	0.007	0.003	−0.055	0.13	0.016

and 1 to 27 atm. They did not report their measurements directly, but they did give the constants in the Beattie-Bridgman equation which fit the data. From these constants, their measured vapor pressure, and heat capacities available in the literature supplemented with some empirical estimates, they calculated and tabulated volume, enthalpy, and entropy of the liquid and gas, and the compressibility and fugacity of the gas in this range. This equation of state does not seem to be very accurate for pressures below one atmosphere. Ambrose and Townsend [1963] measured the orthobaric volumes of liquid and vapor from 146 °C to the critical temperature.

J. D. Cox [1961] expressed the second virial coefficient, derived from P-V-T measurements from 105 to 150°, in the form

$$\log\,(-B_p{}')=15.359-4.8\log T.$$

Beynon and McKetta [1963] fit their vapor heat capacity data to an equation of state containing second and fourth virial coefficients which was based on the usual model of monomers, dimers, and tetramers. When converted to the mathematical form corresponding to that used for the other alcohols, the second and fourth virial coefficients may be represented as

$$B_p{}'=63-5.777\times10^{-3}T\exp\left(\frac{2311}{T}\right)\text{ml mol}^{-1}$$

$$D_p{}'=-2.670\times10^{-16}T\exp\left(\frac{12634}{T}\right)\text{ml atm}^{-2}\text{ mol}^{-1}.$$

The constant term in the equation for $B_p{}'$ was estimated by comparison with the second virial coefficient of Cox. For the formation of dimers and tetramers from the monomers, this gives $\Delta H_2=-4.59$ kcal mol^{-1}, $\Delta S_2=-19.0$ cal deg^{-1} mol^{-1}, $\Delta H_4=-25.1$ kcal mol^{-1}, and $\Delta S_4=-82.2$ cal deg^{-1} mol^{-1}.

Heat Capacity

The vapor heat capacity has been measured at 138 and 160 °C at one atmosphere by Reynolds and De Vries [1950] and at several temperatures from 86 to 164 °C at 750mm by Sinke and De Vries [1953]. Beynon and McKetta [1963] measured the heat capacity of the gas with their flow calorimeter at pressures and temperatures in the range of 92 to 164 °C and ⅓ to ⅔ atm. They expressed the pressure dependence of the heat capacity in terms of the second and fourth virial coefficients given in the preceding section. All three sets of data show good agreement with this equation.

Corrections to the Ideal Gas State

The deviations of the real gas from the ideal gas shown in table 97 are calculated from the equations of state of J. D. Cox [1961], Krone and Johnson [1956], and Beynon and McKetta [1963]. These results are widely scattered. Krone and Johnson made their measurements at higher temperatures and pressures; therefore, the values calculated from their equation cannot be considered reliable. The values calculated from the second virial coefficient of Cox are also uncertain since higher terms were neglected. This procedure has been found to give a heat capacity correction which is too small for this alcohol as well as for the other alcohols. Therefore, the selected values were taken primarily from the calculations based on the equation of Beynon and McKetta, with the modification obtained by adding a constant term in B as previously described.

Solid-Vapor Equilibria

Vapor Pressure at the Triple Point

Since the vapor pressure of the solid at 25.82 °C is equal to that of the liquid at this temperature, it was calculated from the Antoine constants.

Vapor Pressure at 25 °C

This value was calculated from the vapor pressure of the undercooled liquid at 25 °C, extrapolated by the Antoine equation, and from the thermodynamic properties of liquid and crystalline phases. This procedure was described in the section on vapor pressure.

TABLE 98. 2-Methyl-2-propanol. Comparison of virial coefficients and compressibility factor, Z, derived from experimental measurements

	Virial coefficients			Pressure, atmospheres						
	B_p' cm^3	C_p' cm^3 atm^{-1}	D_p' cm^3 atm^{-2}	0.05	0.1	0.25	0.5	1	2	5
				Values of $(1-Z)\times 100$						
Temperature = 50 °C										
Cox, J. D. [1961]	(−2060)			(0.388)	(0.777)	(1.942)				
Beynon and McKetta [1963]	(−2319)		(−8227)	(.441)	(.906)	(2.671)				
Temperature = 100 °C										
Cox, J. D. [1961]	−1033			(0.169)	(0.337)	(0.843)	1.687	(3.37)	(6.75)	
Beynon and McKetta [1963]	−992		−50.42	(.162)	(.324)	.813	1.640	3.40	(7.80)	
Temperature = 150 °C										
Cox, J. D. [1961]	−565			(0.081)	(0.163)	(0.407)	0.814	(1.627)	(3.25)	(8.14)
Beynon and McKetta [1963]	−513		−1.05	(.074)	(.148)	.369	.739	1.480	(2.98)	(7.76)
Temperature = 200 °C										
Cox, J. D. [1961]	(−330)			(0.042)	(0.085)	(0.212)	(0.425)	(0.850)	(1.70)	(4.25)
Beynon and McKetta [1963]	(−298)		(−0.0499)	(.038)	(.077)	(.192)	(.384)	(0.768)	(1.54)	(3.85)

Values in parenthesis have been extrapolated outside the experimental range of temperature or pressure.

Heat of Sublimation at 25 °C

The heat of sublimation is equal to the sum of the heat of vaporization of the undercooled liquid and the heat of fusion at 25 °C.

Temperature Derivative of the Heat of Sublimation

The equation of state of Beynon and McKetta [1963] and the heat capacities of the solid and gas give $d\Delta H/dT = -8.7$ cal deg^{-1} mol^{-1}.

Vapor-Liquid Equilibrium at 25 °C

Vapor Pressure

The value listed on the summary sheets was calculated from the Antoine constants.

Heat of Vaporization

The selected value was from Wadso [1966]. This was also very close to the value calculated from the equation derived by Beynon and McKetta [1963] to represent their observed data at higher temperatures.

Temperature Derivative of the Heat of Vaporization

The equation of Beynon and McKetta [1963] for heat of vaporization as a function of temperature gives $d\Delta H/dT = -29.0$ cal deg^{-1} mol^{-1} at 25 °C. Their equation of state of the gas, along with the heat capacities of the liquid and gas, predicts -26.0 cal deg^{-1} mol^{-1}. In a similar manner, the equation of state of J. D. Cox [1961] predicts -24.3 cal deg^{-1} mol^{-1}. All three of these values depend upon the use of equations outside the range of the data used in the original derivation. However, the difference between ΔC_p for vaporization and $d\Delta H/dT$ at 25 °C is small, and therefore the uncertainty in $d\Delta H/dT$ calculated from ΔC_p is less than when it is calculated from the heat of vaporization equation based on data at higher temperatures.

Vapor-Liquid Equilibrium at the Normal Boiling Point

Normal Boiling Point

The boiling point listed on the summary sheets was calculated from the selected Antoine constants. It is about 0.1 °C higher than the three most recent values in table 91. The values for Biddiscombe, Collerson, Handley, Herington, Martin, and Sprake [1963] and Beynon and McKetta [1963] were calculated from the Antoine equation adjusted to fit their vapor pressure data.

Heat of Vaporization

Beynon and McKetta [1963] report the following equation which represents their calorimetric measurements of heat of vaporization in the range of 57 to 82.5 °C:

$$\Delta H_v = 596.95(235.0 - t)^{0.54692} \text{ cal mol}^{-1}$$

where t is the temperature in degrees Celsius. The ΔH_v value at the normal boiling point calculated from the above equation was considered the most reliable. It is fairly close to the values calculated by Biddiscombe, Collerson, Handley, Herington, Martin, and Sprake [1963] from their second virial coefficients and from the selected Antoine constants.

Heat Capacity of the Liquid

No direct measurements at this temperature have been located. The value shown in table 88 was calculated from the equation

$$C_p = -16.656 + 0.26970T - 1.2367 \times 10^{-4} T^2 \text{ cal deg}^{-1} \text{ mol}^{-1}$$

where T is the temperature in degrees Kelvin. This equation was obtained by a least squares fit of the observed heat capacities of Oetting [1963] from 303 to 331 K.

Temperature Derivative of the Heat of Vaporization

The heat of vaporization equation of Beynon and McKetta [1963] gives $d\Delta H/dT = -33.5$ cal deg^{-1} mol^{-1} at 82.42 °C. Since they did not carry out measurements at any higher temperatures, the derivative at this temperature may not be very accurate. The correction of ΔC_p to $d\Delta H/dT$ using the equation of state of the gas of J. D. Cox [1961] gives -28.3 cal deg^{-1} mol^{-1}, while that of Beynon and McKetta [1963] gives -38.0 cal deg^{-1} mol^{-1}. Thus, the uncertainty in this derivative is rather large.

Properties of the Ideal Gas State

Molecular Parameters

The vibration frequencies and other molecular properties have been studied more extensively for 2-methyl-2-propanol than for the other C_4 alcohols. This is probably the result of the higher symmetry of this molecule as compared to the others. Pritchard and Nelson [1960] selected some of the fundamental frequencies. A more complete study, including normal coordinate analysis, was conducted by Tanaka [1960 and 1962a]. Beynon and McKetta [1963] adopted Tanaka's assignments in their calculation of the thermodynamic functions, except for some modifications of the $-CH_3$ rocking frequencies. The assignments of Pritchard and Nelson and of Tanaka as modified by Beynon and McKetta are shown in table 99. The designations of the vibrational modes adopted by Beynon and McKetta were used in this table, although they are not entirely consistent with the ones listed by Pritchard and Nelson.

Recently Durocher and Sandorfy [1965] obtained the fundamental frequency of 3617.5 cm^{-1} for the OH stretching mode in carbon tetrachloride solution. They also identified the corresponding vibration in dimers and higher polymers and obtained anharmonic contributions. Similar studies have been reported by Hammaker [1961] and Ramiah and Puranik [1962]. The Raman spectrum has been given by Venkateswarlu and Mariam [1962] and microwave absorption by Rathmann, Curtis, McGeer, and Smyth [1956]. Additional references to molecular properties are listed in the Index to the Bibliography.

Beynon and McKetta [1963] adopted barriers to internal rotation of 3800 cal mol^{-1} for the three methyl groups and 900 cal mol^{-1} for the hydroxyl group. These were selected so as to be consistent with their heat capacity measurements and with the third law entropy, and also to be similar to internal rotation barriers found in hydrocarbons of similar structure.

TABLE 99. 2-Methyl-2-propanol. Reported values. Fundamental vibration frequencies

Type of Vibration	Frequencies, cm^{-1}	
	Pritchard and Nelson [1960]	Tanaka [1962], Beynon and McKetta [1963]
a' OH rock	3362	3643
a' CH stretch	2970(6)	2980(6)
a' CH stretch	(ca. 2920)(2)	2910(2)
a'' CH stretch		2880
a' CH bend	1472(6)	1472(5)
a' CH bend		1450
a' CH bend	1389	1395
a', a'' CH bend	1364	1374(2)
a' CC stretch	1380	1330
a'' CC stretch	1239(2)	1230
a' CO stretch	1215	1215
a', a'' CH_3 rock	1027	1106(2)
a' OH bend	1189	1140
a'', a', a'' CH_3 rock		1013(3)
a' CH_3 rock	914	919
a' CC stretch	747	748
a', a'' CCO bend	465(2)	462(2)
a' CCC bend	424	424
a'' CCC bend	346(2)	356
a' CCC bend		344

Entropy at 25 °C

The third law entropy for the ideal gas based on the low temperature calorimetry of Oetting [1963], the selected heat of vaporization, and other auxiliary data is 78.06 cal deg^{-1} mol^{-1}. This differs from the statistical calculation of Beynon and McKetta, [1963] by only 0.08 cal deg^{-1} mol^{-1}. A weighted average, which is within the uncertainties of both values, was selected.

Heat Capacity

Beynon and McKetta [1963] report the following equation for the ideal gas heat capacity:

$$C_p{}^0 = 10.836 + 0.049648T + 0.24070 \times 10^{-4}T^2 \text{ cal deg}^{-1}\text{ mol}^{-1}$$

They obtained this equation by extrapolating their experimental measurements in the range of 365 to 437 K to zero pressure. Within this range of temperatures, this equation agrees with the heat capacity calculated from the partition function to within 0.1 cal deg^{-1} mol^{-1} or better.

Thermodynamic Functions

The only published tables of thermodynamic functions of 2-methyl-2-propanol are those of Beynon and McKetta [1963]. These are calculated from the partition functions based on the vibrational assignments and other parameters previously described. The values of $\Delta H_f{}^0$ and $\Delta G_f{}^0$ have been adjusted to agree with the selections shown in table 88.

Chemical Equilibria

No experimental measurements of equilibrium constants of reactions in the gas phase were found.

Tests of Internal Consistency

The following cycle shows that the vapor-liquid equilibrum data are internally consistent within the estimated uncertainties. Lack of experimental measurements on the liquid heat capacity above 58 °C contributes considerably to the overall uncertainty.

	ΔH kcal mol^{-1}	ΔS cal deg^{-1} mol^{-1}
liquid (25 °C)→real gas (25 °C, 42.0 mmHg)	11.15±0.03	37.40±0.1
real gas (25 °C)→ideal gas (25 °C)	0.05±0.01	0.27±0.04
ideal gas (25 °C)→ideal gas (82.42 °C)	1.67±0.02	5.12±0.04
ideal gas (42.0 mmHg)→ideal gas (760 mmHg)	0.0	−5.755±0.005
ideal gas (82.42 °C, 760 mmHg)→real gas (82.42 °C, 760 mmHg)	−0.29±0.02	−0.71±0.03
real gas (82.42 °C)→liquid (82.42 °C)	−9.32±0.05	−26.21±0.15
liquid (82.42 °C)→liquid (25 °C)	−3.35±0.05	−10.26±0.15
Sum	−0.09±0.08	−0.15±0.25

Miscellaneous

Dannhauser and Bahe [1964] have measured the dielectric constant of the liquid at 1 atm from 25 to 230 °C and have interpreted the results in terms of hydrogen bond formation. Harris, Haycock, and Alder [1953] report dielectric constant data from 14 to 50 °C and at pressures up to 200 atm. Nemeth and Reed [1964] obtained a collision diameter of 7.40 Å from measurement of gas phase viscosity.

Recommendations for Future Work

The thermodynamic properties of 2-methyl-2-propanol have been studied more thoroughly than those of any of the other butanols. The readiness with which it crystallizes has simplified determinations of low temperature heat capacity and third law entropy. Because of its molecular symmetry, calculation of the thermodynamic functions by statistical mechanics is easier than for the other C_4 alcohols. Finally, the theoretical problem of the effect of steric hindrance of the methyl groups on the hydroxyl group has increased interest in the properties of this compound. The principal gap in thermodynamic properties at present is in the heat capacity of the liquid above room temperature. As for the other alcohols, some additional careful measurements of the effect of air on the melting point (as compared to the triple point) would be of interest. More definite identification and characterization of metastable crystalline forms should also be carried out. Also, as for the other alcohols, the existence and types of polymeric species in the gas phase needs further clarification.

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1-Pentanol

Properties of the Liquid Phase at Various Temperatures

Refractive Index

An extensive list of references to the refractive index of 1-pentanol throughout the visible spectrum and at temperatures from 15 to 46 °C may be found in the Index to the Bibliography. Most of the values for the sodium D-line at 20 and 25 °C listed in table 103 fall within 0.0002 of the selected ones. The selected values at other temperatures given in table 100 were taken from the best straight line through the observed values reported by Lievens [1924], Simon, I. [1929], Timmermans and Hennaut-Roland [1932], Nevgi and Jatkar [1934], and Weissler [1948]. Venkataraman [1939] also reported values in the range of 26.4 to 46.5 °C. Although his measured values for methanol, ethanol, 1-propanol, and 1-butanol were close to the results of other investigators, his values of 1-pentanol appeared to be about 0.002 too low. The selected value at 40 °C was obtained by applying the temperature coefficient found by Venkataraman to the value selected at 30 °C.

TABLE 100. 1-Pentanol. Selected values. Physical and thermodynamic properties

Temp. °C	Refractive Index, n_D	Density g cm^{-3}	Vapor Pressure, mmHg
−20		0.8421	
−10		.8358	
0		.8291	
+10		.8222	
15	1.4119		
20	1.4100	.8148	
25	1.4080	.8112	
30	1.4058	.8079	
40	1.4015	.8005	
44.7			10
45			10.2
50		.7930	14.1
55			19.3
60		.7853	26.0
65			34.5
70		.7774	45.4
75			58.9
80		.7694	75.7
85			96.4
85.8			100
90		.7612	121.5
95			151.8
100		.7529	188.2
101.5			200
105			231.4
110		.7445	282.4
115			342.2
119.2			400
120		.736	412.0
125			492.9
130			586.1
135			692.9
137.8			760
140			814.8
145			953.2

Data For Phase Transitions

Initial	Final	Temp. °C	dt/dP deg mm^{-1}	Pressure mmHg	ΔH kcal mol^{-1}	$d\Delta H/dt$	ΔS	ΔC_p
						cal deg^{-1} mol^{-1}		
c	liq	−78.2		760	2.34±0.05	−18.0±1	12.0±0.2	−18.0±1
liq	g	25	5.24	2.35±0.2	13.61±0.05	−18±0.4	45.65±0.15	
liq	g	137.8±0.1	0.0407	760	10.6±0.2	−27±5	25.8±0.4	−21±5

Condensed Phase Heat Capacity

State	Temp. °C	C_p
		cal deg^{-1} mol^{-1}
c	−78.2	31.3±0.8
liq	−78.2	37.9±0.8
liq	137.8	67±5

Properties of the Saturated Real Gas

Temp. °C	H^r-H^0	S^r-S^0	$C_p{}^r-C_p{}^0$
	kcal mol^{-1}	cal deg^{-1} mol^{-1}	
25	0.00	0.00	0.0
137.8	−0.±0.05	−0.35±0.1	5.5±2

Data for the Standard States at 25 °C

State	Heat of Combustion $\Delta H_c{}^0$ kcal mol^{-1}	Heat of Formation $\Delta H_f{}^0$ kcal mol^{-1}	Entropy S^0 cal deg^{-1} mol^{-1}	Gibbs Energy of Formation $\Delta G_f{}^0$ kcal mol^{-1}	Heat Capacity, C_p cal deg^{-1} mol^{-1}
liq	−795.1±0.3	−85.0±0.3	62.0±0.5	−38.3±0.3	49.8±0.2
g	−808.7±0.3	−71.4±0.3	96.2±0.3	−34.9±0.3	31.8±0.3

Critical Constants

Temp. 313. °C, 586. K	Pressure atm	Density 0.27 g cm^{-3}

Constants in Vapor Pressure and Density Equation

Antoine Equation				Francis Equation				
Temp. Range	*A*	*B*	*C*	Temp. Range	*A*	$B \times 10^3$	*C*	*E*
37 to 138 °C	7.17758	1314.56	168.11	−20 to 120 °C	0.97611	0.3874	73.73	500

TABLE 101. 1-Pentanol. Selected values. Thermodynamic functions of the ideal gas at one atmosphere

Temperature K	Etrnopy S^0 cal deg^{-1} mol^{-1}	Heat Capacity C_p^0 cal deg^{-1} mol^{-1}	Enthalpy Function $(H^0-H_0^0)/T$ cal deg^{-1} mol^{-1}	Gibbs Energy Function $(G^0-H_0^0)/T$ cal deg^{-1} mol^{-1}	Heat of Formation ΔH_f^0 kcal mol^{-1}	Gibbs Energy of Formation ΔG_f^0 kcal mol^{-1}
0	0	0	0	0	−63.27	−63.27
273.15	93.56	29.89	20.25	−73.31	−70.81	−37.94
298.15	96.21	31.76	21.14	−75.07	−71.40	−34.90
300	96.39	31.91	21.20	−75.19	−71.45	−34.68
400	106.55	39.74	24.86	−81.69	−73.62	−22.04
500	116.18	47.01	28.58	−87.60	−75.42	−8.91
600	125.26	53.24	32.17	−93.09	−76.87	+4.55
700	133.85	58.59	35.55	−98.30	−78.01	18.23
800	141.99	63.18	38.74	−103.25	−78.85	32.04
900	149.68	67.15	41.68	−107.96	−79.42	45.95
1000	156.91	70.59	44.40	−112.51	−79.78	59.91

TABLE 102. 1-Pentanol. Selected values. Refractive index at various temperatures and wavelengths

Symbol	Wavelength, Å	Refractive Index, n		
		15 °C	20 °C	25 °C
$\mathrm{He_{red}}$	6678.2	1.4095	1.4077	1.4057
$\mathrm{H_C}$	6562.8	1.4098	1.4080	1.4060
$\mathrm{Na_D}$	5892.6	1.4119	1.4100	1.4080
$\mathrm{Hg_e}$	5460.7	1.4136	1.4117	1.4097
$\mathrm{He_{blue}}$	5015.7	1.4158	1.4140	1.4121
$\mathrm{H_F}$	4861.3	1.4169	1.4150	1.4131
$\mathrm{Hg_g}$	4358.3	1.4210	1.4191	1.4172
$\mathrm{H_{G'}}$	4340.5	1.4211	1.4192	1.4173

Refractive indices at wavelengths other than the sodium D-line have been reported by Landolt and Jahn [1892], Lievens [1934], Simon, I. [1929], and Timmermans and Hennaut-Roland [1932]. The selected values in table 102 were obtained by graphically smoothing these data.

Density

Constants in the Francis equation and the corresponding selected values of the density from −20 to 120 °C are given in table 100. Accurate experimental values at 20 and 25 °C are listed in table 103. The selected values are within about 0.0004 g cm^{-3} of most of these. Measurements at other temperatures have been reported by Vogel [1948] from 20 to 85 °C, Philip [1939] from 30 to 65 °C, Thomas and Meatyard [1963] from 30 to 123 °C, and Costello and Bowden [1958] from −60 to 180 °C. The selected densities were within 0.0003 g cm^{-3} of those reported by Thomas and Meatyard. The values of Costello and Bowden were about 0.0016 g cm^{-3} below the selected ones from 20 to 100 °C, but were within 0.0002 g cm^{-3} of the selected values at other temperatures. The data of Vogel were also lower than the selected densities by 0.0011 to 0.0015 g cm^{-3}. The uncertainties in the selected densities are probably of the order of 0.0003 g cm^{-3} from 0 to 80 °C and range up to about twice this amount at lower and higher temperatures within the range of experimental data shown in table 100. Sackmann and Sauerwald [1950] report a density of 0.8868 gm ml^{-1} at −78.2 °C, the freezing point. Efremov [1966] has reported densities to three significant figures from 0 °C to the critical temperature. These data are within 0.005 g cm^{-3} of the selected values up to 140 °C.

Vapor Pressure and Boiling Point

The vapor pressures and boiling points listed in table 100 were based on the Antoine constants obtained from a least squares fit of the experimental data. Vapor pressures below 1 atm were based mainly on the work of Thomas and Meatyard [1963] and Butler, Ramchandani, and Thomson [1935]. These two sets of data agree to within about 2 mmHg except at the higher temperatures where the values of Butler, Ramchandani, and Thomson were 4 to 6 mmHg higher. No data above the normal boiling point were found.

Kopp [1854] first reported a normal boiling point of 131.1 °C. Since then over 50 values, identified in the Index to the Bibliography, have been published. Accurate measurements at 1 atm are summarized in table 103. Nearly all of these are within about 0.2 °C of the value calculated from the Antoine equation.

Critical Properties

Critical Temperature and Density

The only experimental values are from Efremov [1966]; so, these were selected. The critical temperature was obtained by observing the disappearanec of the meniscus, and the uncertainty is about one degree. The density was obtained by extrapolation of orthobaric liquid and vapor densities.

Critical Pressure

There are no directly measured values. Efremov [1966] calculated a critical pressure of 38.3 atm by an empirical relation based on his observed critical temperature and pressure.

Solid-Liquid Phase Equilibria

Normal Melting Point

The significant values of the melting point which have been reported are listed in table 103. None of these measurements are very accurate in terms of modern standards. Whitmore, Karnatz, and Popkin [1938] used a carefully purified sample in their measurements, and the boiling point, refractive index, and density which they reported agreed closely with the selected values given in table 100. Therefore, their value was the principal basis of the selected value. However, they did not describe their technique of measurement nor the type of thermometer used.

Heat Capacity of the Solid and Liquid at the Melting Point

These were obtained by graphical extrapolation of the specific heats observed by Parks, Huffman, and Barmore [1933].

Heat of Fusion

Parks, Huffman, and Barmore [1933] are the source of the only measured value.

TABLE 103. 1-Pentanol. Reported values. Simple physical properties

Investigators		Vapor Pressures and Boiling Points		Freezing Point	Density, d g cm^{-3}		Refractive Index, n_D	
		°C	mmHg	t_m, °C	20 °C	25 °C	20 °C	25 °C
1-Pentanol, $C_5H_{12}O$, mol wt. 88.151, state at 25 °C liq								
Zander	[1884]	137.8–137.9	760					
Kishner	[1913]				0.8147		1.4101	
Timmermans and Mattaar	[1921]	137.8	760	−78.5				
Bourgom	[1924]	137.95	760					
Lievens	[1924]	137.95	760	−78.5			1.4085	
Norris and Cortese	[1927]	138.0–138.1	760			0.8110	1.4077	
Verkade and Coops	[1927]	137.6	760					
Lloyd, Brown, Bonnell, and Jones	[1928]	137.2	760			.80942		
Malone and Reid	[1929]	137.8	760	−78.5				
Simon	[1929]	138.00	760					1.40815
Ellis and Reid	[1932]	137.8	760			.81159		1.4077
Timmermans and Hennaut-Roland	[1932]	138.25	760	−78.85	.8145		1.40903	
Butler, Thomson, and Maclennan	[1933]	137.6–137.7	760		.81146		1.41043	
Parks, Huffman, and Barmore	[1933]	137.9	760	−79.0				
Butler, Ramchandani, and Thomson	[1935]	137.75	760		.81253		1.41113	
Wojciechowski	[1936]	138.06	760					
Ginnings and Baum	[1937]	137.6–138.3	760		.8110			
Whitmore, Karnatz, and Popkin	[1938]	137.8	760	−78.24	.8144		1.40988	
Larson and Hunt	[1939]					.8095		
Jones, Bowden, Yarnold, and Jones	[1948]					.8083		
Vogel	[1948]	136.6	760		.8136		1.40999	
Tschamler, Richter, and Wettig	[1949b]	138.0	760	−78.5		.8091		
Mumford and Phillips	[1950]	137.5	760		.8146	.8110	1.4103	
Adkins and Rosenthal	[1950]							1.4080
Mears, Fookson, Pomerantz, Rich, Dussinger, and Howard	[1950]						1.4101	
Pichler, Ziesecke, and Traeger	[1950]	138.0	760		.8144		1.4099	
Sackmann and Sauerwald	[1950]			−78.5				
Cook	[1952]	138.0	760	−77	.8149		1.4098	
Hill and Van Winkle	[1952]	137.0	760				1.41146	
Staveley and Spice	[1952]	137.92	760		.8152			
Timmermans	[1952]			−78.85				
Hellwig and Van Winkle	[1953]	137.5	760				1.41129	
McKenna, Tartar, and Lingafelter	[1953]	138.0	760					1.4062
Costello and Bowden	[1958]	137.9	760		0.8133			
Union Carbide Corporation	[1958]	137.8	760	−78.9	0.8225			
Lishanskii, Korotkov, Andreeva, and Zak	[1959]	135–137	760				1.4108	
Thomas and Meatyard	[1963]	137.9	760			0.8150	1.4120	
Selected value	[1967]	137.8±0.1 44.7±0.2	760 10	−78.2 ±0.2	0.8148 ±0.0002	0.8112 ±0.0003	1.4100 ±0.003	1.4080 ±0.0004

Antoine constants: *A* 7.17758, *B* 1314.56, *C* 168.11

dt/dp at 760 mmHg, 0.0407 °C/mmHg

Properties of the Liquid at 25 °C

Heat Capacity

A linear extrapolation of these data to 25 °C is shown in table 105. The selected value is a weighted average of the two values listed in this table.

Absolute Entropy

The third law value of Parks, Huffman, and Barmore [1933], based on experimental heat capacity measurements down to 94 K, is 60.9 cal deg^{-1} mol^{-1}. The selected value was taken to be consistent with the entropy of the gas and with the selected heat of vaporization.

Heat of Combustion

The available data are summarized in table 108. The only reliable values are those of Verkade and Coops [1927] and Chao and Rossini [1965]. The value of Verkade and Coops in this table has been corrected to current standard state conditions for the liquid by the National Bureau of Standards. A value intermediate between these two, but closer to that of Verkade and Coops, was selected. Further discussion on this point is given in appendix F.

Properties of the Real Gas

Equation of State

Efremov [1966] reported the densities of the saturated vapor from 180 °C to the critical temperature. However, since the accuracy of these measurements was low and since the pressures were not measured, these data cannot be used to establish an equation of state. The observed critical temperature and calculated critical pressure gives by Efremov, along with the selected Antoine constants, gives an acentric factor, as defined by Pitzer et al.[4], of 0.59. This corresponds to a second virial coefficient, B, of -1.32 liters at 137.8 °C, the normal boiling point. Another estimation procedure based on critical temperature and liquid density, which has been found to be reliable for hydrocarbons, predicts $B=-0.97$ liters at 137.8 °C. However, in analogy with the lower alcohols, we would expect 1-pentanol vapor to be appreciably associated at pressures in the vicinity of 1 atm. This conclusion is also supported by the heat capacity data discussed in the next section. Neither of these methods of estimation gives reliable results for substances which are associated in the vapor state. Thus we would expect B to be at least -1.5 liters and probably larger, at 137.8 °C, and also expect a significant contribution from higher terms in the virial equation.

Heat Capacity

The only measured vapor heat capacity data are those of Sinke and De Vries [1953] shown in table 107. They were measured in a vapor flow calorimeter at 750 mmHg. Their estimated uncertainty is ± 1 cal deg^{-1} mol^{-1} at the two lower temperatures and ± 0.2 cal deg^{-1} mol^{-1} at 437 K. Also shown in table 107 are the ideal gas heat capacities interpolated at the corresponding temperatures from the ideal gas thermodynamic functions shown in table 101. The fourth column shows the difference between the observed real gas values and the calculated ideal gas data. The last column shows the difference between the heat capacity of the real gas at 1 atm and the ideal gas predicted by the acentric factor of 0.59. Thus the data of Sinke and De Vries suggest an extent of association comparable to what has been found for the butanols. Extrapolation down to the boiling point is uncertain, but it appears that the heat capacity of the saturated real gas at the boiling point is at least 5 cal deg^{-1} mol^{-1} greater than the ideal gas. This is larger than the corresponding value of 1-butanol and similar to what has been observed for 2-butanol, 2-methyl-1-propanol, and 2-methyl-2-propanol.

Corrections to the Ideal Gas State

Because of the low vapor pressure, the differences between properties of the real gas in equilibrium with the liquid at 25 °C and the ideal gas are negligible. The acentric factor of 0.59 predicts $H^0-H^r=125$ cal mol^{-1}, $S^0-S^r=0.23$ cal deg^{-1} mol^{-1}, and $C_p{}^0-C_p{}^r=-0.98$ cal deg^{-1} mol^{-1} for the saturated vapor at the boiling point If the heat capacity data of Sinke and De Vries are even approximately correct, we would expect the correct values to be somewhat larger than these. The heat capacity is more strongly affected by association than the other properties; and analogy with 2-butanol and 2-methyl-1-propanol, which have a similar difference in heat capacity at their boiling point, suggests $H^0-H^r=180$ cal mol^{-1} and $S^0-S^r=0.35$ cal deg^{-1} mol^{-1} for 1-pentanol.

Vapor-Liquid Equilibrium at 25 °C

Vapor Pressure

The vapor pressure at 25 °C was calculated from the Antoine equation using the selected constants. This is about 10 °C below the lowest experimental value used in the evaluation of these constants, but the uncertainty in this extrapolation is not likely to be more than 0.1 or 0.2 mmHg.

Heat of Vaporization

Wadso [1966] measured the heat of vaporization at 25 °C by direct calorimetry, and his value was selected. Table 104 shows his result, as well as heats of vaporization calculated from vapor pressure.

TABLE 104. 1-Pentanol. Reported values. Heats of vaporization

Investigator	ΔH_v at 25 °C	ΔH_v at t_b	Method and Remarks
Schall [1884]		10.7	Calorimetric.
Green [1960]	13.80		Calculated from vapor pressure.
Wadso [1966]	13.610		Calorimetric.
Selected Antoine constants	14.3	10.37	Calculated.

Temperature Derivative of the Heat of Vaporization

At the equilibrium vapor pressure found at 25 °C, the vapor may be considered to behave as an ideal gas. The temperature derivative of the heat of vaporization is therefore equal to the difference in heat capacities.

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[4] Pitzer, J. Am. Chem. Soc. 77, 3427 (1955); Pitzer, Lippmann, Curl, Huggins and Peterson, J. Am. Chem. Soc. 77, 4344 (1955); Pitzer and Curl, J. Am. Chem. Soc. 79, 2369 (1957).

Vapor-Liquid Equilibrium at the Normal Boiling Point

Normal Boiling Point

The boiling point at 1 atm was calculated from the Antoine constants.

Heat of Vaporization

The only direct calorimetric measurement is the old value of Schall [1884]. The heat of vaporization calculated from the Antoine constants by use of the Clapeyron equation, with second virial coefficients of -1.5 liters mol^{-1}, is shown in table 104. This value was adjusted slightly to obtain the selected value.

Heat Capacity of the Liquid

Leech [1949] measured the heat capacity of the liquid from 40 to 70 °C and expressed his results as $C_p = 45.9 + 0.132\ t$ cal deg^{-1} mol^{-1}. von Reis [1881] measured the enthalpy change from temperatures of 100.1, 111.6, and 124.5 °C to around 20 °C. Combining these results with those of Leech, the equation $C_p = 43.0 + 0.173\ t$ cal deg^{-1} mol^{-1} was taken as giving the best representation of the heat capacity from 70 to 124 °C. The heat capacity at the boiling point was calculated from this equation.

TABLE 105. 1-Pentanol. Reported values. Heat capacity and entropy of the liquid at 25 °C

Investigator	$C_p^0(\text{l})$	Remarks	$S^0(\text{l})$, Third Law
Parks, Huffman and Barmore [1933]	50.0	Graphical interpolation	60.9
Leech [1949]	49.2	Extrapolated by equation	

TABLE 106. 1-Pentanol. Reported values. Heat capacity and entropy of the ideal gas

T K	C_p^0, cal deg^{-1} mol^{-1}		S^0, cal deg^{-1} mol^{-1}	
	Green [1961a]	Chermin [1961]	Green [1961a]	Chermin [1961]
298.15	31.76	31.6	96.21	95.9
600	53.24	54.0	125.26	125.5
1000	70.59	71.2	156.91	157.6

Temperature Derivation of the Heat of Vaporization

If the equation of state of the gas phase is taken to be $V = RT/P + B$, then the total derivative of the heat of vaporization is given by,

$$\frac{d\Delta H}{dT} = \Delta C_p + \frac{(H^r - H^0)\Delta H_v}{(RT - BP)T}.$$

Substitution of the other selected data into this equation gives -26.8 cal deg^{-1} mol^{-1}.

Properties of the Ideal Gas State

No statistical calculations of the thermodynamic properties of the ideal gas have been published. Chermin [1961] and Green [1961] have prepared tables of the ideal gas thermodynamic functions of the 1-alkanols from methanol to decanol. For alkanols above 1-propanol Green applied the methylene increments established by Person and Pimentel, J. Am. Chem. Soc. 75, 532 [1953]. For alcohols above 1-butanol Chermin assumed that the difference between the property of a C_n alkanol and the corresponding property of 1-butanol was equal to the difference in the same property between the normal C_n+1 alkane and 1-pentane. The thermodynamic properties of alkanes were taken from "Selected Values of Properties of Hydrocarbons and Related Compounds," American Petroleum Institute Research Project 44, Thermodynamics Research Center, Texas A&M University, College Station, Texas. In effect this means that both sets of tables are based on the same methylene increment for alcohols above 1-butanol. The principal difference between the two sets of tables is the result of differences in the properties of 1-butanol. Green calculated the properties of 1-butanol by adding the methylene increment to n-propanol, and Chermin calculated the properties of 1-butanol statistically using the molecular parameters of Dyatkina [1954]. A comparison of the heat capacity and entropy obtained by these methods for three different temperatures is given in table 106. The third law entropy of the ideal gas at 298.15 K, based on the entropy of the liquid published by Parks, Huffman, and Barmore [1933], is 95.1 cal deg^{-1} mol^{-1}. However, the uncertainty in this figure is at least 1 cal deg^{-1} mol^{-1}.

Since thermodynamic properties published by Green were selected for 1-butanol, his values were also selected for 1-pentanol in order to retain internal consistency.

TABLE 107. 1-Pentanol. Comparison of observed and calculated vapor heat capacity

Temperature T K	C_p^r, experimental real gas, 750 mm Hg	C_p^0 interpolated ideal gas	$C_p^r - C_p^0$ by difference	$C_p^r - C_p^0$ acentric factor
417	44.72	41.05	3.67	0.89
428	43.92	41.88	2.04	0.88
437	44.27	42.55	1.72	0.69

C_p^r from Sinke and De Vries [1953].

Tests for Internal Consistency

The internal consistency among vapor and liquid heat capacities, heats and entropies of vaporization, vapor pressure, and ideal gas corrections can be tested by calculating the net change of enthalpy and entropy through a cycle, starting with the liquid at 25 °C, going through the gas at the boiling point and returning back to the initial state. If all of these properties are internally consistent, the results should be zero.

Table 108. 1-Pentanol. Reported values. Heat of combustion of the liquid at 25 °C

Investigator	$-\Delta H_c^0(\mathrm{l})$ kcal mole^{-1}
Louguinine [1880]	793.8
Zubov [1898] (recalculated by Swietoslawski [1920])	792.3
Verkade and Coops [1927] (recalculated by NBS)	795.27
Chao and Rossini [1965]	794.61

	ΔH kcal mol^{-1}	ΔS cal deg^{-1} mol^{-1}
liquid (25 °C)→real gas (25 °C, 2.35 mmHg)	13.61±0.05	45.65±0.15
real gas (25 °C)→ideal gas (25 °C)	0.00±0.01	0.00±0.05
ideal gas (25 °C)→ideal gas (137.8 °C)	4.08±0.2	11.42±0.6
ideal gas (2.35 mmHg)→ideal gas (760 mmHg)	0.00	−11.49±0.3
ideal gas (137.8 °C, 760 mmHg)→real gas (137.8 °C, 760 mmHg)	−0.18±0.05	−00.35±0.1
real gas (137.8 °C)→liquid (137.8 °C)	−10.6±0.2	−25.8±0.5
liquid (137.8 °C)→liquid (25 °C)	−6.5±0.4	−18.4±1.5
Sum	+0.4±0.5	1.1±1.7

The change in the enthalpy and entropy of the liquid between 25 and 137.8 °C was calculated from the heat capacity equations previously given. These quantities contribute the largest uncertainty to the calculations.

Index to the Bibliography

Numbers refer to the Bibliography, page 1–389.

References to data used in the selection of refractive index, density, boilng point, vapor pressure, and melting point are in boldface type.

Numbers in parentheses refer to sources of reviews, or theoretical calculations only.

Reference numbers under each property are listed in the order of date of publication.

Refractive Index
840, 990, **909**, **1066**, 1748, **1273**, **1622**, **486**, **1781**, **254**, 695, **253**, 1112, **1925**, **1843**, 799, 6, **1856**, **1893**, **13**, 1159, 1224, **1377**, **338**, **1865**, **760**, 1387, 1903, **737**, 1152, 459, 1426, 630, 811, **1073**, 1758, 1279

Density at 20–30 °C Only
989, 840, **909**, 1748, **1273**, **1075**, **486**, **254**, 1262, **253**, 1112, 1287, 598, **1925**, 997, 799, 1222, 6, 981, 1893, **853**, 1807, **1377**, 1224, **338**, **1865**, 1682, 459, 811, 1823, 1073, **1758**

Density at all Temperatures
941, 1061, **2012**, **990**, 1409, **188**, **1066**, 1848, **1622**, **1781**, 1371, **1856**, 1527, **347**, 1154, 481

Normal Boiling Point
941, 989, 1504, 1291, 2012, 990, 188, **1066**, 1994, 1748, **1273**, 907, 1075, 1622, 1121, 12, 375, **486**, 1781, **1323**, **254**, **253**, 1287, **1977**, **598**, **1925**, 799, 1396, 731, 6, 1554, 981, 1007, 1011, 1807, 1224, 1377, 760, **338**, 1387, **1682**, 194, 1902, **1865**, 737, **1152**, 1426, 630, 365, **1823**, 1073

Vapor Pressure and Boiling Points at Other Pressures
1061, 909, 1785, 1409, **870**, **1848**, 1262, **253**, 799, 1856, 1159, 459, 1823, **1758**

Critical Temperature
749, (1433), (347), 481

Critical Volume and Density
481

Heat Capacity of the Solid
1323

Normal Melting Point
1785, 1066, 1622, **1781**, **1323**, **1925**, **1807**, 1527, 338, 1777, 1823

Heat of Fusion
1323

Heat Capacity of the Liquid
1866, 1323, 1011, 1823

Heat Capacity of the Real Gas
1627

Calorimetric Heat of Vaporization at 25 °C
(626), 1870

Calorimetric Heats of Vaporization at the Normal Boiling Point
1555

Heat of Combustion
1084, 2033, (1721), 1848, (1507), (626), 287, 288

Third Law Entropy of the Liquid at 25 °C
1323

Molecular Vibration Frequencies and Spectra
1440, 619, 46, 243, 1844, 379, 456, 1012, 977 668

Thermodynamic Functions of the Ideal Gas
623, 291

Association in the Liquid Phase
1115, 1105, 1104, 1683, 1114, 1383, 1757, 1758, 78

2-Pentanol

Properties of the Liquid Phase at Various Temperatures

Refractive Index

Values used as a basis for the final selection of n_D at 20 and 25 °C are listed in table 111. Only a few values at other temperatures or wavelengths were found. Nevgi and Jatkar [1934] report a value at 30 °C. Eykman [1919] reports values at several wavelengths at 18 °C, and Timmermans and Hennaut-Roland [1932] report values at various wavelengths at 15 °C. The selected values in table 110 were read from a smooth curve drawn through values of refractive index plotted against $1/(\lambda-1000)^{1.6}$ taken from Timmermans and Hennaut-Roland. Converting the value of n_D obtained from this curve at 15 to 20 °C, using the temperature coefficient given by Hennaut-Roland, gave a result which was very close to the n_D selected from the data in table 111. The data in table 110 for other wavelengths at 20 °C were obtained by applying these temperature coefficients to the data at 15 °C.

Density

The selected data listed in table 109 were calculated from the Francis equation with substitution of the constants also listed in table 109. The values calculated for 20 and 25 °C are within about 0.0005 g cm^{-1} of the better observed data in table 111. At other temperatures the Francis equation constants were based primarily on the data of Timmermans and Hennaut-Roland [1932], Pickard and Kenyon [1911], Costello and Bowden [1958], and Thomas and Meatyard [1963]. Generally the density values of Costello and Bowden were lower, and those of Thomas and Meatyard higher, than the calculated values.

Vapor Pressure and Boiling Point

A selection of the best values of the normal boiling point is given in table 111. On the average these run a little higher than the value given in table 109 which was calculated from the Antoine equation, where the constants were adjusted to fit all of the reliable observed values of vapor pressure and boiling point. Vapor pressures at other than 1 atm are reported by Butler, Ramchandani, and Thomon [1935], 25 to 110 °C; Brauns [1943], 57 to 119 °C; and Thomas and Meatyard [1964], 25 to 119 °C. The data of Brauns were weighted heavily in fitting the Antoine equation, and the calculated pressures are within 2 mmHg of his below 119 °C.

Critical Properties

No experimental values have been reported in the literature.

Solid-Liquid Phase Equilibria

Normal Melting Point

Cook [1952] stated that 2-pentanol sets to a glass between −95 and −90 °C. No other information on the melting point was found.

Properties of the Liquid at 25 °C

The only property of the liquid, besides those already discussed, which has been found is the heat of combustion by Chao [1961] and Chao and Rossini [1965]. This was used to calculate the heat of formation reported in table 109.

Vapor-Liquid Equilibrium at 25 °C

Vapor Pressure

The value calculated from the Antoine constants was increased slightly to agree better with experimental data in this vicinity.

Heat of Vaporization

The result of McCurdy and Laidler [1963] obtained by direct calorimetry was the only experimental data. The Antoine constants gave 13.5 kcal mol^{-1} with the assumption of a second virial coefficient of −3 liter mol^{-1}. However, this is not expected to be accurate at so low a temperature. There is no information which would permit a calculation of the temperature derivative of the heat of vaporization.

Vapor-Liquid Equilibrium at the Normal Boiling Point

Normal Boiling Point

This was calculated from the selected constants in the Antoine equation.

TABLE 109. 2-Pentanol. Selected values. Physical and thermodynamic properties

Temp. °C	Refractive Index, n_D	Density g cm^{-3}	Vapor Pressure, mmHg
−20		0.8396	
−10		.8324	
0		.8249	
+10		.8172	
15	1.4083		
20	1.4064	.8093	
25	1.4044	.8053	
30	1.4025	.8012	8.47
32.3			10
35			12.1
40		.7928	17.0
45			23.4
50		.7841	31.9
55			42.9
60		.7751	56.8
65			74.4
70		.7656	96.4
70.7			100
75			123.6
80		.7558	156.9
85			197.3
85.3			200
90		.7454	245.9
95			303.9
100		.7344	372.7
101.8			400
105			453.7
110		.7104	548.5
115			658.7
119.0			760
120			786.0
125			932.
130			1100.

Data For Phase Transitions

Initial	Final	Temp. °C	dt/dP deg mm^{-1}	Pressure mmHg	ΔH kcal mol^{-1}	$d\Delta H/dt$ cal deg^{-1} mol^{-1}	ΔS cal deg^{-1} mol^{-1}	ΔC_p cal deg^{-1} mol^{-1}
liq	g	25	2.21	5.9±0.2	12.7±0.3		42.6±1	
liq	g	119.0±0.3	0.0376	760	10.3±0.5		26.3±1	

Condensed Phase Heat Capacity

State	Temp. °C	C_p cal deg^{-1} mol^{-1}

Properties of the Saturated Real Gas

Temp. °C	H^r-H^0 kcal mol^{-1}	S^r-S^0 cal deg^{-1} mol^{-1}	$C_p^r-C_p^0$ cal deg^{-1} mol^{-1}

Data for the Standard States at 25 °C

State	Heat of Combustion ΔH_c^0 kcal mol^{-1}	Heat of Formation ΔH_f^0 kcal mol^{-1}	Entropy S^0 cal deg^{-1} mol^{-1}	Gibbs Energy of Formation ΔG_f^0 kcal mol^{-1}	Heat Capacity, C_p cal deg^{-1} mol^{-1}
liq	−792.4±0.3	−87.7±0.3			
g	−805.1±0.4	−75.0±0.4			

Critical Constants

Temp. °C, K	Pressure atm	Density g cm^{-3}

Constants in Vapor Pressure and Density Equation

Antoine Equation

Temp. Range	A	B	C
25 to 120 °C	7.27575	1271.92	170.37

Francis Equation

Temp. Range	A	$B\times10^3$	C	E
−20 to 110 °C	0.91413	0.4585	26.772	300

TABLE 110. 2-Pentanol. Selected values. Refractive index at various temperatures and wavelengths

Symbol	Wavelength, Å	Refractive Index, *n*	
		15 °C	20 °C
He_{red}	6678.2	1.4059	1.4040
H_c	6562.8	1.4062	1.4043
Na_D	5892.6	1.4083	1.4064
Hg_e	5460.7	1.4101	1.4082
He_{blue}	5015.7	1.4125	1.4106
H_F	4861.3	1.4135	1.4116
Hg_g	4358.3	1.4176	1.4155
$H_{G'}$	4340.5	1.4177	1.4157

Heat of Vaporization

No calorimetric measurements have been reported. The selected value was calculated from the Antoine constants with the assumption that the second virial coefficient is -1 liter mol^{-1} at this temperature.

Index to the Bibliography

Numbers refer to the Bibliography, page 1–389.

References to data used in the selection of refractive index, density, boiling point, vapor pressure, and melting point are in boldface type.

TABLE 111. 2-Pentanol. Reported values. Simple physical properties

Investigators	Vapor Pressures and Boiling Points		Freezing Point	Density, *d* g cm^{-3}		Refractive Index, n_D	
	°C	mmHg	t_m, °C	20 °C	25 °C	20 °C	25 °C
2-Pentanol, $C_5H_{12}O$, mol wt. 88.151, state at 25 °C liq							
Linnemann [1876]	118.5–119.5	760		0.8102			
Pickard and Kenyon [1911]	118.5–119.5	760		.8103		1.4053	
Willcox and Brunel [1916]	118.9	760					
Brunel [1923]	119.50	760			0.80483		1.4043
Clough and Johns [1923]	119.2	760		.8088			
Munch [1926]	119.0	760			.8091		
Norris and Cortese [1927]	119.16–119.26	760			.8068		
Malone and Reid [1929]	119.3	760					
Ellis and Reid [1932]	119.5	760			.80528		1.4041
Timmermans and Hennaut-Roland [1932]	119.85	760		.80919		1.40642	
Kailan and Raff [1932]	119.0	760					
Lauer and Stodola [1934]	118.4–119.9	760				1.4067	
Butler, Ramchandani, and Thomson [1935]	119.89	760			.80525	1.41787	
Norton and Hass [1936]	118.3	760			.8083		1.4046
Ginnings and Baum [1937]	119.2–119.7	760			.8056		
Whitmore and Karnatz [1938b]	118.7–119.3	760					
Brauns [1943]	119.4	760		.8101		1.4056	
Huston and Bostwick [1948]						1.4068	
Pichler, Ziesecke, and Traeger [1950]	119.2	760		0.8088		1.4064	
Huston and Tiefenthal [1951]						1.4068	
Cook [1952]	119.5	760		.8097		1.4065	
Pines, Rudin, and Ipatieff [1952]	117.0–117.5	760				1.4060	
McKenna, Tartar, and Lingafelter [1953]	119.2	760					1.4025
Zeiss and Tsutsui [1953]	118–119	760					1.4047
Pomerantz, Fookson, Mears, Rothberg, and Howard [1954]				.8098		1.4065	
Brown and Nakagawa [1955]	118.4–118.9	760				1.4060	
Costello and Bowden [1958]	119.1	760		.8089			
Thomas and Meatyard [1963]	119.2	760		.8070			
Selected value [1967]	119.0±0.3	760		.8093	.8053	1.4064	1.4044
	32.3±0.4	10		±0.0003	±0.0004	±0.0004	±0.0004

Antoine constants: *A* 7.27575, *B* 1271.92, *C* 170.37

dt/*dp* at 760 mmHg, 0.0376 °C/mmHg

Numbers in parentheses refer to sources of reviews, or theoretical calculations only.

Reference numbers under each property are listed in the order of date of publication.

Refractive Index
1378, 1838, **509**, **238**, 512, **1227**, **1273**, 1605, **486**, **1781**, 1001, **1262**, 253, **1275**, **1924**, **202**, **803**, **1377**, **808**, **338**, **1387**, 1152, **2016**, **1407**, **226**, 233, 610, 505, 1193

Density at 20–30 °C Only
238, 311, 1227, 1273, 486, **253**, 1275, 598, **202**, 1377, **338**, 1407, 610, 1147, **1758**

Density at all Temperatures
1070, **1378**, 1838, 509, 512, **486**, **1781**, 92, **347**

Normal Boiling Point
1070, 1526, 1435, 1378, 1838, **1960**, **238**, 311, 1983, 512, **1227**, 573, 907, **1273**, 1605, 1121, 1022, 1597, 620, **1781**, **486**, 870, 921, 1001, **253**, **1275**, **598**, 1924, 92, 1007, 1554, 803, **1377**, 808, **338**, 1387, 194, 720, 2016, 1152, 1407, **226**, 610, 505, 1193

Vapor Pressure and Boiling Points at Other Pressures
1262, **253**, **202**, **347**, **1758**

Critical Temperature
748, (347)

Normal Melting Point
338

Calorimetric Heat of Vaporization at 25 °C
1147

Heat of Combustion
287, 288

Molecular Vibration Frequencies and Spectra
243, 530, 1376

Association in the Liquid Phase
1705, 530

3-Pentanol

Properties of the Liquid Phase at Various Temperatures

Refractive Index

The data used as a basis for selecting the refractive indices for the sodium D-line at 20 and 25 °C are reported in table 114. The uncertainty in the selections is about 0.0005. In addition, Nevgi and Jatkar [1934], Weissler [1948], and Laddha and Smith [1950] have reported values at 30 °C, and Vavon [1914] and Thomas and Meatyard [1963] have reported values at 15 °C. Selections at these temperatures are reported in table 112. Eykman [1919] has measured refractive indices at several wavelengths at 16 °C, and Timmermans and Hennaut-Roland [1932] have carried out similar measurements at 15 °C. The data in table 113 were taken from smoothed curves plotted in the usual manner. When the temperature coefficient of Timmermans and Hennaut-Roland was applied to the selected refractive index at the sodium D-line at 20 °C, the value calculated for 15 °C was about 0.0004 larger than their observed value. Therefore all of their measurements were corrected by this amount to give the data at 15 °C reported in table 113. The values at 20 °C were taken from a parallel curve drawn through the selected value of n_D at 20 °C.

Density

Experimental density values at 20 and 25 °C are listed in table 114. Timmermans and Hennaut-Roland [1932] report values at 0, 15, and 30 °C, and Nevgi and Jatkar [1934] and Weissler [1948] report values of the density at 30 °C. The only data at higher temperatures are those of Thomas and Meatyard [1963], which cover the range from 19 to 108 °C. The selected values listed in table 112 were calculated from the constants in the Francis equation which were adjusted to fit the experimental data. Weissler's value is 0.0017 g cm^{-3} below the calculated one. Experimental values at temperatures other than 20 and 25 °C are within about 0.0005 g cm^{-3} of the calculated ones.

Vapor Pressure and Boiling Point

The best values of the normal boiling point are listed in table 114. The only significant source of vapor pressure data below 1 atm is Thomas and Meatyard [1963]. These data are the basis of the Antoine constants and vapor pressures given in table 112.

Critical Properties

No experimental values have been reported in the literature.

Solid-Liquid Phase Equilibria

Normal Melting Point

Union Carbide Chemicals Company reports 3-pentanol as forming a glass at −50 °C. Cook [1952] gives the melting point as −69±2 °C. These are the only available data.

Properties of the Liquid at 25 °C

Heat Capacity

Leech [1949] measured the heat capacity from 40 to 70 °C and fitted his points to a linear function of temperature. The selected value was obtained by extrapolation of these data to 25 °C using the equation.

TABLE 112. 3-Pentanol. Selected values. Physical and thermodynamic properties

Temp. °C	Refractive Index, n_D	Density g cm^{-3}	Vapor Pressure, mmHg
0		0.8372	
10		.8288	
15	1.4126		
20	1.4104	.8203	
25	1.4079	.8160	8.24
27.7			10
30	1.4055	.8116	11.7
35			16.4
40		.8077	22.5
45			30.6
50		.7935	40.9
55			54.2
60		.7840	70.9
65			91.7
66.7			100
70		.7743	117.5
75			149.1
80		.7642	187.5
81.4			200
85			233.8
90		.7538	289.2
95			354.9
98.			400
100		.7429	432.4
105			523.3
110		.7316	629.2
115			751.9
115.3			760
120			893.2

Data For Phase Transitions

Initial	Final	Temp. °C	dt/dP deg mm^{-1}	Pressure mmHg	ΔH kcal mol^{-1}	$d\Delta H/dt$	ΔS	ΔC_p
						cal deg^{-1} mol^{-1}		
c	liq	−59		760				
liq	g	25	1.70	8.2±0.3	12.8±0.3		42.9±1	
liq	g	115.3±0.3	0.0376	760	10.1±0.5		26.0±1	

Condensed Phase Heat Capacity

State	Temp. °C	C_p
		cal deg^{-1} mol^{-1}
liq	115.3	68±3

Properties of the Saturated Real Gas

Temp. °C	H^r-H^0	S^r-S^0	$C_p^r-C_p^0$
	kcal mol^{-1}	cal deg^{-1} mol^{-1}	

Data for the Standard States at 25 °C

State	Heat of Combustion ΔH_c^0 kcal mol^{-1}	Heat of Formation ΔH_f^0 kcal mol^{-1}	Entropy S^0 cal deg^{-1} mol^{-1}	Gibbs Energy of Formation ΔG_f^0 kcal mol^{-1}	Heat Capacity, C_p cal deg^{-1} mol^{-1}
liq	−791.7±0.2	−88.5±.2	57.4±1	−40.4±0.3	60.0±0.5
g	−804.5±0.3	−75.7±0.3	91.3±0.3	−37.8±0.4	

Critical Constants

Temp. °C, K	Pressure atm	Density g cm^{-3}

Constants in Vapor Pressure and Density Equation

Antoine Equation				Francis Equation				
Temp. Range	A	B	C	Temp. Range	A	$B\times10^3$	C	E
21 to 116 °C	7.41493	1354.42	183.41	0 to 110 °C	0.94094	0.5274	36.322	350

TABLE 113. 3-Pentanol. Selected values. Refractive index at various temperatures and wavelengths

Symbol	Wavelength, Å	Refractive Index, *n*	
		15 °C	20 °C
He_{red}	6687.2	1.4102	1.4081
H_c	6562.8	1.4105	1.4084
Na_D	5892.6	1.4125	1.4104
Hg_e	5460.7	1.4143	1.4122
He_{blue}	5015.7	1.4167	1.4145
H_F	4861.3	1.4177	1.4155
Hg_g	4358.3	1.4218	1.4196
$H_{G'}$	4340.5	1.4219	1.4198

Absolute Entropy

There is no third law value. The entropy at 25 °C was calculated from the entropy of the ideal gas, along with other appropriate auxiliary data.

Heat of Combustion

The value listed in table 112 was obtained by Chao [1961] and Chao and Rossini [1965].

Vapor-Liquid Equilibrium at 25 °C

Vapor Pressure

This was calculated from the selected Antoine constants.

Heat of Vaporization

McCurdy and Laidler [1963] have made the only calorimetric measurement. They obtained 12.65 kcal mol^{-1}. The selected Antoine constants gave 12.67 K cal mol^{-1}, when the second virial coefficient of −3 liter mol is assumed. The selected value was obtained by adjusting the result of McCurdy and Laidler slightly to correspond to the other related data.

TABLE 114. 3-Pentanol. Reported values. Simple physical properties

Investigators	Vapor Pressures and Boiling Points		Freezing Point	Density, *d* g cm^{-3}		Refractive Index, n_D	
	°C	mmHg	t_m, °C	20 °C	25 °C	20 °C	25 °C
3-Pentanol, $C_5H_{12}O$, mol wt. 88.151, state at 25 °C liq							
Pickard and Kenyon [1913]	114.8	760		0.8198		1.4094	
Timmermans [1913]	115.53	760					
Willcox and Brunel [1916]	114.8–115.2	760					
Brunel [1923]	115.63	760			0.8154		1.4077
Norris and Cortese [1927]	115.8–116.0	760			.8154		1.4079
Timmermans and Hennaut-Roland [1932]	116.10	760		.82061		1.41012	
Kailan and Raff [1932]	116.5	760					
Spells [1936]				.81546			
Ginnings and Baum [1937]	115.4–115.9	760			.8195		
Whitmore and Karnatz [1938b]	115.6–116.0	760				1.4100	
Whitmore and Surmatis [1940]	115.2	760		.8218		1.4104	
Laddha and Smith [1950]	113.5–115.5	760		.8202			
Pichler, Ziesecke, and Traeger [1950]	115.3	760		.8203		1.4104	
Braun, Spooner, and Fenske [1950]						1.4108	
Cook [1952]	115.7	760	−69	.8208		1.4104	
Anisimov [1953b]					.81046		1.40781
McKenna, Tartar, and Lingafelter [1953]	116.2	760					1.4072
Union Carbide Corporation [1953]	115.9	760		.8155			
Zeiss and Tsutsui [1953]	116–116.5	760					1.4058
Pomerantz, Fookson, Mears, Rothberg, and Howard [1954]	115.9	760		.8155			
Brown and Nakagawa [1955]	114.4–114.5	760				1.4097	
Benkeser, Hazdra, and Burrous [1959]						1.4090	
Thomas and Meatyard [1963]	115.50	760		.8203		1.4103	
Selected value [1967]	115.3±0.3	760	−69	.8203	0.8160	1.4104	1.4079
	27.7±0.4	10	±3	±0.0005	±0.0007	±0.0005	±0.0005

Antoine constants: *A* 7.41493, *B* 1354.42, *C* 183.41

dt/*dp* at 760 mmHg, 0.0376 °C/mmHg

Vapor-Liquid Equilibrium at the Normal Boiling Point

Normal Boiling Point

This was calculated from the selected Antoine constants.

Heat of Vaporization

The value listed on the summary sheet was calculated from the Antoine constants along with the assumption of the second virial coefficient of -1 liter mol^{-1}.

Properties of the Ideal Gas State

The heat of formation in the ideal gas state was calculated from the heat of combustion of the liquid and the selected heat of vaporization. The entropy was obtained from the gas phase dehydrogenation equilibrium described below.

Chemical Equilibria

Buckley and Herington [1965] measured the equilibrium constant for the gas phase reaction,

$$CH_3CH_2CHOHCH_2CH_2 \rightarrow CH_3CH_2COCH_2CH_3 + H_2$$

over the temperature range of 388 to 526 K. Their equilibrium constant, when converted to the Gibbs energy change for this reaction, could be expressed as a function of temperature by

$$\Delta G^0 = 11890 - 13.49T \log T + 10.75T - 1.15 \times 10^{-3}T^2$$

$$+ 0.33 \times 10^{-5}T^3 \text{ cal mol}^{-1}.$$

This equation yields

$$\Delta H^0 = 13.56 \text{ kcal mol}^{-1} \text{ and } \Delta G^0 = 5.12 \text{ kcal mol}^{-1}$$

for the dehydrogenation reaction at 25 °C. Using values for the enthalpy and entropy of formation of 3-pentanone in the gas phase, Buckley and Herington calculate

$$\Delta Hf^0(g) = -75.38 \pm 0.32 \text{ kcal mol}^{-1} \text{ and}$$

$$S^0(g) = 91.35 \pm 0.31 \text{ cal deg}^{-1} \text{ mol}^{-1}$$

for 3-pentanol. The heat of formation derived from the heat of combustion is within their estimated uncertainty. Their value of entropy was selected and used to calculate the entropy of the liquid at 25 °C.

Index to the Bibliography

Numbers refer to the Bibliography, page 1–389.

References to data used in the selection of refractive index, density, boiling point, vapor pressure, and melting point are in boldface type.

Numbers in parentheses refer to sources of reviews, or theoretical calculations only.

Reference numbers under each property are listed in the order of date of publication.

Refractive Index
1379, 1838, **509**, **238**, **1273**, **1781**, **1262**, 1301, 1017, **1924**, **1945**, 857, **1893**, **201**, 980, **1377**, 1378, 1387, **36**, **1152**, 2016, **1407**, 226, 610, 901, **1594**, 124, 872, **1758**

Density at 20–30 °C Only
1379, **238**, **1273**, **1262**, 1017, **1667**, **598**, **1945**, **1893**, **980**, **1377**, **338**, 36, 1823, **1407**, 610, 1147

Density at all Temperatures
1838, 509, **1781**, **1758**

Normal Boiling Point
1408, 1526, **1769**, 1379, 1838, 1960, 509, **238**, **1273**, 907, 621, **1781**, 870, 921, 1301, 215, 1017, 598, 1923, 1943, 1952, 1945, 857, 1396, 1554, 1155, 1007, 1011, **1377**, 980, **194**, 1387, **338**, 2016, **1152**, **1823**, **1407**, 226, 610, 1594, 901, 124, 696

Vapor Pressure and Boiling Points at Other Pressures
1823, **1262**, 872, **1758**

Normal Melting Point
338, 1823

Heat Capacity of the Liquid
1011

Calorimetric Heat of Vaporization at 25 °C
1147

Heat of Combustion
287, 288

Equilibrium Constants of Gas Phase Reactions
245

Molecular Vibration Frequencies and Spectra
243, 379, 1376

2-Methyl-1-butanol

Properties of the Liquid Phase at Various Temperatures

Refractive Index

2-Methyl-1-butanol may be resolved into optically active isomers. However, there is no indication that the physical properties of the liquid, other than specific rotation, are any different for the *d*-mixture than for the optically active form. The refractive indices reported in the literature for 20 and 25 °C scatter more widely than they do for the first three pentanols discussed so far. Data considered in the choice of the selected values are listed in table 116. The uncertainty in the selected values is about 0.0008. No data at wavelengths other than the sodium D-line were located. Nevgi and Jatkar [1934] and Weissler [1948] reported values at 30 °C, which along with an estimated temperature coefficient were used to select the value at 30 °C. Thomas and Meatyard [1963] gave a value at 15 °C which seemed to be about 0.0009 too small when compared to an extrapolation from 20 °C.

Density

Ikeda, Kepner, and Webb [1958] have obtained a density of 0.8150 g cm^{-3} at 25 °C on a sample carefully purified by fractional distillation. This matches exactly the selected value. Norris and Cortese [1927] had previously obtained a very similar result. Brauns [1937], Whitmore and Olewine [1938], and Cook [1952] have reported densities at 20 °C which are close to the selected value. Ginnings and Baum [1937] obtained a density of 0.8106 g cm^{-3} at 25 °C from what appeared to be a reliable measurement; however, it is obviously too low. The value of Nevgi and Jatkar [1934] at 30 °C is too high and that of Weissler [1948] too low at this temperature. The selected values at 30 °C and above are based largely on the results of Thomas and Meatyard [1963]. There are no reliable data below 20 °C.

Vapor Pressure and Boiling Point

Vapor pressures have been accurately measured from 65.7 to 128.7 °C by Brauns [1937]. These results and those of Thomas and Meatyard [1963] from 33.6 to 128.2 °C are the only significant data below the normal boiling point. Reliable boiling points are listed in table 116. The selected temperature of 128.7 °C may be about 0.1 or 0.2 °C below the best experimental values.

Critical Properties

No experimental data are available.

Solid-Liquid Phase Equilibria

Normal Melting Point

Cook [1952] found that 2-methyl-1-butanol sets to a glass in the range from −105 to −90 °C.

Properties of the Liquid at 25 °C

Heat Capacity

Leech [1949] has measured the liquid heat capacity from 40 to 70 °C. The selected value was obtained by extrapolating these data.

Heat of Combustion

The only measurement has been reported by Chao [1961] and Chao and Rossini [1965].

Vapor-Liquid Equilibrium at 25 °C

Vapor Pressure

The vapor pressure was calculated from the Antoine constants.

Heat of Vaporization

The selected value was measured calorimetrically by McCurdy and Laidler [1962].

Vapor-Liquid Equilibrium at the Normal Boiling Point

Normal Boiling Point

This was calculated from the Antoine constants.

Heat of Vaporization

No direct calorimetric measurements have been made. The selected value was calculated from the Antoine constants with a second virial coefficient of −1 liter mol^{-1}.

Heat Capacity of the Liquid

The data of Leech [1949] were extrapolated to the boiling point by means of the equation which he reported.

TABLE 115. 2-Methyl-1-Butanol. Selected values. Physical and thermodynamic properties

Temp. °C	Refractive Index, n_D	Density g cm^{-3}	Vapor Pressure, mmHg
20	1.4107	0.8190	
25	1.4086	.8150	
30	1.4062	.8109	
40		.8026	
40.2			10
45			14.0
50		.7942	19.4
55			26.6
60		.7856	35.9
65			47.8
70		.7770	62.8
75			81.6
79.0			100
80		.7682	104.8
85			133.3
90		.7593	167.8
93.9			200
95			209.4
100		.7502	259.1
105			317.9
110		.7410	387.1
110.9			400
115			468.0
120		.7316	561.9
125			670.2
128.7			760
130			794.6
135			936.6
140			1097.9

Data For Phase Transitions

Initial	Final	Temp. °C	dt/dP deg mm^{-1}	Pressure mmHg	ΔH kcal mol^{-1}	$d\Delta H/dt$ cal deg^{-1} mol^{-1}	ΔS cal deg^{-1} mol^{-1}	ΔC_p cal deg^{-1} mol^{-1}
liq	g	25	3.87	3.1±0.4	12.9±0.3		43.3±1	
liq	g	128.7±0.4	0.0390	760	10.5±0.5		26.1±1.3	

Condensed Phase Heat Capacity

State	Temp. °C	C_p cal deg^{-1} mol^{-1}
liq	128.7	64±2

Properties of the Saturated Real Gas

Temp. °C	H^r-H^0 kcal mol^{-1}	S^r-S^0 cal deg^{-1} mol^{-1}	$C_p^r-C_p^0$ cal deg^{-1} mol^{-1}

Data for the Standard States at 25 °C

State	Heat of Combustion ΔH_c^0 kcal mol^{-1}	Heat of Formation ΔH_f^0 kcal mol^{-1}	Entropy S^0 cal deg^{-1} mol^{-1}	Gibbs Energy of Formation ΔG_f^0 kcal mol^{-1}	Heat Capacity, C_p cal deg^{-1} mol^{-1}
liq	−794.9±0.2	−85.2±0.2			52.6±0.5
g	−807.8±0.3	−72.3±0.3			

Critical Constants

Temp. °C, K	Pressure atm	Density g cm^{-3}

Constants in Vapor Pressure and Density Equation

Antoine Equation

Temp. Range	A	B	C
34 to 129 °C	7.06730	1195.26	156.83

Francis Equation

Temp. Range	A	$B\times10^3$	C	E
20 to 120 °C	1.15748	0.3880	257.93	800

TABLE 116. 2-Methyl-1-butanol. Reported values. Simple physical properties

Investigators		Vapor Pressures and Boiling Points		Freezing Point	Density, *d* g cm^{-3}		Refractive Index, n_D	
		°C	mmHg	t_m, °C	20 °C	25 °C	20 °C	25 °C
2-Methyl-1-butanol, $C_5H_{12}O$, mol wt. 88.151, state at 25 °C liq								
Perkin	[1884]	130.5–131.5	760			0.8067		
Thorpe and Rodgers	[1894]	128.7	760					
Willcox and Brunel	[1916]	128.0–128.05	760		0.8169			
Norris and Cortese	[1927]	129.4	760			.8152		1.4087
Graves	[1931]	128–130	760					
Brauns	[1937]	138.9	760		.8193		1.4107	
Ginnings and Baum	[1937]	128.4–129.1	760			.8106		
Whitmore and Olewine	[1938b]	128–129	760		.8189		1.4109	
Houtman, Steenis, and Heertjes	[1946]						1.4092	
Hafslund and Lovell	[1946]						1.41084	
Brokaw and Brode	[1948]	129	760				1.4102	
Baker and Linn	[1949]						1.4100	
Braun, Spooner, and Fenske	[1950]						1.4105	
Pichler, Ziesecke, and Traeger	[1950]	128.8	760		.816		1.4111	
Lyubomilov and Terent'ev	[1951]	128–129	760		.8200		1.4102	
Cook	[1952]	128.9	760		.8198		1.4108	
Nerdel and Henkel	[1953]	128–129	760					
McKenna, Tartar, and Lingafelter	[1953]	128.6						1.4066
Urry, Stacy, Huyser, and Juveland	[1954]						1.4052	
Ikeda, Kepner, and Webb	[1956]					.8150		1.4088
Thomas and Meatyard	[1963]	128.2	760			.815	1.4099	
Zweifel, Ayyangar, Munekata, and Brown	[1964]						1.4106	
Selected value	[1967]	128.7±0.4 40.2±0.5	760 10		.8190 ±0.0005	.8150 ±0.0005	1.4107 ±0.0005	1.4086 ±0.0005

Antoine constants: *A* 7.06730, *B* 1195.26, *C* 156.83

dt/*dp* at 760 mmHg, 0.0390 °C/mmHg

Index to the Bibliography

Numbers refer to the Bibliography, page 1–389.

References to data used in the selection of refractive index, density, boiling point, vapor pressure, and melting point are in boldface type.

Numbers in parentheses refer to sources of reviews, or theoretical calculations only.

Reference numbers under each property are listed in the order of date of publication.

Refractive Index
1764, 1765, 1123, 564, 483, 1124, 1960, 1983, **1273**, 907, 1026, 1597, 1034, 621, 1518, 921, **1262**, 660, 598, **203**, **1936**, 92, 1554, **674**, **783**, **214**, **72**, 1011, 429, **201**, 1276, 1377, **1102**, 194, **338**, 736, **1152**, 1259, 900, 1426, 1650, **811**, 336, **2036**

Density at 20–30 °C Only
1123, 1960, 1273, 660, 598, 203, **1935**, **1936**, 214, 1893, 1377, **1102**, **338**, 736, **811**, **1758**, 1147

Density at all Temperatures
1349, 92, **674**

Normal Boiling Point
1347, 1349, 1764, 1765, 1123, 564, 483, 1124, **1960**, 1983, 907, **1273**, 1026, 1597, 1034, 621, 1518, 921, 660, **598**, **203**, 1936, 92, 1554, 783, 214, 1011, 429, 1276, **1377**, 1102, 194, **338**, **1152**, 1259, 900, 1426, 1650, 900, 336

Vapor Pressure and Boiling Points at Other Pressures
1262, **203**, **1935**, 1824, 1365, 1310, **1758**

Normal Melting Point
338

Heat Capacity of the Liquid
1011

Calorimetric Heat of Vaporization at 25 °C
1147

Heat of Combustion
287, 288

Association in the Liquid Phase
1705

3-Methyl-1-Butanol

Properties of the Liquid Phase at Various Temperatures

Refractive Index

Because of its industrial importance, there is more information on the properties of 3-methyl-1-butanol (isoamyl alcohol) than on any of the other pentanols except 1-pentanol. Data used to select the refractive index at the sodium D-line at 20 and 25 °C are shown in table 119. Values at other temperatures in the range of 11 to 30 °C have been reported by Brühl and Schröder [1904], Cheneveau [1907], de Lattre [1927], Timmermans and Hennaut-Roland [1929], Nevgi and Jatkar [1934], Udovenko and Frid [1948], Weissler [1948], Bonauguri, Bicelli, and Spiller [1951], and Wheeler and Jones [1952]. The values listed in table 117 for 10 and 30 °C were taken from a straight line drawn through a plot of these points. Refractive indices at other wavelengths have been reported by Brühl and Schröder [1904], Timmermans and Hennaut-Roland [1929], and Vogel [1948]. The values of n_D of Brühl and Schröder were about 0.0005 high and those of Timmermans and Hennaut-Roland were about 0.0006 low, relative to the selected values. The values in table 118 were taken from curves of n plotted against $1/(\lambda-1000)^{1.6}$ which passed through the selected n_D at 15 and 20 °C and were parallel to the data of Brühl and Schröder and Timmermans and Hennaut-Roland.

Density

In spite of the comparatively large number of published density values, only a few represent measurements of high accuracy. At 20 and 25 °C the data of Krchma and Williams [1927], Lloyd, Brown, Bonnell, and Jones [1928], Ginnings and Baum [1937], Cook [1952], and Ikeda, Kepner, and Webb [1958] are within about 0.0015 g cm^{-3} of the selected values. Values published by Norris and Cortese [1927] and Butler, Ramchandani, and Thomson [1935], which appear to be based on careful measurements, deviate even further. There has been no systematic study of density over a wide range of temperature. Therefore the Francis constants were determined on scattered points by a variety of investigators. Timmermans and Hennaut-Roland [1929] list values at 0, 15, and 30 °C which lie 0.001 to 0.002 g cm^{-3} above the selected values listed in table 117. Vogel [1948] reported data from 20 to 87 °C, and Udovenko, Kalabanovskoya, and Prokop'eva [1949] from 40 to 80 °C. Above 87 °C the density temperature curve is anchored by only one value which was determined by Schiff [1884] at 131.4 °C. Thus there is a marked scarcity of accurate modern density data for this compound.

Vapor Pressure and Boiling Point

The older vapor pressure data of Richardson [1886] and of Schmidt [1891a] at low pressures deviate significantly from more recent measurements. The Antoine constants and vapor pressures in table 117 were based primarily on the vapor pressures reported by Schmidt [1891a] above 760 mmHg, Ramchandani and Thomson [1935], and Udovenko and Frid [1948a,b], and on the more reliable boiling point data from Table 119. Although several calorimetric values of the heat of vaporization are available, they could not be used to evaluate the Antoine constants because of the lack of information on the second virial coefficient of the vapor phase.

Critical Properties

Critical Temperature

Four measurements of critical temperature have been reported in the literature, and they are listed in table 120. Since Kreglewski [1954] used a carefully purified sample, and the purity of the samples used by the previous three investigators were unknown, the value of Kreglewski was selected.

Critical Pressure and Density

No experimental measurements have been reported.

Solid-Liquid Phase Equilibria

Normal Melting Point

Cook [1952] found that 3-methyl-1-butanol formed a glass in the range from −120 to −105 °C, and Union Carbide Chemicals Company reports that it forms a glass below −117 °C.

Properties of the Liquid at 25 °C

Heat Capacity

There have been a comparatively large number of measurements of heat capacity of 3-methyl-1-butanol, although none of these could be considered as accurate by modern standards. Regnault [1862] determined the average specific heat from 10 to 117 °C, and Louguinine [1898] made a similar measurement between 21 and 130 °C which he used in his heat of vaporization measurement. Schiff [1886] carried out a series of enthalpy

TABLE 117. 3-Methyl-1-Butanol. Selected values. Physical and thermodynamic properties

Temp. °C	Refractive Index, n_D	Density g cm^{-3}	Vapor Pressure, mmHg
0		0.8229	
10	1.4111	.8167	
20	1.4072	.8103	
25	1.4052	.8070	
30	1.4032	.8036	
40		.7967	
41.0			10
45			13.1
50		.7896	18.1
55			24.7
60		.7821	33.1
65			43.9
70		.7744	57.6
75			74.6
80		.7662	95.7
80.9			100
85			121.6
90		.7576	153.0
95			190.9
96.1			200
100		.7485	236.2
105			289.9
110		.7389	353.4
113.2			400
115			427.7
120		.7285	514.3
125			614.5
130		.7174	729.9
131.2			760
135			862.0
140			1012.6

Data For Phase Transitions

Initial	Final	Temp. °C	dt/dP deg mm^{-1}	Pressure mmHg	ΔH kcal mol^{-1}	$d\Delta H/dt$	ΔS	ΔC_p
						cal deg^{-1} mol^{-1}		
liq	g	25	3.65	3.1±0.2	13.0±0.3		43.6±1	
liq	g	131.2±0.4	0.0392	760	10.54±0.2		26.1±0.5	

Condensed Phase Heat Capacity

State	Temp. °C	C_p
		cal deg^{-1} mol^{-1}
liq	131.2	78.0±1

Properties of the Saturated Real Gas

Temp. °C	H^r-H^0	S^r-S^0	$C_p{}^r-C_p{}^0$
	kcal mol^{-1}	cal deg^{-1} mol^{-1}	

Data for the Standard States at 25 °C

State	Heat of Combustion $\Delta H_c{}^0$ kcal mol^{-1}	Heat of Formation $\Delta H_f{}^0$ kcal mol^{-1}	Entropy S^0 cal deg^{-1} mol^{-1}	Gibbs Energy of Formation $\Delta G_f{}^0$ kcal mol^{-1}	Heat Capacity, C_p cal deg^{-1} mol^{-1}
liq	−795.0±0.2	−85.2±0.2			
g	−808.0±0.3	−72.2±0.3			50.3±0.4

Critical Constants

Temp. 306.3 °C, 579.5 K	Pressure atm	Density g cm^{-3}

Constants in Vapor Pressure and Density Equation

Antoine Equation				Francis Equation				
Temp. Range	A	B	C	Temp. Range	A	$B\times10^3$	C	E
25 to 153 °C	7.25821	1314.36	169.06	0 to 130 °C	0.89972	0.3604	23.031	300

measurements with a mixing calorimeter with upper temperatures ranging from 63.5 °C to around 111 °C and lower temperatures from 9 to 18 °C. He fitted these data to a linear equation for specific heat, $C_p/M = 0.5012 + 0.00270\ t$ cal deg^{-1} g^{-1}. Lussana [1913] measured the specific heat at several temperatures and at pressures up to 872 atm. Williams and Daniels [1924] measured the specific heat at temperatures from 30 to 80 °C and expressed their data as a quadratic function of temperature. A quadratic equation for specific heat as a function of temperature based on these data and a few other isolated values was given in Volume 5 of the International Critical Tables, McGraw-Hill Book Co. [1929]. Battelli [1907] measured the heat capacity from 0 down to −160 °C. More recently Leech [1949] measured the liquid heat capacity from 40 to 70 °C in a conduction calorimeter and expressed his results as a linear function of temperature. The equation of Williams and Daniels gives a heat capacity of 48.8 cal deg^{-1} mol^{-1} at 25 °C; the other three equations give values ranging from 49.9 to 50.9 cal deg^{-1} mol^{-1}.

TABLE 118. 3-Methyl-1-butanol. Selected values. Refractive index at various temperatures and wavelengths

Symbol	Wavelength, Å	Refractive Index, n	
		15 °C	20 °C
He_{red}	6678.2	1.4068	1.4050
H_c	6562.8	1.4071	1.4052
Na_D	5892.6	1.4092	1.4072
Hg_e	4560.7	1.4109	1.4089
He_{blue}	5015.7	1.4132	1.4113
H_F	4861.3	1.4142	1.4122
Hg_g	4358.3	1.4183	1.4162
$H_{G'}$	4340.5	1.4184	1.4163

Heat of Combustion

Chao [1961] and Chao and Rossini [1965] report the only modern heat of combustion measurement, and their value was adopted. Thomsen [1886] listed the enthalpy of combustion of gas as −820.0 kcal mol^{-1}. The selected value yields −808.0 kcal mol^{-1} for the gas.

Properties of the Real Gas

There have been no measurements of any of the real gas properties.

Vapor-Liquid Equilibrium at 25 °C

Vapor Pressure

Vapor pressure was calculated from the Antoine equation.

Heat of Vaporization

McCurdy and Laidler [1963] have made the only calorimetric measurement. Their value, along with the one calculated from the selected Antoine constants and the assumption of $B = -3$ liters mol^{-1}, is shown in table 121. Since the Antoine constants cannot be expected to give a reliable vapor pressure slope at 25 °C, the value of McCurdy and Laidler was selected.

Vapor-Liquid Equilibrium at the Normal Boiling Point

Normal Boiling Point

The boiling point at 1 atm was calculated from the Antoine equation.

Heat of Vaporization

The three calorimetric values are listed in table 121. The value obtained by Mathews [1926] agrees very well with the one calculated from the Antoine constants where B is taken as −1.1 liters mol^{-1}.

TABLE 119. 3-Methyl-1-butanol. Reported values. Simple physical properties

Investigators		Vapor Pressures and Boiling Points		Freezing Point	Density, d g cm^{-3}		Refractive Index, n_D	
		°C	mmHg	t_m, °C	20 °C	25 °C	20 °C	25 °C
3-Methyl-1-butanol, $C_5H_{12}O$, mol wt. 88.151, state at 25 °C liq								
Perkin	[1884]	131.5	760			0.80539		
Thorpe and Rodgers	[1884]	131.29	760					
Beckmann, Fuchs, and Gernhardt	[1895]	132.5	760					
Louguinine	[1898]	130.11	760					
Young and Fortey	[1902]	132.05	760					
Richards and Mathews	[1908]	131	760		0.8121			
English and Turner	[1914]					.8086		
Wroth and Reid	[1916]					.81225		
Willcox and Brunel	[1916]	131.2–131.6	760					
Cox	[1921]	131–132	760				1.4053	
Reilly and Hickinbottom	[1921]	130.6–131.6	760		.8021			
Grimm and Patrick	[1923]	131.6	760					
Williams and Daniels	[1924]	131.1–131.3	760					1.4061
Palmer and Constable	[1925]	131.1–131.2	760					
Munch	[1926]	130.0	760			.8095		1.4042
Mathews	[1926]	131.35	760		.8105			
Krchma and Williams	[1927]	131.2–131.7	760			.8083		1.40568
Norris and Cortese	[1927]	132.0–132.1	760			.8044		1.4046
Timmermans	[1927]	132.0	760					
Lloyd, Brown, Bonnell, and Jones	[1928]	130.8	760			.80484		
Mondain-Monval	[1928]				.8102		1.4070	
Timmermans and Hennaut-Roland	[1929]	132.0	760		.80922		1.4066	
Longinov and Pryanishnikov	[1931]	129–132	760				1.4072	
Kailan and Raff	[1932]	130.1	760					
Carter and Jones	[1934]	130.8	760				1.4096	
							1.4075	
Webb and Lindsley	[1934]	131.8–132.0	760				1.4068	
Butler, Ramchandani, and Thomson	[1935]	131.35	760			.81022	1.40964	
Coull and Hope	[1935]	130.5	760			.8061		
Spells	[1936]				.81411			
Tomanari	[1936]	130–131	760		.8119		1.40774	
Ginnings and Baum	[1937]	131.5–131.7	760			.8071		
Hafslund and Lovell	[1946]						1.40937	
Houtman, Stennis, and Heertjes	[1946]						1.4071	
Vogel	[1948]	130.4	760		.8128		1.40731	
							1.40865	
Pichler, Ziesecke, and Traeger	[1950]	131.6	760		.8071		1.4066	
Cook	[1952]	131.7			.8095		1.4065	
Wheeler and Jones	[1952]							1.40495
McKenna, Tartar, and Lingafelter	[1953]	131.8	760					1.4055
Kreglewski	[1954]	132.04	760					
Mathers and Pro	[1954]							1.40460
Ikeda, Kepner, and Webb	[1956]	132.0				0.8056		1.4046
Toropov	[1956]				0.8086			
Union Carbide Corporation	[1957]	131.9	760		.8092		1.4065	
Arnold and Washburn	[1958]	131.9	760			.8051		1.4048
								1.4052
Selected value	[1967]	131.2±0.4	760		.8103	.8070	1.4072	1.4052
		41.0±0.3	10		±0.0005	±0.0005	±0.0005	±0.005

Antoine constants: *A* 7.25821, *B* 1314.36, *C* 169.06

dt/*dp* at 760 mmHg, 0.0392 °C/mmHg

TABLE 120. 3-Methyl-1-butanol. Reported values. Critical properties

Investigator	Critical Temperature t_c, °C
Pawlewski [1882]	306.6
Brown, J. C. [1906]	309.77
Fischer and Reichel [1943]	307.2
Kreglewski [1954]	306.25

TABLE 121. 3-Methyl-1-butanol. Reported values. Heats of vaporization

Investigator	ΔH_v at 25 °C	ΔH_v at t_b	Method and Remarks
Louguinine [1898]		10.16	Mixing calorimeter.
Brown, J. C. [1903]		11.06	Calorimetric.
Mathews [1926]		10.54	Calorimetric.
McCurdy and Laidler [1963]	12.98		Calorimetric.
Selected Antoine Constants	14.19	10.54	Calculated.

Index to the Bibliography

Numbers refer to the Bibliography, page 1–389.

References to data used in the selection of refractive index, density, boiling point, vapor pressure, and melting point are in boldface type.

Numbers in parentheses refer to sources of reviews, or theoretical calculations only.

Reference numbers under each property are listed in the order of date of publication.

Refractive Index
237, **289**, 354, **1961**, 1227, **406**, **956**, **1273**, 1201, **1783**, **1080**, **1803**, **274**, **1262**, **1891**, **253**, **351**, 1112, **1792**, 799, 1222, 532, 6, **674**, **783**, **1819**, **1856**, **1893**, **1377**, **180**, **338**, **1909**, **1152**, **1139**, 811, 1365, 1823, 48, 1279

Density at 20–30 °C Only
1801, **1481**, **488**, 1992, 1140, **1227**, 1273, **956**, **1201**, 1075, 707, 1262, **253**, 1112, **351**, **1792**, 1667, **598**, 799, 1222, 176, 6, **1893**, 1377, **338**, **811**, 1365, **48**, 1823, 1147

Density at all Temperatures
74, **1349**, **1560**, **1556**, **237**, 289, **1587**, **1471**, 1409, **1783**, 173, **674**, **1856**, **1820**, 1797

Normal Boiling Point
490, 1347, 74, 868, 1349, 1560, 909, 1556, 1562, 1764, 1765, 119, **1083**, **2002**, 1526, 1395, 1481, 1525, 538, 1336, 1768, 1838, 280, **1960**, 1261, 355, **1471**, 642, 1961, 1994, 864, 1308, 533, **1227**, **1140**, 1009, 956, **1772**, 907, **1273**, **1075**, 1201, **1783**, 1597, 1080, 375, 870, **1803**, **274**, 1891, 351, **253**, 1792, **598**, 1979, 1842, 799, 168, 174, 929, 6, **1856**, 1606, 1011, 1007, 1820, **1377**, 180, 1902, 194, **338**, **1152**, 111, **1823**, 811, 1365, 48

Vapor Pressure and Boiling Points at Other Pressures
868, **1483**, **1571**, **253**, **1819**, **1818**, 1262

Critical Temperature
532, 218, 1344

Normal Melting Point
338, 1823

Heat Capacity of the Liquid
1466, 1562, 1083, 103, 1097, 1961, 1011

Calorimetric Heats of Vaporization at 25 °C
1147

Calorimetric Heats of Vaporization at the Normal Boiling Point
1083, 219, 1140

Heat of Combustion
1762, 287, 288

Molecular Vibration Frequencies and Spectra
1190, 1844, 456, 528

Association in the Liquid Phase
(1754), 1705, 528

2-Methyl-2-butanol

Properties of the Liquid Phase at Various Temperatures

Refractive Index

Data used in selecting the refractive index, n_D, at 20 and 25 °C are given in table 124. Uncertainty in the selected value is about 0.0004 at 20 °C and probably a little larger at 25 °C. Data at other temperatures in the range from 10 to 30 °C have been published by Norris and Reuter [1927], Nevgi and Jatkar [1934], Weissler [1948], and Bonauguri, Bicelli and Spiller [1951]. Eykman [1919] measured the refractive index over a range of wavelengths at 13 and 79 °C, and Timmermans and Hennaut-Roland [1932] also made similar measurements at 15 °C. The values of n_D selected from 10 to 30 °C were taken from a straight line drawn through the data in this range. The values in table 123 were taken from smooth curves drawn through plots of the refractive indices of Eykman and of Timmermans and Hennaut-Roland against $1/(\lambda - 1000)^{1.6}$, after correcting to the temperature shown using the available data on temperature coefficients. The values of Eykman and of Timmermans and Hennaut-Roland agreed well with the values selected at the sodium D-line based on the other published data. The values listed for 80 °C in tables 122 and 123 were based on measurements of Eykman, by converting them from 79 to 80 °C. From 10 to 30 °C the refractive index is a linear function of temperature to within the uncertainty of the data. The values at 80 °C imply some curvature in this function above 30 °C, so values between 30 and 80 °C cannot be obtained accurately by interpolation.

TABLE 122. 2-Methyl-2-Butanol. Selected values. Physical and thermodynamic properties

Temp. °C	Refractive Index, n_D	Density g cm^{-3}	Vapor Pressure, mmHg
0		0.8267	
10	1.4100	.8180	
20	1.4050	.8090	
21			10
25	1.4020	.8044	13.6
30	1.3994	.7998	19.8
35			28.2
40		.7903	39.3
45			53.8
50		.7806	72.4
55			96.0
55.7			100
60		.7706	125.4
65			161.7
69.4			200
70		.7603	205.9
75			259.3
80	1.3738	.7497	322.9
85			398.2
85.1			400
90		.7388	486.5
95			589.2
100		.7276	707.9
102.0			760
105			843.9
110		.7160	998.9
115			1174.5
120		.7041	
130		.6918	

Data For Phase Transitions

Initial	Final	Temp. °C	dt/dP deg mm^{-1}	Pressure mmHg	ΔH kcal mol^{-1}	$d\Delta H/dt$	ΔS	ΔC_p
						cal deg^{-1} mol^{-1}		
c,II	c,I	−127.2±0.5			0.47±0.02	6.5±0.5	3.2±0.2	3.3±0.5
c,I	liq	8.8±0.2			1.06±0.02	31. ±2	4.03±0.1	8.9±2
liq	g	25	0.95	13.6	11.9±0.5		40.0±1.5	
liq	g	102.0±0.3	0.0373	760	9.6±0.4		25.6±1	

Condensed Phase Heat Capacity

State	Temp. °C	C_p
		cal deg^{-1} mol^{-1}
c	−8.8	40.5±2
liq	−8.8	49.4±1
liq	102.0	75.0±1

Properties of the Saturated Real Gas

Temp. °C	$H^r - H^0$	$S^r - S^0$	$C_p^r - C_p^0$
	kcal mol^{-1}	cal deg^{-1} mol^{-1}	

Data for the Standard States at 25 °C

State	Heat of Combustion ΔH_c^0 kcal mol^{-1}	Heat of Formation ΔH_f^0 kcal mol^{-1}	Entropy S^0 cal deg^{-1} mol^{-1}	Gibbs Energy of Formation ΔG_f^0 kcal mol^{-1}	Heat Capacity, C_p cal deg^{-1} mol^{-1}
liq	−789.5±0.2	−90.7±0.2	54.8±0.5	−41.9±0.3	59.2±0.5
g	−801.4±0.5	−78.8±0.5	86.7±1.6	−39.5±0.7	

Critical Constants

Temp. 272. °C, 545. K	Pressure atm	Density g cm^{-3}

Constants in Vapor Pressure and Density Equation

Antoine Equation				Francis Equation				
Temp. Range	*A*	*B*	*C*	Temp. Range	*A*	$B \times 10^3$	*C*	*E*
25 to 102 °C	6.5193	863.4	135.3	0 to 140 °C	1.54925	−0.0407	578.02	800

TABLE 123. 2-Methyl-2-butanol. Selected values. Refractive index at various temperatures and wavelengths

Symbol	Wavelength, Å	Refractive Index, *n*		
		15 °C	20 °C	80 °C
He_{red}	6678.2	1.4050	1.4028	1.3717
H_c	6562.8	1.4053	1.4031	1.3720
Na_D	5892.6	1.4075	1.4050	1.3738
Hg_e	5460.7	1.4093	1.4068	1.3754
He_{blue}	5015.7	1.4116	1.4091	1.3775
H_F	4861.3	1.4125	1.4101	1.3784
Hg_g	4358.3	1.4166	1.4141	1.3820
$H_{G'}$	4340.5	1.4168	1.4143	1.3822

Density

Accurate density values at 20 °C have been published by Cook [1952]; Soehring, Frey and Endres [1955]; Petrov, Sushchinskii, Zakharov, and Rogozhnikova [1957]; and Costello and Bowden [1958]. They are all within about 0.0005 g cm^{-3} of the value calculated from the Francis equation. Density at 25 °C has been measured by Norris and Reuter [1927], Butler, Ramchandani, and Thomson [1935], and Ginnings and Baum [1937] and are within 0.00015 of the selected value. Densities at other temperatures depend largely on the data of Timmermans and Hennaut-Roland (1932) at 0, 15, and 30 °C and of Costello and Bowden in the range of 0 to 180 °C. The only other datum above 30 °C used for evaluating the constants in the Francis equation was that of Schiff [1883] at 101.6 °C.

Vapor Pressure and Boiling Point

There have been several precise measurements of the normal boiling point, which are summarized in table 124. The selected value based on the Antoine equation is 102.0 °C, and the true value is certainly within 0.2 °C of this temperature. Other than about three isolated points, the vapor pressures below 1 atm are based on the measurements of Butler, Ramchandani, and Thomson [1935] and the available heats of vaporization. The calculated vapor pressures fall one or two mm below the values reported by Butler, Ramchandani, and Thomson.

Critical Properties

Brown, J. C. (1906) obtained a critical temperature of 271.77 °C. Critical pressure and density have not been measured.

Solid-Solid Phase Equilibria

Transition Temperature

Parks, Huffman, and Barmore [1933] found a transition from crystal II to crystal I at −127.2 °C in the course of their low temperature heat capacity measurements.

Heat Capacity of the Solid Phases

These were taken from Parks, Huffman, and Barmore [1933].

Heat of Transition

Parks, Huffman, and Barmore [1933] obtained 5.32 cal g^{-1} by measurement in their adiabatic calorimeter.

Solid-Liquid Phase Equilibria

Normal Melting Point

Significant values of the normal melting point in air are listed in table 124. Parks, Huffman, and Barmore [1933] did not clearly state whether their values were

TABLE 124. 2-Methyl-2-butanol. Reported values. Simple physical properties

Investigators		Vapor Pressures and Boiling Points		Freezing Point	Density, *d* g cm^{-3}		Refractive Index, n_D	
		°C	mmHg	t_m, °C	20 °C	25 °C	20 °C	25 °C
2-Methyl-2-butanol, $C_5H_{12}O$, mol wt. 88.151, state at 25 °C liq								
Wischnegradsky	[1878]	102.4	760	−12.5				
Perkin	[1884]	101.5–102.0	760			0.80453		
Thorpe and Rodgers	[1894]	101.81	760					
Louginine	[1898]	101.81	760					
Richard	[1910]	101–103	760	−12				
Atkins and Wallace	[1913]	102.30–102.33	760					
Timmermans	[1913]	102.0	760					
Willcox and Brunel	[1910]	101.7–102.1	760					
Cox	[1921]	102–103	760				1.4042	
Munch	[1926]	101.6	760			.8098		1.4020
Norris and Reuter	[1927]	101.76	760	−11.9		.80475	1.4052	
Norris and Cortese	[1927]							1.4024
Timmermans and Hennaut-Roland	[1932]	102.35	760	−8.55	0.8089		1.4050	
Parks, Huffman, and Barmore	[1933]	102.33–102.35	760	−9.1				
Butler, Ramchandani, and Thomson	[1935]	101.90				.80599	1.40580	
Deffet	[1935]			−8.55				
Ginnings and Baum	[1937]	101.9–102.1	760			.8055		
Owens, Quayle, and Beavers	[1939]					.8018		
Whitmore, Rowland, Wrenn, and Kilmer	[1942]	101.7	760				1.4049	
Braun, Spooner, and Fenske	[1950]						1.4046	
Adkins and Rosenthal	[1950]							1.4061
Huston and Brault	[1950]						1.4020	
Pichler, Ziesecke, and Traeger	[1950]	101.8	760		.8063		1.4047	
Levina, Fainzil'berg, Tantsyreva, and Treshcheva	[1951]						1.4061	
Saunders, Slocombe, and Hardy	[1951]	102–102.5	760					
Cook	[1952]	102.3		−9	.8095		1.4049	
Philpotts and Thain	[1952]						1.4050	
West, Senise, and Burkhalter	[1952]	101.0–101.8	760					
McKenna, Tarter, and Lingafelter	[1953]	101.9	760					1.4018
Urry, Stacey, Huyser, and Juveland	[1954]						1.4052	
Brown and Nakagawa	[1955]	101.5	760				1.4043	
Soehring, Frey, and Endres	[1955]	102–102.5	760		.8089		1.4051	
Petrov, Sushchinskii, Zakharov, and Rogozhnikova	[1957]	100.9–102.4	760		.8087		1.4056	
Costello and Bowden	[1958]	102.6	760	−9.0	0.8084			
Pansevich-Kolyada and Osipenko	[1958]	101.9	760		0.8108		1.4058	
Selected value	[1967]	102.0±0.3 21.0±1	760 10	−8.8 ±0.2	0.8090 ±0.0005	0.8044 ±0.0007	1.4050 ±0.0005	1.4020 ±0.0007

Antoine constants: *A* 6.5193, *B* 363.4, *C* 135.3

dt/*dp* at 760 mmHg, 0.0373 °C/mmHg

obtained in air or in the presence of the vapor phase only. However, the accuracy was not sufficiently high to make this distinction an important one. On the basis of these data, it appears that the melting point is between −8.5 and −9.0 °C. The selected value was a weighted average of these data.

Heat Capacity of the Solid and Liquid at the Melting Point

The only data in this range are those of Parks, Huffman, and Barmore [1933].

Heat of Fusion

Parks, Huffman, and Barmore [1933] have made the only measurements.

Properties of the Liquid at 25 °C

Heat Capacity

Parks, Huffman, and Barmore [1933] measured the liquid heat capacity from 275 to 294 K. Extrapolation of these data up to 25 °C gives 59.1 cal deg^{-1} mol^{-1}. Leech [1949] measured the heat capacity from 40 to 70 °C and expressed his results as a linear function of temperature. His equation gives 59.9 cal deg^{-1} mol^{-1} at 25 °C.

Absolute Entropy

Parks, Huffman, and Barmore [1933] calculated a third law entropy from their experimental heat capacity measurements down to 92 K. They estimated the entropy at 90 K as 11.18 cal deg^{-1} mol^{-1}. This is the only source of entropy data.

Heat of Combustion

Heat of combustion data are listed in table 126. The value of Chao and Rossini [1965] is the only one of significant accuracy, and it was selected.

Properties of the Real Gas

There have been no experimental measurements of gas phase properties.

Vapor-Liquid Equilibrium at 25 °C

Vapor Pressure

The value listed was calculated from the Antoine equation.

Heat of Vaporization

The only calorimetric value is that of McCurdy and Laidler [1963]. Table 125 shows it to be 1.9 kcal mol^{-1} lower than the value calculated from the Antoine constants. However, since the Antoine equation cannot be expected to give an accurate vapor pressure slope at the lower end of the range of vapor pressure data, the selected value was close to the calorimetric one.

TABLE 125. 2-Methyl-2-butanol. Reported values. Heats of vaporization

Investigator	ΔH_v at 25 °C	ΔH_v at t_b	Method and Remarks
Louguinine [1898]		9.31	Mixing calorimeter.
Brown [1905]		10.11	Calorimetric.
McCurdy and Laidler [1963]	11.75	9.52	Calorimetric.
Selected Antoine Constants	13.64		Calculated.

TABLE 126. 2-Methyl-2-butanol. Reported values. Heat of combustion of the liquid at 25 °C

Investigator	$-\Delta H_c^0$(l) kcal mol^{-1}
Louguinine [1880]	788.4
Thomsen [1886]	*798.4
Zubov [1898] (recalculated by Swietoslawski [1920])	785.2
Chao and Rossini [1965]	789.45

* ΔH_c of gas reported, value converted to the liquid.

Vapor-Liquid Equilibrium at the Normal Boiling Point

Normal Boiling Point

This was calculated from the Antoine equation.

Heat of Vaporization

The three values shown in table 125 cover a range of 0.8 kcal mol^{-1}. Since the value based on vapor pressure data should be fairly close to the true value, a compromise close to this value was selected.

Heat Capacity of the Liquid

Leech [1949] has reported the specific heat as a linear function of temperature based on measurements in a conduction calorimeter from 40 to 70 °C. The change in enthalpy calculated from this equation for a temperature change from 20 to 98.5 °C agrees to within 0.2 percent of the measured value reported by Louguinine [1898]. The heat capacity at the boiling point was calculated from the equation of Leech.

Index to the Bibliography

Numbers refer to the Bibliography, page, 1–389.

References to data used in the selection of refractive index, density, boiling point, vapor pressure, and melting point are in boldface type.

Numbers in parentheses refer to sources of reviews, or theoretical calculations only.

Reference numbers under each property are listed in the order of date of publication.

Refractive Index
509, **354**, **1227**, **1273**, **1274**, **1781**, **1262**, **253**, 1112, **1942**, **1893**, 13, **201**, 804, **1377**, **180**, **1049**, 1547, 1388, **383**, 1375, **1152**, **1824**, 226, **1650**, **1365**, 1594, **1310**, 819

Density at 20–30 °C Only
1227, 1262, 1112, **253**, 1337, **598**, 1893, 1377, **338**, 1049, 1650, 1365, 1310, 1147

Density at all Temperatures
1974, **1559**, **1349**, 1560, 1477, 509, **1274**, **1781**, **1300**, **347**

Normal Boiling Point
19070, 1974, 1559, 1560, 1349, 1764, 119, **1083**, 1765, 2033, 1257, 1477, 652, **55**, **1769**, **280**, **1960**, 355, 1859, **1227**, 1009, **1274**, 1940, **1781**, **1323**, 1089, 296, 1582, 598, 1942, 1554, 1606, 1007, 1011, 1876, 1377, 804, 1049, 1311, 1388, 180, 1547, 819, 1902, **338**, **1152**, 1650, 755, **226**, 811, **1823**, 1594, 347, 1148

Vapor Pressure and Boiling Points at Other Pressures
509, 1942, **1262**, **253**, **1824**, 1365, 1310

Critical Temperature
218, (347)

Heat Capacity of the Solid
1323

Normal Melting Point
1970, 1974, 1477, 1769, 1274, 1781, 399, 1378, 347

Heat of Fusion
1323

Heat Capacity of the Liquid
984, 1323, 1011

Calorimetric Heat of Vaporization at 25 °C
1147

Calorimetric Heat of Vaporization at the Normal Boiling Point
1083, 220

Heat of Combustion
1084, 1762, 2033, (1721), 237, 288

Third Law Entropy of the Liquid at 25 °C
1323

Molecular Vibration Frequencies and Spectra
45, 1844, 379

Association in the Liquid Phase
(1755), 713, 1705, 439, 810, 461

3-methyl-2-butanol

Properties of the Liquid Phase at Various Temperatures

Refractive Index

There is only a relatively small amount of experimental data on the properties of 3-methyl-2-butanol. The only values of refractive index which have been directly published are at the sodium D-line and at 20 and 25 °C. The significant values are summarized in table 128. Thomas and Meatyard [1963] report a temperature coefficient, $dn/dt = -0.00042$, based on measurements from 10 to 25 °C.

Density

Densities reported by Pickard and Kenyon [1912], Cook [1952], and Pichler, Ziesecke, and Traeger [1950] are within 0.0004 g cm^{-3} of the selected value. Ginnings and Baum [1937] found the density to be 0.8134 g cm^{-3} at 25 °C, and McCurdy and Laidler obtained 0.8150 g cm^{-3}. Data at other temperatures which were used in fitting the Francis equation were from Pickard and Kenyon [1921] at 15.8, 51 and 71 °C and Thomas and Meatyard [1963] from 29.4 to 105 °C. Winogradow [1878] reported 0.8308 at 0 °C, but this was not used in fitting the equation. A few other scattered values identified in the Index to the Bibliography of uncertain reliability have been published.

Vapor Pressure and Boiling Point

No high accuracy measurements of the normal boiling point have been reported. The best available data are listed in table 128, and these scatter over about a three degree range. The Antoine equation used to calculate the selected boiling points and vapor pressures is based on these measurements, the vapor pressure data of Thomas and Meatyard, and two values of the heat of vaporization.

Critical Properties

There are no experimental data.

Solid-Liquid Phase Equilibria

Normal Melting Point

Cook [1952] found that 3-methyl-2-butanol formed a glass in the range from −100 to −85 °C.

TABLE 127. 3-Methyl-2-Butanol. Selected values. Physical and thermodynamic properties

Temp. °C	Refractive Index, n_D	Density g cm^{-3}	Vapor Pressure, mmHg
10		0.826	
20	1.4096	.8179	
25	1.4075	.8137	8.97
26.0			10
30		.8095	13.0
35			18.4
40		.8007	25.6
45			35.1
50		.7916	47.4
55			63.1
60		.7821	82.8
63.6			100
65			107.5
70		.7722	137.9
75			174.9
77.9			200
80		.7619	219.8
85			273.5
90		.7512	337.3
94.2			400
95			412.7
100		.7400	500.9
105			603.4
110		.7283	722.0
111.5			760
115			858.1
120			1013.6

Data For Phase Transitions

Initial	Final	Temp. °C	dt/dP deg mm^{-1}	Pressure mmHg	ΔH kcal mol^{-1}	$d\Delta H/dt$	ΔS	ΔC_p
						cal deg^{-1} mol^{-1}		
liq	g	25	1.47	9.0±0.3	12.4±0.3		41.6±1	
liq	g	111.5±0.7	0.0378	760	9.9±0.4		25.7±1	

Condensed Phase Heat Capacity

State	Temp. °C	C_p
		cal deg^{-1} mol^{-1}

Properties of the Saturated Real Gas

Temp. °C	H^r-H^0	S^r-S^0	$C_p{}^r-C_p{}^0$
	kcal mol^{-1}	cal deg^{-1} mol^{-1}	

Data for the Standard States at 25 °C

State	Heat of Combustion $\Delta H_c{}^0$ kcal mol^{-1}	Heat of Formation $\Delta H_f{}^0$ kcal mol^{-1}	Entropy S^0 cal deg^{-1} mol^{-1}	Gibbs Energy of Formation $\Delta G_f{}^0$ kcal mol^{-1}	Heat Capacity, C_p cal deg^{-1} mol^{-1}
liq	−792.5±0.2	−87.5±0.2			55.5±2
g	−804.9±0.3	−75.1±0.3			

Critical Constants

Temp. °C, K	Pressure atm	Density g cm^{-3}

Constants in Vapor Pressure and Density Equation

Antoine Equation

Temp. Range	A	B	C
25 to 111 °C	6.9421	1090.9	157.2

Francis Equation

Temp. Range	A	$B\times10^3$	C	E
15 to 105 °C	1.56856	−0.2865	514.33	700

TABLE 128. 3-Methyl-2-butanol. Reported values. Simple physical properties

Investigators	Vapor Pressures and Boiling Points		Freezing Point	Density, d g cm^{-3}		Refractive Index, n_D	
	°C	mmHg	t_m, °C	20 °C	25 °C	20 °C	25 °C
3-Methyl-2-butanol. Reported values. Simple physical properties							
Picard and Kenyon [1912]				0.8180		1.3973	
Willcox and Brunel [1916]	112.9–113.9	760					
Stevens [1932]	112.6–112.8	760				1.4093	
Kohlrausch and Koppl [1933]	111.9–112.1	760					
Ginnings and Baum [1937]	111.1–111.9	760			0.8134		
Karantz and Whitmore [1938]	112.5	760				1.4096	
Whitmore and Johnston [1938]	111–112	760		.818		1.4090	
Baker and Adkins [1940]	111.8	760					1.4071
Mosher [1940]	112.7	760				1.4092	
Whitmore, Whitaker, Mosher, Brevik, Wheeler, Miner, Sutherland, Wagner, Clapper, Lewis, Lux, and Popkin [1941]	111–114	760				1.4085–1.4098	
McMahon, Roper, Utermohler, Hasek, Harris, and Brant [1948]	111–115	760			.8116	1.4098	
Pichler, Ziesecke, and Traeger [1950]	113–114	760		.8182		1.402	
Cook [1952]	111.8			.8175		1.4097	
Winstein and Ingraham [1952]	111.8–111.9	760					
McKenna, Tartar, and Lingafelter [1953]	112.4						1.4076
Zeiss and Tsutsui [1953]	111–112	760					1.4069
Brown and Subba Rao [1959]	110.2–111.2	760				1.4091	
Thomas and Meatyard [1963]	111.4	760			.815	1.4093	
Selected value [1967]	111.5±0.7 26.0±1	760 10		.8179 ±0.0007	.8137 ±0.0007	1.4096 ±0.0005	1.4075 ±0.0007

Antoine constants: A 6.9421, B 1090.9, C 157.2

dt/dp at 760 mmHg, 0.0378 °C/mmHg

Properties of the Liquid at 25 °C

Heat Capacity

There are no directly measured heat capacity data at 25 °C. Louguinine [1898] has measured the enthalpy change from 21.7 to 128 °C in a mixing calorimeter. He has also made similar measurements for two other isomeric pentanols. If these data are compared with the selected heat capacities at 25 °C for the other pentanols, a value of 55.5 cal deg^{-1} mol^{-1} can be predicted for 3-methyl-2-butanol.

Heat of Combustion

The only heat of combustion measurement has been made by Chao and Rossini [1965].

Properties of the Real Gas

No gas phase properties have been measured.

Vapor-Liquid Equilibrium at 25 °C

Vapor Pressure

This was calculated from the Antoine equation.

Heat of Vaporization

McCurdy and Laidler [1963] obtained 12.35 kcal mol^{-1} by microcalorimetry. The Antoine constants gave 13.35 kcal mol^{-1}. The calorimetric value was selected.

Vapor-Liquid Equilibrium at the Normal Boiling Point

Normal Boiling Point

This was calculated from the Antoine equation.

Heat of Vaporization

Louguinine [1898] obtained 10.02 kcal mol^{-1} with a mixing calorimeter. The selected Antoine constants gave 9.88 kcal mol^{-1}, with the second virial coefficient estimated at −1.1 liter mol^{-1}. Considering the possible sources of error in both values, this is a good agreement.

Index to the Bibliography

Numbers refer to the Bibliography, page 1–389.

References to data used in the selection of refractive index, density, boiling point, vapor pressure, and melting point are in boldface type.

Numbers in parentheses refer to sources of reviews, or theoretical calculations only.

Reference numbers under each property are listed in the order of date of publication.

Refractive Index
1380, 1690, 874, 1922, 71, 1209, 1155, 804, 1377, **338, 1152, 2016**, 1594, **232, 1758**

Density at 20–30 °C
1228, 1974, **1380**, 1691, **598**, 1922, 1155, 1377, **338, 1758**, 1147

Density at all Temperatures
1970

Normal Boiling Point
1228, 1974, 1970, **1960**, 1409, 1007, 621, **1690**, 448, 921, **598**, 1922, **874**, 1209, 71, 1947, 1554, 1155, 506, 1377, 804, 194, 1973, **338**, 127, 2016, **1152**, 1594, 1193

Vapor Pressure and Boiling Points at Other Pressures
1922, 1267, 232, 1758

Normal Melting Point
338

Calorimetric Heat of Vaporization at 25 °C
1147

Calorimetric Heat of Vaporization at the Normal Boiling Point
1083

Heat of Combustion
287, 288

Association in the Liquid Phase
1705

2,2-Dimethyl-1-propanol

Properties of the Liquid Phase at Various Temperatures

Refractive Index and Density

Since 2,2-dimethyl-1-propanol (neopentyl alcohol) melts at 52 °C, there are very few data on the liquid phase below this temperature. Whitmore, Whitaker, Mosher, Breivik, Wheeler, Miner, Sutherland, Wagner, Clapper, Lewis, Lux, and Popkin [1941] report $n_D = 1.3950$ at 20 °C, and Pichler, Ziesecke, and Traeger [1950] report $n_D = 1.4080$ at 20 °C. Very little explanation was given in these sources. If these actually applied to 2,2-dimethyl-1-propanol, they must refer to the undercooled liquid. No values of refractive index or density above the melting point have been located.

Vapor Pressure and Boiling Point

Only very approximate boiling point data have been published. Table 130 lists those values which seem to be most reliable. The value calculated from the Antoine equation is 113.1 °C, but the uncertainty is at least one degree. Scattered boiling point measurements at lower pressures have been reported by Richard [1910]; Greenwood, Whitmore, and Crooks [1938]; Whitmore, Meyer, Pedlow, and Popkin [1938]; Whitmore [1938]; Gerrard, Nechvatal, and Wilson [1950]; Sommer, Blankman, and Miller [1954]; and Criegee and Schröder [1960]. The Antoine constants were adjusted to give the best fit among these data. The result can be considered only as approximate.

Critical Properties

There have been no experimental measurements.

Solid-Liquid Phase Equilibria

Normal Melting Point

There is a relatively large number of melting points reported in the literature. This is largely because it melts at a more convenient temperature than most of the other alcohols. Values from references listed in the Index to the Bibliography range from 44 to 56 °C. A selection of some of the better ones is given in table 130. This poor agreement reflects the difficulty of preparing pure samples. McKenna, Tartar, and Lingafelter [1933] and Hoffman and Boord [1955] seemed to have spent some effort in purifying their samples, although their melting points differ by three degrees. The selected value is close to that of Hoffman and Boord, but the uncertainty is at least two degrees.

TABLE 129. Selected values. 2,2-Dimethyl-1-propanol. Vapor pressure of the liquid

Temperature °C	Vapor Pressure mmHg	Antoine Constants
55	60.0	*A* 7.8753
60	78.0	*B* 1604.7
65	100.4	*C* 208.2
70	128.0	
75	161.8	
80	202.9	
85	252.	
90	312.	
95	383.	
96.	400	
100	466.	
105	565.	
110	680.	
113.1	760	
115	813.	
120	968.	
125	1146.	

TABLE 130. 2,2-Dimethyl-1-propanol. Reported values. Simple physical properties

Investigators		Vapor Pressures and Boiling Points		Freezing Point	Density, *d* g cm^{-3}		Refractive Index, n_D	
		°C	mmHg	t_m, °C	20 °C	25 °C	20 °C	25 °C
2,2-Dimethyl-1-propanol, $C_5H_{12}O$, mol wt. 88.151, state at 25 °C *c*								
Samec	[1907]	113	760	48				
Richard	[1910]	113–115	760	50				
Franke and Hinterberger	[1923]	112–113	760					
Conant, Webb, and Mendum	[1929]	112–114	760	47–49				
Kohlrausch and Koppl	[1933]	112.2–113.8	760					
Ginnings and Baum	[1937]	113.0–114.0	760	48–49				
Whitmore	[1938]			50				
Cook and Percival	[1949]	112	760	50				
Pichler, Ziesecke, and Traeger	[1950]	112–113	760	48				
Bradley, Mehrotra, and Wardlaw	[1952]	113.7	760					
McKenna, Tartar, and Lingafelter	[1953]			51.8				
Sokolova	[1953]	112–114						
Sommer, Blankman, and Miller	[1954]			51–52				
Hoffman and Boord	[1955]			54.5–55.5				
Kornblum and Iffland	[1955]	110–111	760	55–56				
Searles, Pollart, and Lutz	[1959]	110–111	760	52				
Pillai and Pines	[1961]	112–114						
Lawesson and Lang	[1959]	113–115		44				
Selected value	[1967]	113.1±0.5	760	54±1				

Antoine constants: *A* 7.8753, *B* 1604.7, *C* 208.2

dt/dp at 760 mmHg, °C/mmHg 0.0368

Heats of Vaporization

No other thermodynamic properties have been measured. The heat of vaporization calculated from the Antoine constants at 25 °C is 12.0 kcal mol^{-1}, which refers to the undercooled liquid. Similarly, at the normal boiling point a value of 10.3 kcal mol^{-1} was obtained. Because of the uncertainty in the vapor pressure data, little reliance can be placed on these results.

Index to the Bibliography

Numbers refer to the Bibliography, page 1–389.

References to data used in the selection of refractive index, density, boiling point, vapor pressure, and melting point are in boldface type.

Numbers in parentheses refer to sources of reviews, or theoretical calculations only.

Reference numbers under each property are listed in the order of date of publication.

Refractive Index
1947, 1377

Normal Boiling Point
1788, 1534, **557**, 332, 921, **598**, 367, 1476, 1842, 902, 1554, **10**, 339, **1377**, **194**, 181, 1652, 1658, 945, 767, 1539, 1594, 181, 1003, 1148, 1385

Vapor Pressure and Boiling Points at Other Pressures
1477, 632, **1934**, 1947, 1939, 1910, **590**, **1658**, 362

Normal Melting Point
1534, 1477, 332, **1940**, 598, **1934**, 367, **632**, 1476, 1910, 902, 1554, 339, 590, 1377, 2016, **1152**, 1658, **767**, 945, 1539, 1594, 1003, 280

1-Hexanol

Properties of the Liquid Phase at Various Temperatures

Refractive Index

Data on refractive index scatter rather widely. For example, values of n_D at 20 °C reported in the references listed in the Index to the Bibliography range from 1.413 to 1.421 and at 25 °C from 1.413 to 1.418. A selection of the most reliable data is shown in table 134 and was used to arrive at the final selections for these two temperatures. This situation probably reflects the difficulty of obtaining pure samples, which is the usual situation for the higher alcohols. A few measurements have been made at other temperatures and wavelengths. Values of n_D from 13.5 to 30 °C have been reported by Hovorka, Lankelma, and Stanford [1938], Weissler [1948], Bonauguri, Bicelli, and Spiller [1951], and Colonge and Falcotet [1957]. Bilterys and Gisseleire [1935] have reported values at various wavelengths at 15 °C, and Vogel [1948] has reported values at a few wavelengths other than the Na$_D$ line at 20 °C. Vogel's value of n_D agrees well with the selected value, and the data in table 133 were taken from a smooth curve drawn through his data at 20 °C. The values at 15 °C were taken from a parallel curve which passed through the selected value of n_D at 15 °C. These were about 0.0008 higher than the data of Bilterys and Gisseleire.

Density

The literature on density is fairly extensive. Accurate measurements at 20 and 25 °C have been made by Ellis and Reid [1932], Butler, Thomson, and Maclennan [1933], Mumford and Phillips [1950], and Cook [1952]. The selected values as calculated from the Francis equation are within 0.0004 g cm^{-3} of these. Lieben and Janecek [1877] measured the density from 0 to 40 °C. Although these data were not considered in the selection, they were surprisingly close to the final values based on more modern data. Measurements over an extended range of temperatures have been published by Carrara and Ferrari [1906], 25 to 86 °C; Hovorka, Lankelma, and Stanford [1938], 5 to 159 °C; and Costello and Bowden [1958], −20 to 240 °C. Bilterys and Gisseleire [1935] made accurate measurements from 0 to 30 °C, and McKinney, Skinner, and Staveley [1959] obtained an accurate value at 0 °C. The data of Carrara and Ferrari above 40 °C were decidedly low and were omitted from the calculation. The final selected values ran about 0.0005 g cm^{-3} above those of Hovorka, Lankelma, and Stanford within their range of temperature, and about 0.0020 to 0.0025 below those of Costello and Bowden. The data used in the curve fitting calculation were terminated at about 160 °C, even though Costello and Bowden reported values at higher temperatures. Sackmann and Sauerwald [1950] reported a density of 0.8698 g cm^{-1} at −50.5 °C. Efremov [1966] reported densities having a lower order of accuracy from 20 to 337 °C.

Vapor Pressure and Boiling Point

A selection of boiling point data is presented in table 134. The better values range from about 157.0 to 157.5 °C, although few of these can be regarded as resulting from high precision measurements. The average is a little higher than the value of 157.0 °C calculated from the selected Antoine constants. Vapor pressures below one atmosphere depend primarily on the work of Butler, Ramchandani, and Thomson [1935], who covered the range from 60 to 153 °C; Hovorka, Lankelma, and Stanford [1938], from 35 to 160 °C; and Rose and Supina [1961], from 60 to 108 °C. The selected Antoine constants were based on these data plus a few scattered boiling points at various pressures. The most accurate set of data was from Rose and Supina, and these were given the greatest weight in the curve fit. Except for the value at 108 °C which is 1.3 mmHg low, the calculated vapor pressures are within about 0.5 mmHg of their observed ones. The vapor pressures of Butler, Ramchandani, and Thomson are close to those of Rose and Supina's at the low temperature end but become about 3 mmHg higher at the high temperature end of their range. Hovorka, Lankelma, and Stanford's values run 1 to 2 mm high in this same range.

Critical Properties

Critical Temperature and Density

Efremov [1966] has made the only measurements. He used a "chemically pure" grade and determined the critical temperature by observing the disappearance of the meniscus. His results were selected.

Solid-Liquid Phase Equilibria

Normal Melting Point

The observed melting points listed in table 134 scatter over a wide range of temperature. This situation undoubtedly reflects the effect of impurities, as well as the usual difficulty in obtaining sharp melting points for the higher alcohols. In such cases the higher values are usually more likely to be correct, and therefore the selected melting point was close to the one obtained in the laboratories of the Union Carbide Chemicals Company.

TABLE 131. 1-Hexanol. Selected values. Physical and thermodynamic properties

Temp. °C	Refractive Index, n_D	Density g cm^{-3}	Vapor Pressure, mmHg
−20		0.8468	
−10		.8403	
0		.8336	
10		.8267	
15	1.4201		
20	1.4181	.8198	
25	1.4161	.8162	
30	1.4141	.8127	
40		.8054	2.6
50		.7979	5.2
60		.7903	10.0
60.1			10
65			13.5
70		.7826	18.0
75			23.8
80		.7746	31.2
85			40.5
90		.7664	52.0
95			66.3
100		.7581	83.8
103.9			100
105			105.2
110		.7407	131.0
115			161.9
120		.7316	198.8
120.2			200
125			242.6
130			294.3
135			354.9
138.3			400
140			425.5
145			507.5
150			602.3
155			711.3
157.0			760
160			810.
165			978.

Data For Phase Transitions

Initial	Final	Temp. °C	dt/dP deg mm^{-1}	Pressure mmHg	ΔH kcal mol^{-1}	$d\Delta H/dt$	ΔS	ΔC_p
						cal deg^{-1} mol^{-1}		
c	liq	−44.0±1		760	3.68±0.05	28.0±0.5	16.0±0.2	12.0±0.5
liq	g	25	15.	0.8±0.2	14.8±0.2	−19.5±0.8	49.6±0.6	−19.4±0.7
liq	g	157.0±0.5	0.0406	760	11.6±0.4		27.0±1	

Condensed Phase Heat Capacity

State	Temp. °C	C_p
		cal deg^{-1} mol^{-1}
c	−44.0	34.5±0.3
liq	−44.0	46.5±0.3

Properties of the Saturated Real Gas

Temp. °C	$H^r - H^0$	$S^r - S^0$	$C_p{}^r - C_p{}^0$
	kcal mol^{-1}	cal deg^{-1} mol^{-1}	
25	0.0	0.0	0.0

Data for the Standard States at 25 °C

State	Heat of Combustion $\Delta H_c{}^0$ kcal mol^{-1}	Heat of Formation $\Delta H_f{}^0$ kcal mol^{-1}	Entropy S^0 cal deg^{-1} mol^{-1}	Gibbs Energy of Formation $\Delta G_f{}^0$ kcal mol^{-1}	Heat Capacity, C_p cal deg^{-1} mol^{-1}
liq	−951.9±0.3	−90.7±0.3	69.2±1	−36.4±0.4	56.6±0.5
g	−966.7±0.3	−75.9±0.3	105.5±0.6	−32.4±0.4	37.2±0.5

Critical Constants

Temp. 337. °C, 610. K	Pressure atm	Density 0.268 g cm^{-3}

Constants in Vapor Pressure and Density Equation

Antoine Equation				Francis Equation				
Temp. Range	A	B	C	Temp. Range	A	$B \times 10^3$	C	E
35 to 157 °C	7.86045	1761.26	196.66	−20 to 159 °C	1.16584	0.2013	232.59	700

TABLE 132. 1-Hexanol. Selected values. Thermodynamic functions of the ideal gas at one atmosphere

Temperature K	Entropy S^0 cal deg^{-1} mol^{-1}	Heat Capacity C_p^0 cal deg^{-1} mol^{-1}	Enthalpy Function $(H^0-H^0_0)/T$ cal deg^{-1} mol^{-1}	Gibbs Energy Function $(G^0-H^0_0)/T$ cal deg^{-1} mol^{-1}	Heat of Formation ΔHf^0 kcal mol^{-1}	Gibbs Energy of Formation ΔGf^0 kcal mol^{-1}
0	0	0	0	0	−66.5	−66.5
273.15	102.41	35.00	23.40	−79.01	−75.2	−36.1
298.15	105.52	37.23	24.47	−81.05	−75.9	−32.4
300	105.73	37.41	24.54	−81.19	−76.0	−32.2
400	117.67	46.68	28.92	−88.75	−78.4	−17.2
500	129.00	55.26	33.35	−95.65	−80.5	−1.6
600	139.67	62.58	37.61	−102.06	−82.2	14.4
700	149.77	68.87	41.61	−108.16	−83.5	30.6
800	159.32	74.25	45.38	−113.96	−84.4	46.9
900	168.33	78.90	48.86	−119.47	−85.0	63.4
1000	176.87	82.92	52.06	−124.81	−85.4	79.9

TABLE 133. 1-Hexanol. Selected values. Refractive index at various temperatures and wavelengths

Symbol	Wavelength, Å	Refractive Index, n	
		15 °C	20 °C
He_{red}	6678.2	1.4178	1.4157
H_c	6562.8	1.4181	1.4160
Na_D	5892.6	1.4201	1.4181
Hg_e	5460.7	1.4219	1.4199
He_{blue}	5015.7	1.4242	1.4222
H_F	4861.3	1.4252	1.4232
Hg_g	4358.3	1.4294	1.4274
$H_{G'}$	4340.5	1.4296	1.4276

Heat of Fusion

Kelley [1929a] has made the only measurement of heat of fusion, and this was selected. His heat capacity data were extrapolated to obtain the heat capacity of the solid and liquid at the melting point.

Properties of the Liquid at 25 °C

Absolute Entropy

Kelley [1929a] reported the entropy of the liquid at 25 °C as 68.6 cal deg^{-1} mol^{-1} as obtained from a third-law calculation based on his observed heat capacity data down to 18 K. This is 0.6 cal deg^{-1} mol^{-1} lower than the result obtained by converting the selected ideal gas entropy to the liquid. Considering the uncertainties inherent in both procedures, this is about as close an agreement as could be expected. The entropy was selected so as to be consistent with the ideal gas value.

Heat Capacity

The only heat capacity data are those of Kelley [1929a]. His values were extrapolated to 25 °C.

Heat of Combustion

Two directly measured values are available. When converted to modern units and standard conditions, Verkade and Coops [1927] found it to be −951.54 kcal mol^{-1}. Chao and Rossini [1965] obtained −951.90 kcal mol^{-1}, which is within the combined experimental uncertainties.

Vapor-Liquid Equilibrium at 25 °C

Vapor Pressure

This was calculated from the selected Antoine constants and is thus obtained from an extrapolation of 10 °C below the lowest experimental measurement.

Heat of Vaporization

Wadso [1966] obtained 14.73 kcal mol^{-1} by direct calorimetry. This should be fairly accurate, although 14.8 kcal mol^{-1} was selected to reduce slightly the discrepancy between the third law entropy and the selected entropy for the ideal gas. The selected Antoine constants predict $\Delta H_v = 14.56$ kcal mol^{-1} at 25 °C. Butler, Ramchandani, and Thomson [1935] calculated 15.02 kcal mol^{-1} from their vapor pressure data.

Temperature Derivative of the Heat of Vaporization

The vapor should be very nearly ideal at the saturation pressure, and therefore $d\Delta H/dT$ can be taken as nearly equal to the difference between the heat capacity of the ideal gas and the liquid.

Vapor-Liquid Equilibrium at the Normal Boiling Point

Normal Boiling Point

This was calculated from the selected Antoine constants.

TABLE 134. 1-Hexanol. Reported values. Simple physical properties

Investigators		Vapor Pressures and Boiling Points		Freezing Point	Density, d g cm^{-3}		Refractive Index, n_D	
		°C	mmHg	t_m, °C	20 °C	25 °C	20 °C	25 °C
1-Hexanol, $C_6H_{14}O$, mol wt. 102.178, state at 25 °C liq								
Carrara and Ferrari	[1906]	158.0	760			0.8152		
Willcox and Brunel	[1916]	155.2–155.7	760					
Timmermans	[1922a]	155.8	760	−51.6				
Wood and Comley	[1924]	157.0	760					
Lecat	[1927]	157.8	760					
Norris and Cortese	[1927]	157.6–157.7	760			.8153		1.4162
Verkade and Coops	[1927]	157.5	760					
Kelley	[1929a]	157.0–157.1	760	−47.4		.8156		
Malone and Reid	[1929]	156.2	760					
Walbaum and Rosenthal	[1930]						1.41755	
Ellis and Reid	[1932]	156.5	760			.81581		1.4161
Butler, Thomson, and Maclennan	[1933]	155.7	760			.81648	1.41778	
Bilterys and Gisseleire	[1935]	157.47	760	−46.1		.81547	1.4176	
Butler, Ramchandani, and Thomson	[1935]					.81835	1.41827	
Hovorka, Lankelma, and Stanford	[1938]	157.04	760			.81556		1.4158
Goldwasser and Taylor	[1939]	156.4	760		0.8189		1.4161	
Komarewsky and Coley	[1941a]	155.0–156 0	760					
Komarewsky and Coley	[1941b]							1.4170
Addison	[1945]						1.4182	
Jones, Bowden, Yarnold, and Jones	[1948]					.8124		
Vogel	[1948]	156.5	760				1.41816	
Tschamler, Richter, and Wettig	[1949b]	155.7	760					
Gorin	[1950]						1.4172	
Mumford and Phillips	[1950]	156.6	760		.8198	.8164	1.4174	
Pichler, Ziesecke, and Traeger	[1950]	157.0	760		.8191		1.4178	
Sackmann and Sauerwald	[1950]			−50.5				
Winsor	[1950]						1.4185	
Ziegler and Gellert	[1950]			−47.2				
Bonauguri, Bicelli, and Spiller	[1951]	157.8	760				1.42166	
Cook	[1952]	157.3	760	−46	.8195		1.4171	
von Erichsen	[1952]	156.9–157.0	760		.8191		1.8184	
Staveley and Spice	[1952]	157.12	760		.8191			
Timmermans	[1952]			−46.7				
McKenna, Tartar, and Lingafelter	[1953]	157.4	760					1.4150
Union Carbide Corporation	[1953]	157.1	760	−44.6	.8188			
Costello and Bowden	[1958]	157.5	760		0.8217			
Lin and Tuan	[1958]	154.5–155.5	760			0.81876		1.4159
Brown and Smith	[1962b]	157.5	760			.81531		1.41607
Selected value	[1967]	157.0±0.5	760	−44.0	.8198	.8162	1.4181	1.4161
		60.1±0.5	10	±1	±0.0003	±0.0005	±0.0005	±0.0005

Antoine constants: *A* 7.86045, *B* 1761.26, *C* 196.66

dt/dp at 760 mmHg, 0.0406 °C/mmHg

Heat of Vaporization

There are no calorimetric measurements. The Antoine constants predict 11.57 kcal mol^{-1} when the second virial coefficient is taken to be −1 liter mol^{-1}. This is the selected value. Hovorka, Lankelma, and Stanford [1938] calculated a heat of vaporization of 12.10 kcal mol^{-1} from the slope of their vapor pressure data at the boiling point.

Since no heat capacity measurements have been made above 25 °C, it is not possible to calculate the temperature derivative of the heat of vaporization at the normal boiling point nor to test the vapor-liquid equilibrium data for internal consistency by carrying out a cycle between 25 °C and the boiling point.

Properties of the Ideal Gas State

Ideal gas thermodynamic functions have been published by Chermin [1961] and Green [1961]. Both sets of tables were obtained by adding the methylene increment, as derived from the normal alkanes, to data for the lower alcohols. Additional details are discussed in the section on 1-pentanol. The two sets of tables give heat capacity and entropy within 0.2 cal deg^{-1} mol^{-1} of each other at 298.15 K and within 1 cal deg^{-1} mol^{-1} throughout the range from 298 to 1000 K. Green's values were selected.

Index to the Bibliography

Numbers refer to the Bibliography, page 1–389.

References to data used in the selection of refractive index, density, boiling point, vapor pressure, and melting point are in boldface type.

Numbers in parentheses refer to sources of reviews, or theoretical calculations only.

Reference numbers under each property are listed in the order of date of publication.

Refractive Index
123, **1273**, 1113, **1874**, **486**, **252**, **146**, **253**, **789**, 613, **926**, **927**, 1222, **6**, 7, **1856**, **1893**, 13, 617, **1224**, **1377**, **1971**, **180**, **338**, **1865**, 1152, 943, 327, **1067**, 999, 1188, **231**, 165

Density at 20–30 °C Only
123, **1273**, **885**, 1113, **486**, **254**, **253**, **789**, **613**, 6, **853**, 981, **1377**, **1224**, 1682, 1865, **338**, 1252, 1823, 327, **1067**, **231**, 165, 481

Density at all Temperatures
1059, 562, **2012**, **273**, **1848**, **1874**, **146**, 173, 1893, **1856**, 1527, **617**, **347**, **1154**

Normal Boiling Point
1504, 1059, 562, 2012, 1216, 273, 2018, 1960, 123, 1896, 1774, 1850, **1981**, **1273**, **1848**, 1008, 1121, **885**, **1007**, **146**, 1287, 525, 1978, 613, 450, 799, 926, 6, 1554, 349, 981, 1856, 1807, 195, 617, **1377**, 1224, 752, 180, 1902, **1682**, 323, **338**, 1152, 1249, 1823, 473, 1067, **347**, 327, 232, 1188, 231, 1852, 165

Vapor Pressure and Boiling Points at Other Pressures
1874, **486**, 254, **253**, **789**, **173**, **174**, 7, 1823, **943**, **1499**

Critical Temperature
347, 481

Critical Volume and Density
481

Normal Melting Point
1774, **885**, **146**, 1807, **2027**, 1527, 338, **1777**, **1823**, 165

Heat of Fusion
885

Heat Capacity of the Liquid
885

Calorimetric Heat of Vaporization at 25 °C
1870

Heat of Combustion
1848, (1507), (626), 287, 288
Third Law Entropy of the Liquid at 25 °C
885

Molecular Vibration Frequencies and Spectra
93, 619, 46, 1012, 456, 530, 797

Thermodynamic Functions of the Ideal Gas
623, 291

Association in the Liquid Phase
1115, 1104, 1105, 78, 1683, 182, 530, 1383, 1114

Isomeric Hexanols

Refractive Index

A list of the most significant observed values of n_D at 20 and 25 °C and their sources is given in the unnumbered tables on the following pages for the isomeric hexanols other than 1-hexanol. Where more than one observation has been reported, the selected values are shown at the end of the table for each individual compound. A complete list of sources of refractive index data is given in the Index to the Bibliography for the isomeric hexanols on page 1–176. Smoothed selected values of the refractive index over a wider range of temperatures have been listed in numbered tables for those compounds for which the measurements have been reported.

The principal reasons for discrepancies among observed refractive indices, as well as other physical properties, of the higher alcohols are the presence of impurities in the samples. While it is impractical to discuss the reasons for selecting particular values of each property for each compound, in general the greatest weight was given to those data which were accompanied by the best evidence of sample purity. Also, data which resulted from systematic studies of physical properties of one or more compounds were favored over data from isolated measurements or which were incidental to some other type of investigation.

Among the hexanols the bulk of the accurate data on the simple physical properties has been produced by Hovorka and his co-workers in the decade following 1933. They measured refractive index from around room temperature up to 45 °C and sometimes higher for most of the isomeric hexanols. They also measured density, vapor pressure, viscosity, and surface tension from room temperature up to or near the boiling point. These data were used to calculate the parachor and other additive properties for this series of compounds. Except for 3-methyl-3-pentanol which is discussed below, their data were usually given the greatest consideration in the selections. Their values generally were close to careful measurements reported by other investigators. Other sources of reliable data at 20 and 25 °C are Ellis and Reid [1932], Norton and Hass [1936], Ginnings and Webb [1938], Howard, Mears, Fookson, Pomerantz, and Brooks [1947], Pichler, Ziesecke, and Traeger [1950], and Cook [1952]. There are very few data outside this temperature range, other than those reported by Hovorka et al.

TABLE 135. Isomeric Hexanols. Selected values. Physical properties of the liquid

2-Hexanol				3-Hexanol				2-Methyl-1-pentanol			
Temp. °C	Refractive Index, n_D	Density g cm^{-3}	Vapor Pressure, mmHg	Temp. °C	Refractive Index, n_D	Density g cm^{-3}	Vapor Pressure, mmHg	Temp. °C	Refractive Index, n_D	Density g cm^{-3}	Vapor Pressure, mmHg
0		0.8295		0		0.8347		0		0.8382	
10		.8220		10		.8267		10		.8313	
15	1.4167			15	1.4180			15	1.4208		
20	1.4147	.8144		20	1.4160	.8185		20	1.4190	.8242	
25	1.4128	.8105		25	1.4140	.8144	5.1	25	1.4172	.8206	1.8
30	1.4106	.8065	3.7	30	1.4117	.8101	7.0	30	1.4151	.8169	2.6
40	1.4061	.7984	7.4	35			9.4	40	1.4120	.8094	5.1
44.7			10	36			10	50	1.4069	.8016	9.7
45			10.2	40	1.4068	.8016	12.5	50.5			10
50	1.4015	.7901	13.8	45			16.5	55			13.1
55			18.6	50	1.4017	.7928	21.5	60		.7937	17.5
60		.7815	24.7	55			27.9	65			23.2
65			32.5	60		.7838	36.0	70		.7855	30.3
70		.7727	42.3	65			46.0	75			39.3
75			54.6	70		.7746	58.3	80		.7770	50.5
80		.7636	69.8	75			73.4	85			64.4
85			88.5	80		.7651	91.9	90		.7684	81.3
87.7			100	81.9			100	94.6			100
90		.7542	111.3	85			114.2	95			102.0
95			138.9	90		.7554	141.2	100		.7594	127.0
100		.7445	172.0	95			173.5	105			156.9
103.6			200	98.5			200	110		.7502	192.7
105			211.7	100		.7454	212.0	110.9			200
110		.7344	258.7	105			257.6	115			235.1
115			314.3	110		.7532	311.5	120		.7407	285.1
120		.7240	379.4	115			374.8	125			343.8
121.4			400	116.8			400	129.2			400
125			455.5	120		.7246	448.8	130		.7309	412.3
130		.7133	543.8	125			535.0	135			491.7
135			645.9	130		.7137	634.8	140		.7208	583.6
139.9			760	135			750.2	145			689.2
140		.7021	763.3	135.4			760	148.0			760
145			897.8	140		.7025	883.0	150			810.2
				145			1034.	155			946.2

2-Hexanol						3-Hexanol						2-Methyl-1-pentanol					
Constants	Temp. Range	A	B	C	E	Constants	Temp Range	A	B	C	E	Constants	Temp. Range	A	B	C	E
Antoine eq	28 to 142 °C	7.80733	1696.19	204.43		Antoine eq	25 to 138 °C	8.66522	2340.10	296.16		Antoine eq	25 to 150 °C	7.86701	1775.12	208.00	
Francis eq	0 to 140 °C	1.46575	1.645×10^{-4}	205.66	600	Francis eq	0 to 135 °C	1.13170	2.993×10^{-4}	178.17	600	Francis eq	5 to 150 °C	1.46575	-0.778×10^{-4}	517.38	824.5

TABLE 136. Isomeric Hexanols. Selected values. Physical properties of the liquid

3-Methyl-1-pentanol			
Temp. °C	Refractive Index, n_D	Density g cm^{-3}	Vapor Pressure, mmHg
0		0.8372	
10		.8305	
15	1.4212		
20	1.4193	.8237	1.0
25	1.4175	.8202	1.6
30	1.4152	.8167	3.4
40	1.4116	.8095	6.8
50		.8020	9.5
55.9			10
60		.7943	12.9
65			17.5
70		.7864	23.3
75			30.7
80		.7782	40.1
85			51.8
90		.7697	66.2
95			83.9
98.8			100
100		.7610	105.4
105			131.4
110		.7519	162.5
115			199.6
115.1			200
120		.7425	243.3
125			294.8
130		.7328	354.8
133.3			400
135			424.6
140		.7227	505.2
145			597.9
150			703.9
152.4			760
155			825.
160			962.

Constants	Temp. Range	A	B	C	E
Antoine eq	25 to 154 °C	7.40170	1485.39	176.16	
Francis eq	5 to 150 °C	1.15883	1.188×10^{-4}	192.98	600

4-Methyl-1-pentanol			
Temp. °C	Refractive Index, n_D	Density g cm^{-3}	Vapor Pressure, mmHg
0		0.8264	
10		.8198	
15	1.4172		
20	1.4154	.8130	0.8
25	1.4135	.8095	1.3
30	1.4114	.8060	3.0
40	1.4073	.7988	6.2
50		.7915	8.8
56.9			10
60		.7839	12.3
65			16.8
70		.7761	22.7
75			30.2
80		.7680	39.7
85			51.7
90		.7597	66.5
95			84.8
98.6			100
100		75.12	107.0
105			133.8
110		.7423	165.9
114.5			200
115			204.1
120		.7332	249.1
125			302.0
130		.7237	363.5
132.6			400
135			434.9
140		.7139	517.1
145			611.2
150			718.5
151.8			760
155			840.
160			978.

Constants	Temp. Range	A	B	C	E
Antoine eq	25 to 154 °C	7.05114	1273.35	153.56	
Francis eq	0 to 150 °C	1.11945	1.667×10^{-4}	175.81	600

2-Methyl-2-pentanol			
Temp. °C	Refractive Index, n_D	Density g cm ^{3}	Vapor Pressure, mmHg
0		0.8296	
10	1.4161	.8218	
20	1.4113	.8136	4.2
25	1.4089	.8095	6.3
30	1.4068	.8053	9.4
30.8			10
35			13.6
40	1.4021	.7967	19.2
45			26.6
50	1.3972	.7878	36.2
55			48.5
60	1.3921	.7786	63.9
65			82.9
68.8			100
70	1.3868	.7691	106.3
75			134.5
80	1.3820	.7593	168.3
84.0			200
85			208.4
90		.7492	255.4
95			310.3
100		.739	373.7
101.9			400
105			446.5
110			529.4
115			623.4
120			729.1
121.4			760
125			848.
130			980.
135			1126.

Constants	Temp. Range	A	B	C	E
Antoine eq	15 to 123 °C	6.15173	811.05	126.60	
Francis eq	5 to 85 °C	1.22815	1.125×10^{-4}	239.11	600

TABLE 137. Isomeric Hexanols. Selected values. Physical properties of the liquid

3-Methyl-2-pentanol				4-Methyl-2-pentanol				2-Methyl-3-pentanol			
Temp. °C	Refractive Index, n_D	Density g cm^{-3}	Vapor Pressure, mmHg	Temp. °C	Refractive Index, n_D	Density g cm^{-3}	Vapor Pressure, mmHg	Temp. °C	Refractive Index, n_D	Denxity g cm^{-3}	Vapor Pressure, mmHg
0		0.8456		0		0.8244		0		0.8395	
10		.8374		10		.8161		10		.8319	
15	1.4215			15	1.4135			15	1.4189		
20	1.4197	.8291		20	1.4112	.8076	3.7	20	1.4168	.8239	
25	1.4179	.8248	3.2	25	1.4090	.8033	5.2	25	1.4148	.8198	5.3
30	1.4152	.8206	4.7	30	1.4069	.7993	7.3	30	1.4124	.8156	7.6
35			6.7	35.0			10	34.0			10
40	1.4103	.8119	9.5	40	1.4023	.7908	13.7	35			10.7
40.8			10	45			18.4	40	1.4074	.8069	14.9
45			13.2	50	1.3975	.7820	24.4	45			20.3
50		.8030	18.0	55			32.1	50		.7979	27.3
55			24.2	60		.7730	41.7	55			36.3
60		.7940	32.3	65			53.7	60		.7886	47.7
65			42.4	70		.7638	68.4	65			62.0
70		.7847	55.2	75			86.5	70		.7788	79.7
75			71.0	78.2			100	74.7			100
80		.7751	90.5	80		.7544	108.5	75			101.4
82.1			100	85			135.0	80		.7685	127.8
85			114.3	90		.7449	166.8	85			159.6
90		.7654	143.1	94.4			200	90		.7579	197.7
95			177.6	95			204.5	90.3			200
97.8			200	100		.7351	249.1	95			243.0
100		.7553	218.8	105			301.6	100		.7467	296.4
105			267.5	110		.7251	362.9	105			359.0
110		.7450	324.8	112.7			400	107.9			400
115			391.7	115			434.1	110		.7351	431.9
115.6			400	120		.7149	516.4	115			516.4
120		.7343	469.4	125			611.1	120		.7229	613.6
125			559.1	130		.7045	719.6	125			725.0
130		.7233	666.2	131.7			760	126.5			760
134.2			760	135			843.	130		.710	852.
135			780.	140			984.	135			996.
140			914.					140			1158.
145			1066.								

Constants	Temp. Range	A	B	C	E	Constants	Temp. Range	A	B	C	E	Constants	Temp. Range	A	B	C	E
Antoine eq	23 to 135 °C	7.24705	1354.68	176.07		Antoine eq	20 to 133 °C	7.53690	1566.76	204.79		Antoine eq	25 to 128 °C	7.14257	1287.24	175.60	
Francis eq	5 to 125 °C	1.03182	4.372×10^{-4}	93.12	500	Francis eq	0 to 130 °C	0.96569	5.463×10^{-4}	70.38	500	Francis eq	0 to 125 °C	1.36832	-1.295×10^{-4}	317.27	600

TABLE 138. Isomeric Hexanols. Selected values. Physical properties of the liquid

3-Methyl-3-pentanol

Temp. °C	Refractive Index, n_D	Density g cm^{-3}	Vapor Pressure, mmHg
0		0.8440	
10		.8362	
20	1.4186	.8281	
25	1.4163	.8238	
30		.8195	
40		.8105	
50		.8011	
60		.7912	56.4
65			72.9
70		.7808	
71.4			100
75			118.4
80		.770	148.7
85			185.2
86.8			200
90			228.8
95			280.5
100			341.4
104.2			400
105			412.6
110			495.5
115			591.3
120			701.5
122.4			760
125			828.

Constants	Temp. Range	*A*	*B*	*C*	*E*
Antoine eq	65 to 123 °C	7.2252	1313.8	180.0	
Francis eq	0 to 65 °C	1.48966	-3.149×10^{-4}	387.37	600

2-Ethyl-1-butanol

Temp. °C	Refractive Index, n_D	Density g cm^{-3}	Vapor Pressure, mmHg
0		0.8481	
10		.8408	
15	1.4243		
20	1.4224	.8333	
25	1.4205	.8295	1.5
30	1.4185	.8257	2.3
35			6.6
40	1.4146	.8179	5.1
45			7.2
49.8		.8099	10
50			10.1
55		.8017	14.0
60			19.0
65		.7933	25.4
70			33.6
75		.7848	44.0
80			56.8
85		.7759	72.6
90			91.8
91.9			100
95		.7668	115.1
100			142.9
105			176.1
108.2		.7575	200
110			215.2
115		.7478	261.0
120			314.4
125			376.2
126.8		.7379	400
130			447.3
135		.7276	528.6
140			621.2
145			726.1
146.5			760
150			844.
155			977.

Constants	Temp. Range	*A*	*B*	*C*	*E*
Antoine eq	25 to 153 °C	6.84055	1188.69	153.70	
Francis eq	5 to 145 °C	1.02199	3.785×10^{-4}	86.92	500

2,2-Dimethyl-1-butanol

Temp. °C	Refractive Index, n_D	Density g cm^{-3}	Vapor Pressure, mmHg
0		0.8445	
10		.8366	
20	1.4208	.8286	
25	1.4188	.8246	3.2
30	1.4167	.8205	4.7
35		.8122	6.6
40	1.4125		9.3
41.1			10
45		.8038	12.8
50			17.5
55		.7952	23.5
60			31.1
65		.7865	40.7
70			52.8
75		.7775	67.7
80			85.9
83.3			100
85		.7684	108.2
90			135.0
95			167.0
99.4		.7590	200
100			205.0
105		.7494	250.0
110			302.7
115			364.1
117.6		.7395	400
120			435.3
125		.7293	517.2
130			611.2
135			718.3
136.8			760
140			840.
145			977.

Constants	Temp. Range	*A*	*B*	*C*	*E*
Antoine eq	25 to 142 °C	7.15475	1338.45	176.38	
Francis eq	5 to 135 °C	0.96031	5.238×10^{-4}	52.13	450

TABLE 139. Isomeric Hexanols. Selected values. Physical properties of the liquid

2,3-Dimethyl-1-butanol			
Temp. °C	Refractive Index, n_D	Density g cm^{-3}	Vapor Pressure, mmHg
20	1.4205	0.8300	
25	1.4185	.8255	
96.			100
100			120.
105			148.
110			183.
112.			200
115			223.
120			271.
125			328.
130.			400
135			471.
140			561.
145			664.
149.			760

Constants	Temp. Range	A	B	C	E
Antoine eq	100 to 149 °C	8.273	2044.	230.	
Francis eq					

3,3-Dimethyl-1-butanol			
Temp. °C	Refractive Index, n_D	Density g cm^{-3}	Vapor Pressure, mmHg
20	1.4138	0.8147	
25	1.4118	0.8097	
75			48.
80			61.
85			78.
90			78.
91.			100
95			122.
100			151.
105			187.
107.			200
110			229.
115			279.
120			337.
125.			400
130			487.
135			581.
140			690.
143.			760

Constants	Temp. Range	A	B	C	E
Antoine eq	80 to 144 °C	8.271	2010.	230.	
Francis eq					

2,3-Dimethyl-2-butanol			
Temp. °C	Refractive Index, n_D	Density g cm^{-3}	Vapor Pressure, mmHg
0		0.8395	
10		.8312	
15	1.4197		
20	1.4173	.8226	
25	1.4150	.8182	8.8
26.8			10
30	1.4126	.8132	12.4
35			17.1
40	1.4074	.8046	23.3
45			31.2
50		.7952	41.4
55			54.2
60		.7855	70.1
65			89.8
67.2			100
70		.7755	113.9
75			143.2
80		.7652	178.3
82.7			200
85			220.3
90		.7545	270.1
95			328.6
110		.7435	397.1
100.2			400
105			476.6
110		.7321	568.5
115			674.1
118.6			760
120		.7203	795.
130		.708	

Constants	Temp. Range	A	B	C	E
Antoine eq	25 to 120 °C	7.12924	1271.40	180.64	
Francis eq	5 to 115 °C	1.62647	-1.643×10^{-4}	629.58	800

TABLE 140. Isomeric Hexanols. Selected values. Physical properties of the liquid

3,3-Dimethyl-2-butanol

Temp. °C	Refractive Index, n_D	Density g cm^{-3}	Vapor Pressure, mmHg
10		0.8258	
20	1.4151	.8179	
25	1.4132	.8139	
30		.8099	
40		.8015	
50		.7929	
60		.7841	58.6
65			75.5
70		0.7748	96.5
71.			100
75			122.
80		.7652	154.
85			192.
86.			200
90		.7553	238.
95			293.
100		.7449	359.
103.			400
105			437.
110		.734	528.
115			635.
120			760

Constants	Temp. Range	*A*	*B*	*C*	*E*
Antoine eq	65 to 120 °C	8.261	1883.	230.	
Francis eq	15 to 100 °C	0.99379	3.505×10^{-4}	64.16	400

Constants	Temp. Range	*A*	*B*	*C*	*E*
Antoine eq					
Francis eq					

Constants	Temp. Range	*A*	*B*	*C*	*E*
Antoine eq					
Francis eq					

Weissler [1948] and Rao, Ramamurty, and Rao [1958] measured the refractive index of 4-methyl-2-pentanol at 30 °C, and Dupont and Dumas [1959] reported a value at 17 °C. These were all about 0.001 higher than the values of Hovorka, Lankelma, and Stanford [1938]. Weissler has also measured the refractive index for several other hexanols at 30 °C.

The situation for 3-methyl-3-pentanol is very puzzling. Hovorka, Lankelma, and Axelrod [1940] report a refractive index which is about 0.08 lower than other good values, and densities which appear low by about 0.005 g cm^{-3}. The only other values which are close to these were reported by Reformatsky [1887] and Savard [1935]. In addition their boiling point was 1.5 °C below the carefully measured value of Howard, Mears, Fookson, Pomerantz, and Brooks [1947]. Hovorka et al. obtained their sample by fractional distillation of a commercial product and since the properties do not correspond to those of any other hexanol, it seems likely that it was contaminated with some impurity. A common method of preparation of 3-methyl-3-pentanol is by the Grignard reduction of 3-pentanone. The presence of 3-pentanone with the alcohol would give a lower refractive index, density, and boiling point. It may be that they had an azeotrope of 3-methyl-3-pentanol and 3-pentanone. The samples used by Howard et al., and by several other investigators were prepared by procedures which did not involve 3-pentanone. The selection was based on data other than that of Hovorka, Lankelma, and Axelrod.

Smoothed values of the refractive index at wavelengths other than the sodium D-line are presented in table 141 for three of the isomeric hexanols. Data for 2-methyl-2-pentanol were based on data of Eykman [1919] and Krollpfeiffer and Seebaum [1928] at 15 °C; those for 4-methyl-2-pentanol on data of van Risseghem [1933] at 15 °C; and those for 3-methyl-3-pentanol on data of Eykman [1919] at 18.5 °C. In each case the data were converted to 20 °C by applying the temperature coefficient obtained for the Na$_D$ line data.

TABLE 141. Isomeric hexanols. Selected values. Refractive index at various wavelengths at 20 °C

Symbol	Wavelength, Å	2-Methyl-2-pentanol	4-Methyl-2-pentanol	3-Methyl-3-pentanol
He$_{red}$	6678.2	1.4087		1.4163
H$_c$	6562.8	1.4091		1.4166
Na$_D$	5892.6	1.4113	1.4112	1.4186
Hg$_e$	5460.7	1.4129	1.4139	1.4205
He$_{blue}$	5015.7	1.4153	1.4160	1.4228
H$_F$	4861.3	1.4161	1.4171	1.4237
Hg$_g$	4358.3	1.4202	1.4210	1.4276
H$_{G'}$	4340.5	1.4204	1.4212	1.4278

Density

As for the refractive indices, the principal source of accurate density data is the research of Hovorka and co-workers. Reliable densities have been reported at 20 and 25 °C by Brunel [1923], Ellis and Reid [1932], Olivier [1936], Olivier [1937], Ginnings and Webb [1938], Pichler, Ziesecke, and Traeger [1950], and Cook [1952]. Pickard and Kenyon have made the only systematic measurements of density over a range of temperature, besides those of Hovorka et al. Although published in the years 1911 and 1913, Pickard and Kenyon's values show reasonably good agreement with most of those of Hovorka et al.

The significant sources of density at 20 and 25 °C are listed in the unnumbered tables for individual compounds, and a complete bibliography can be generated from the Index on page 1–176. The densities over an extended temperature range which have been listed in the numbered tables of selected data were calculated from the Francis equation using the constants shown at the bottom of each table. The procedure for fitting the constants to the observed data is discussed in appendix B.

For reasons given in the section on Refractive Index, the density data of Hovorka, Lankelma, and Axelrod [1940] were not used to establish the selected values for 3-methyl-3-pentanol. The density of 2-methyl-2-pentanol found by Hovorka, Lankelma, and Naujoks [1933] were about 0.003 to 0.005 g cm^{-3} higher than other comparable data except that of Pichler, Ziesecke, and Traeger [1950]. Thus one set of investigators must have had impure samples. There is no certain way of deciding at this time. The selected values were calculated from the data of Hovorka, Lankelma, and Naujoks. The densities of 4-methyl-2-pentanol calculated from the Francis equation showed some small systematic deviations from the observed data. To correct for this, the calculated values were reduced by 0.0005 to 0.0002 g cm^{-3} from 0 to 30 °C to give the selected values in table 137.

Costello and Bowden [1958] reported the density of "*iso*hexyl alcohol" from −20 to 220 °C. The only isomer which matches their boiling point and density data is 2-ethyl-1-butanol. Their densities run about 0.003 g cm^{-3} below the selected ones.

Vapor Pressure and Boiling Point

Observed values of the boiling points at or near 1 atm are in the unnumbered tables. Additional references, as well as references to boiling points and vapor pressures at other pressures, have been identified in the Index to the Bibliography. The principal source of vapor pressure data at pressures other than 1 atm is the work of Hovorka and associates. Except for 3-methyl-3-pentanol, the selected vapor pressures and boiling points given in the numbered tables were calculated from the Antoine equation using the values of the constants shown at the bottom of the tables. Along with Hovorka et al., accurate normal boiling point measurements have been made by Brunel [1923], Clough and Johns [1923], Ellis and Reid [1932], Norris and Cortese [1927], Olivier [1936], Ginnings and Webb [1938], Howard, Mears, Fookson, Pomerantz, and Brooks [1947], Pichler, Ziesecke, and Traeger [1950], and Cook [1952]. Pickard and Kenyon, Levene et al., and Whitmore et al., and a few others have reported individual boiling point values at various scattered pressures.

Data from Hovorka et al. were not used in establishing the vapor pressure curves of 3-methyl-3-pentanol, 2,3-dimethyl-1-butanol, 3,3-dimethyl-1-butanol, and 3,3-dimethyl-2-butanol. Thus, the accuracy of the data for these compounds is less than that for the other hexanols. The case of 3-methyl-3-pentanol was discussed in the section on Refractive Index. The normal boiling point of this compound is certainly accurate to within a few tenths of a degree, but there were only a few isolated measurements of boiling points at other pressures to establish the vapor pressure curve. These were by Eykman [1919] at 84 mmHg, Norton and Hass [1936] to 50 mm, and Howard, Mears, Fookson, Pomerantz, and Brooks [1947] at 150 mmHg. Hovorka et al. did not conduct measurements on the other three compounds, and temperatures other than the normal boiling points are uncertain by two or three degrees at least.

Heats of Vaporization

Heats of vaporization of the 16 isomeric hexanols at 25 °C and at their respective boiling points are listed in table 142. All of these were calculated from the Antoine constants, with estimated values for the second virial coefficients of -3 liter mol^{-1} at 25 °C and -1 liter mol^{-1} at the boiling point. The heat of vaporization of 3-methyl-3-pentanol at its boiling point is uncertain by about 1 kcal mol^{-1}, and that of 2,3-dimethyl-1-butanol, 3,3-dimethyl-1-butanol, and 3,3-dimethyl-2-butanol by about 2 kcal mol^{-1}. The uncertainties in the other heats of vaporization are about 0.3 to 0.5 kcal mol^{-1} at the boiling points and 0.5 to 1 kcal mol^{-1} at 25 °C.

TABLE 142. Isomeric hexanols. Heats of vaporization calculated from Antoine constants

Name of Compound	at 25 °C		at the boiling point	
	Vapor Pressure mmHg	ΔHv kcal mol^{-1}	t_b, °C	ΔHv kcal mol^{-1}
2-Hexanol	2.6	13.1	139.9	10.84
3-Hexanol	5.1	11.0	135.4	10.59
2-Methyl-1-pentanol	1.8	13.3	148.0	11.04
3-Methyl-1-pentanol	1.0	14.9	152.4	11.07
4-Methyl-1-pentanol	0.8	16.2	151.8	10.96
2-Methyl-2-pentanol	6.3	14.3	121.4	9.10
3-Methyl-2-pentanol	3.2	13.6	134.2	10.36
4-Methyl-2-pentanol	5.2	12.1	131.7	10.07
2-Methyl-3-pentanol	5.3	13.0	126.5	9.99
3-Methyl-3-pentanol			122.4	10.0
2-Ethyl-1-butanol	1.5	15.1	146.5	10.32
2,2-Dimethyl-1-butanol	3.2	13.4	136.8	10.18
2,3-Dimethyl-1-butanol			149.	11.3
3,3-Dimethyl-1-butanol			143.	11.1
2,3-Dimethyl-2-butanol	8.8	12.2	118.6	9.66
3,3-Dimethyl-2-butanol			120.	10.5

Melting Point

The only accurate melting point determination on this group of compounds was made by Howard, Mears, Fookson, Pomerantz, and Brooks [1947] for 2,3-dimethyl-2-butanol. Cook [1952] has reported that 2-hexanol, 3-hexanol, and 4-methyl-1-pentanol form a glass on cooling, and Union Carbide Chemicals Company [1953] also found this phenomenon for 4-methyl-2-pentanol. These glass formations occur in the temperature range of -70 to -110 °C. It is probable that several other hexanols also form glasses, and this tendency is probably responsible for the difficulty in obtaining precise data for most of the other compounds.

Data for isomeric hexanols

Investigators		Vapor Pressures and Boiling Points		Freezing Point	Density, *d* g cm^{-3}		Refractive Index, n_D	
		°C	mmHg	t_m, °C	20 °C	25 °C	20 °C	25 °C
See also table 135		2-Hexanol, $C_6H_{14}O$, mol wt. 102.178, state at 25 °C liq						
Ponzio	[1901]	139.5	760					
Zelinskii and Przheval'skii	[1908]	138–139	732		0.8141		1.4148	
Pickard and Kenyon	[1911]	137–138	760		.8150			1,4139
Clough and Johns	[1923]	139.4–139.6	760		.8159			
Terent'ev	[1926]	136–8	760		.8215		1.4193	
Norris and Cortese	[1927]	140–140.4	760			0.8044		1.4136
Malone and Reid	[1929]	139.7	759					
Ellis and Reid	[1932]	139.8	760			.8098		1.4126
Oliver	[1936]	139.8–140.8	776					
Whitmore	[1938]	130–4	726				1.4144–'52	
Whitmore, Popkin, Whitaker, Mattil, and Zech	[1938]	134–9.5	736				1.4152–'69	
Hovorka, Lankelmz, and Stanford	[1938]	139.9	760			.81036		1.4128
Ginnings and Webb	[1938]	139.0–140.0	760			.8108		
Hargreaves and Owen	[1947]	139–140	760				1.4143	
Airs, Balfe, and Kenyon	[1942]	137–140	760		.8150			
Huston and Bostwick	[1948]	139.5	740				1.4155	
Pichler, Ziesecke, and Traeger	[1950]	139.9	760		.8142		1.4147	
Huston and Tiefethal	[1951]	139.2	743				1.4140	
Cook	[1952]	140.0	760		.8143		1.4147	
Zeiss and Tsutsui	[1953]	138–138	760					1.4131
Zazarou, Kakhniaskvili, and Ryabchenko	[1954]	137–139	759					
Urry, Stacey, Huyser, and Juveland	[1954]						1.4154	
Selected value	[1967]	^{e}139.9±0.2 ^{e}44.7±0.5	760 10		^{d}.8144 ±.0004	^{d}.8105 ±.0004	^{b,c}1.4147 ±0.0002	^{b,c}1.4128 ±0.0002

Antoine constants: *A* 7.80733, *B* 1696.19, *C* 204.43.

dt/*dp* at 760 mmHg, ^{e}0.0399 °C/mmHg

Data for isomeric hexanols—Continued

Investigators		Vapor Pressures and Boiling Points		Freezing Point	Density, *d* g cm^{-3}		Refractive Index, n_D	
		°C	mmHg	t_m, °C	20 °C	25 °C	20 °C	25 °C
3-Hexanol, $C_6H_{14}O$, mol wt. 102.178, state at 25 °C liq								
See also table 135								
Lieben and Volker	[1875]	134.5–135.5	760		0.8188			
de Coninck	[1876]	134	760		**.81825**			
Pickard and Kenyon	[1913]	133	733		.8213		**1.4141**	
Lespieau and Lombard	[1935]	134	760		.820		**1.4176**	
Hovorka, Lankelma, and Stanford	[1938]	**135.52**	760			**0.81428**		**1.4139**
Ginnings and Webb	[1938]	**134.5–135.0**	760			**0.8143**		
Burdick and Adkins	[1939]							1.4180
Airs, Balfe, and Kenyon	[1942]	132.5–133.5	760		.8193			
Henne and Matuszak	[1944]				.8195		1.4168	
Kenyon and Poplett	[1945]	133–134	760				**1.4148**	
Pichler, Ziesecke, and Traeger	[1950]	**135.5**	760		.8186		**1.4159**	
Cook	[1952]	**135.6**	760	−90–−70	.8190		**1.4162**	
Zeiss and Tsutsui	[1953]							**1.4150**
Benkeser, Hazdra, and Burrous	[1959]	132–134	760				**1.4140**	
Selected value	[1967]	^{e} 135.4±0.2	760		^{d} .8185	^{d} 0.8144	^{b,c} 1.4160	^{b,c} 1.4140
		36.±1	10		±.0003	±0.0003	±0.0004	±0.0004
Antoine constants: *A 8.66522, B 2340.10, C 269.16*								*dt/dp at 760 mmHg, ^{e} 0.0400 °C/mmHg*
2-Methyl-1-Pentanol, $C_6H_{14}O$, mol wt., 102.178 state at 25 °C liq								
See also table 135								
Guerbet	[1901a]	148.	762					
Przhevai'skii	[1909]	146–147	749		0.8263		1.4178	
Norris and Cortese	[1927]	**147.9–148.1**	760			0.8192		1.4180
Levene and Mikeska	[1929]	147–147.5	760					
Oliver	[1936]	147.5–148.0	766		.8208			
Shonle, Waldo, Keltch, and Coles	[1936]	146.5	760					
Hovorka, Lankelma, and Stanford	[1938]	**147.93**	760			**.82065**		**1.4172**
Scattergood, Miller, and Gammon	[1945]	147–149	760					
Weizmann, Bergman, and Sulzbacher	[1950]	148	760					
Pichler, Ziesecke, and Traeger	[1950]	**147.9**	760		**.8243**		**1.4190**	
Cook	[1952]	**148.6**	760		.8134		1.4184	
Union Carbide Chemicals Company		**148.0**	760		.8215		1.4192	
Selected value	[1967]	^{e} 148.0±0.2	760		^{d} .8242	^{d} .8206	^{b,c} 1.4190	^{a} 1.4172
		50.5±0.5	10		±0.0003	±.0003	±0.0003	±0.0004
Antoine constants: *A* 7.86701, *B* 1775.12, *C* 208.00								*dt/dp* at 760 mmHg, ^{e} 0.0408 °C/mmHg

Data for isomeric hexanols—Continued

Investigators		Vapor Pressures and Boiling Points		Freezing Point	Density, *d* g cm^{-3}		Refractive Index, n_D	
		°C	mmHg	t_m, °C	20 °C	25 °C	20 °C	25 °C
3-Methyl-1-pentanol, $C_6H_{12}O$, mol wt. 102.178, state at 25 °C liq								
See also table 136								
Hardin	[1908]	151–152	758		0.8265			
Verley	[1924]	153	760					
Norris and Cortese	[1927]	153.7–'4.1	760			0.8205		1.4177
Olivier	[1936]	152.3–'3.0	765		.8242			
Hovorka, Lankelma, and Schneider	[1940]	152.44	760			.81870		1.4169
Cymerman, Heilbron, and Jones	[1945]	152–'3	763				1.4204	
Pichler, Ziesecke, and Traeger	[1950]	152.4			.8224		1.4189	
Mosher and La Combe	[1950a]	151.1–'2.0	760					
Young and Webb	[1951]	152						1.4174
Cook	[1952]	153			.8241		1.4195	
Lardicci and Pino	[1961]	152–153	760					1.4176
Selected value	[1967]	^{e} 152.4±0.2 ^{e} 55.9±0.5	760 10		^{d} 0.8237 ±0.001	^{d} 0.8202 ±0.001	^{b,c} 1.4193 ±0.0005	^{b,c} 1.4175 ±0.0005

Antoine constants: *A* 7.40170, *B* 1485.39, *C* 176.16

dt/dp at 760 mmHg, ^{e} 0.0415 °C/mmHg

4-Methyl-1-pentanol, $C_6H_{14}O$, mol wt. 102.178, state at 25 °C liq

See also table 136

Investigators		°C	mmHg	t_m, °C	20 °C	25 °C	20 °C	25 °C
Levene and Allen	[1916]	153	760					
Norris and Cortese	[1927]	151.8–152.8	760			0.8110		1.4134
Malone and Reid	[1929]	151.7	758					
Olivier	[1936]	151.5–152.5	763		0.8131			
Hovorka, Lankelma, and Schneider	[1940]	151.63				.8094		1.4135
Pichler, Ziesecke, and Traeger	[1950]	151.6			.8129		1.14154	
Searles	[1951]	151–152	752					
Cook	[1952]	152.2			.8142		1.4154	
Selected value	[1967]	^{e} 151.8±0.3 ^{e} 56.9±0.5	760 10		^{d} .8130 ±.0004	^{d} .8095 ±.0004	^{b,c} 1.4154 ±0.0003	^{b} 1.4135 ±0.0003

Antoine constants: *A* 7.05114, *B* 1273.35, *C* 153.56

dt/dp at 760 mmHg, ^{e} 0.0418 °C/mmHg

Data for isomeric hexanols—Continued

Investigators		Vapor Pressures and Boiling Points		Freezing Point	Density, *d* g cm^{-3}		Refractive Index, n_D	
		°C	mmHg	t_m, °C	20 °C	25 °C	20 °C	25 °C
2-Methyl-2-pentanol, $C_6H_{14}O$, mol wt. 102.178, state at 25 °C liq								
See also table 136								
Willcox and Brunel	[1916]	122.1–122.6	760					
Deschamps	[1920]	122.5–123.5	762		0.8312		1.4103	
Owen, Quayle, and Beavers	[1930]					0.8019		
Hovorka, Lankelma, and Navjoks	[1933]	**121.04**	760	**−103**		**.8097**		**1.4089**
Norton and Hass	[1937]	119.3	748			.8071		**1.4089**
Whitmore and Johnston	[1938]	119.5–120.5	738		.808		**1.4103**	
Ginnings and Webb	[1938]	**122.4–122.6**	760			.8053		
Addison	[1945]	122.0			.8048		1.4120	
Huston and Brault	[1950]	117–118	740				1.4125	
Pichler, Ziesecke, and Traeger	[1950]	**121.5**			.8134		**1.4113**	
Searles	[1951]						1.4178	
Levina, Tantsyreva, and Fainzil'berg	[1952]				.8041		1.4087	
Urry, Stacy, Huyser, and Juveland	[1954]							**1.4120**
Brown and Nakagawa	[1955]						1.4105	
Selected value	[1967]	^{e} 121.4±0.3 ^{e} 30.8±0.5	760 10	^{a} −103 ±2	^{d,a} 0.8136 ±0.0001	^{d,a} 0.8095 ±0.0001	^{b,c} 1.4113 ±0.0003	^{b} 1.4089 ±0.0003

Antoine constants: *A* 6.15173, *B* 811.05, *C* 126.60 *dt/dp* at 760 mmHg, ^{e} 0.0433 °C/mmHg

Data for isomeric hexanols—Continued

Investigators		Vapor Pressures and Boiling Points		Freezing Point	Density, *d* g cm^{-3}		Refractive Index, n_D	
		°C	mmHg	t_m, °C	20 °C	25 °C	20 °C	25 °C
3-Methyl-2-pentanol, $C_6H_{14}O$, mol wt. 102.178, state at 25 °C liq.								
See also table 137								
Cotter and Powell	[1936]	132–134	760					
Norton and Hass	[1937]	**134.2–134.4**	749					**1.4179**
Whitmore and Karnatz	[1938a]	132.0–132.5	726				1.4206	
Ginnings and Webb	[1938]	**133.5–134.5**	760			0.8231		
Hovorka, Lankelma, and Bishop	[1941]	**134.32**	760			**0.82475**		**1.4175**
Pichler, Ziesecke, and Traeger	[1950]	134			0.8231			
Selected value	[1967]	^{e} 134.2±0.2 ^{e} 40.8±0.5	760 10		^{d,a} 0.8291 ±0.0004	^{d,a} 0.8248 ±0.0004	^{c} 1.4197 ±0.004	^{b,c} 1.4179 ±0.004

Antoine constants: *A* 7.24705, *B* 1354.68, *C* 176.07 *dt/dp* at 760 mmHg, °C/mmHg ^{e} 0.0406

Data for isomeric hexanols—Continued

4-Methyl-2-pentanol, $C_6H_{14}O$, mol wt. 102.178, state at 25 °C liq.

See also table 137

Investigators		Vapor Pressures and Boiling Points		Freezing Point	Density, *d* g cm^{-3}		Refractive Index, n_D	
		°C	mmHg	t_m, °C	20 °C	25 °C	20 °C	25 °C
Pickard and Kenyon	[1911]	125–132	760		**0.8077**		1.4103	
Willcox and Brunel	[1916]	130–131	766					
Brunel, Crenshaw, and Tobin	[1921]	**131.82**	760			0.8025		1.40895
Brunel	[1923]	131.85	760			.80245		**1.40895**
Van Rissieghem	[1933]	128–132	760					
Whitmore and Johnston	[1938]	**129.5**	734		.807		**1.4112**	
Hovorka, Lankelma, and Stanford	[1938]	**131.60**	760			**.80306**		**1.4091**
Ginnings and Webb	[1938]	**131.6–131.8**	760			.8034		
Schmerling, Friedman, and Ipatieff	[1940]	128–131	760				1.4140	
Henne and Matuszak	[1944]	133.0			**.8075**		**1.4122**	
Scattergood, Miller, and Gammon	[1945]	131.5–132.0	760					
Tuot and Guyard	[1947]				.80708		1.4101	
Huston and Bostwick	[1948]						1.4120	
Pichler, Ziesecke, and Traeger	[1950]	**131.6**	760		.8071		**1.4111**	
Huston and Tiefenthal	[1951]	131.4	745					
Stevenson, Wagner, and Beock	[1952]						**1.4114**	
Zeiss and Tsutsui	[1953]	130–131						**1.4095**
Union Carbide Chemicals Co.	[1955]	**131.8**	760		.8065			
Brown and Nakagawa	[1955]	129–129.5	737				**1.4110**	
Rao, Ramamerty, and Rao	[1958]	130.0–131.5	760					
Mislow, O'Brien, and Schaefer	[1962]	130–131.5	760					**1.4082**
Selected value	[1967]	^{e}131.7±0.2	760		^{d}0.7076	^{d}0.8033	^{b,c}1.4112	^{b,c}1.4090
		^{e}35.0±0.5	10		±0.0005	±0.0005	±0.0002	±0.0003

Antoine constants: *A* 7.53690, *B* 1566.76, *C* 204.79

dt/*dp* at 760 mmHg, ^{e} 0.0413 °C/mmHg

2-Methyl-3-pentanol, $C_6H_{14}O$, mol wt. 102.128, state at 25 °C liq

See also table 137

Investigators		Vapor Pressures and Boiling Points		Freezing Point	Density, *d* g cm^{-3}		Refractive Index, n_D	
		°C	mmHg	t_m, °C	20 °C	25 °C	20 °C	25 °C
Pickard and Kenyon	[1912]				**0.8247**		1.4117	
Behal	[1919]				.8413		1.4135	
Krollpfelffer and Seebaum	[1928]	121–127	760		.823			
Norton and Hass	[1936]	124.6	747			0.8193		**1.4151**
Whitmore and Johnston	[1938]	125–126	742		.824		**1.4170**	
Ginnings and Webb	[1938]	**126.3–127.3**	760			**0.8186**		
Hovorka, Lankelma, and Axelrod	[1940]	**126.68**	760			**0.82064**		**1.4148**
Henne and Matuszak	[1944]				.8230		1.4172	
Huston and Brault	[1950]	127–128	740				**1.4168**	
Pichler, Ziesecke, and Traeger	[1950]	**126.7**			.8249		**1.4168**	
Cook	[1952]	125	735				1.4176	
Greenwood and Cohen	[1963]							**1.4148**
Selected value	[1967]	^{e}126.5±0.3	760		^{d}.8239	^{d}0.8198	^{b,c}1.4168	^{b,c}1.4148
		^{e}34.0±0.5	10		±.0007	±0.0007	±0.0003	±0.0003

Antoine constants: *A* 7.14257, *B* 1287.24, *C* 175.60

dt/*dp* at 760 mmHg, 0.0405 °C/mmHg

Data for isomeric hexanols—Continued

Investigators		Vapor Pressures and Boiling Points		Freezing Point	Density, *d* g cm^{-3}		Refractive Index, n_D	
		°C	mmHg	t_m, °C	20 °C	25 °C	20 °C	25 °C

3-Methyl-3-pentanol, $C_6H_{14}O$, mol wt. 102.178, state at 25 °C liq.

See also table 138

Investigators		°C	mmHg	t_m, °C	20 °C	25 °C	20 °C	25 °C
Reformatsky	[1887]	121–123	764		0.8230	.8186		
Willcox and Brunel	[1916]	122.1–122.9	760					
Eykman	[1919]			−22	.8130			
Pariselle and Simon	[1921]	121	760		.8286	.8246	1.418	
Favorski and Zalesskii-Kibardine	[1925]	121	755					
Norris and Cortese	[1927]	122.8–123.0	760			.8233		1.4166
Church, Whitmore, and McGrew	[1934]	121–122	740					
Savard	[1935]	123	760		.8237			
Norton and Hass	[1936]	120.0–121.3	749			.8240		1.4161
Owen, Quayle, and Beavers	[1939]					0.8215		
Ginnings and Webb	[1938]	122.6–122.8	760			.8242		
Hovorka, Lankelma, and Axelrod	[1940]	120.9	760			.81903		1.4079
Scattergood, Miller, and Gammor	[1945]							
Howard, Mears, Fookson, Pomerants, and Brooks	[1947]	122.4	760	−23.6	.8286	.8243	1.4186	1.4163
			10					
Zal'Manovich	[1948]	122–123	760		.8279			
Pichler, Ziesecke, and Traeger	[1950]	120.9	760		.8237		1.4101	
Young and Webb	[1951]							1.4153
Chancel	[1951]	122	760					
Van Risseghem	[1952]	123.0–123.1	760	−23.7	.8278			
Soehring, Frey, and Enfres	[1955]	120.0–120.5	760		.8284		1.4189	
Sokolova and Fedorou	[1956]				.8617		1.4180	
Lanning and Moore	[1958]						1.4182	
Selected value	[1967]	^{e}122.4±0.5	760	^{a} −23.6	^{d} .8281	^{d} .8238	^{b}1.4186	^{b}1.4163
				±0.2	±.001	±.001	±0.0004	±0.0004

Antoine constants: *A* 7.2252, *B* 1313.8, *C* 180.0

dt/dp at 760 mmHg, ^{e} 0.0398 °C/mmHg

2-Ethyl-1-butanol, $C_6H_{14}O$, mol wt. 102.178, state at 25 °C liq.

See also table 138

Investigators		°C	mmHg	t_m, °C	20 °C	25 °C	20 °C	25 °C
Shonie, Waldo, Keltch, and Coles	[1936]	147.0–147.6	760					
Whitmore and Karnatz	[1938a]	146	732		0.8236		1.4220	
Goldwasser and Taylor	[1939]	148.9	760		.8328		1.4121	
Hovorka, Lankelma, and Smith	[1940]	146.27	760			0.82955		1.4205
Whitmore, Whitaker, Mosher, Brevik, Wheeler, Miner, Sutherland, Wagner, Clapper, Lewis, Lux, and Popkin	[1941]						1.4123	
Scattergood, Miller, and Gammon	[1945]	148–149	760					
Pichler, Ziesecke, and Traeger	[1950]	146.3	760		.8235		1.4224	
Adkins and Rosenthal	[1950]							1.4210
Freedman and Becker	[1951]	149	760					1.4200
Cook	[1952]	148.1			.8331		1.4226	
Union Carbide Carbon Chemicals Co.	[1955]	149.4		−114.4	.8313			
Costello and Bowden	[1958]	146.2	758		.8292			
Selected value	[1967]	^{e}146.5±0.3	760	−114.4	^{d} .8333	^{d} .8295	^{b,c}1.4224	^{b,c}1.4205
		^{e}49.8±0.5	10	±1	±.0002	±.0003	±0.0003	±0.0003

Antoine constants: *A* 6.84055, *B* 1188.69, *C* 153.70

dt/dp at 760 mmHg, ^{e} 0.0433 °C/mmHg

Data for Isomeric Hexanols—Continued

2,2-Dimethyl-1-butanol, $C_6H_{14}O$, mol wt. 102.178, state at 25 °C liq.

See also table 138

Investigators		Vapor Pressures and Boiling Points		Freezing Point	Density, *d* g cm^{-3}		Refractive Index, n_D	
		°C	mmHg	t_m, °C	20 °C	25 °C	20 °C	25 °C
Bouveault and Blanc	[1904b]	135	760	−15				
Conand, Webb, and Mendum	[1929]	130–137	760		0.8048			
Konlrausch and Koppl	[1933]	134.9–135.8	760					
Ginnings and Webb	[1938]	136.9–137.9	760			0.8498		
Hovorka, Lankelma, and Smith	[1940]	136.69				.82429		1.4188
Whitmore and Fosrter	[1942]						1.4208	
Pichler, Ziesecke, and Traeger	[1950]	136.7	760			.8283	1.4208	
Blood and Hagemeyer	[1964]	136	760		.8274			1.4187
Selected value	[1967]	^{e} 136.8±0.3	760	−15	^{d} .8286	^{d} .8246	^{b,c} 1.4208	^{b,c} 1.4188
		^{e} 41.1±0.5	10	±3	±.0004	±.0004	±0.0003	±0.0003

Antoine constants: *A* 7.15475, *B* 1338.45, *C* 176.38

dt/dp at 760 mmHg, ^{e} 0.0419 °C/mmHg

2,3-Dimethyl-1-butanol, $C_6H_{14}O$, mol wt. 102.178, state at 25 °C liq.

See also table 139

Investigators		Vapor Pressures and Boiling Points		Freezing Point	Density, *d* g cm^{-3}		Refractive Index, n_D	
		°C	mmHg	t_m, °C	20 °C	25 °C	20 °C	25 °C
Gorskii	[1913]	144–145	761		0.8298		1.4197	
Conant, Webb, and Mendum	[1924]	133–138	760					
Levene and Marker	[1935]	142	760			0.823		
Sutter	[1938]	145	760					
Pichler, Ziesecke, and Traeger	[1950]	144–145	760		.8301		1.4197	
Cook	[1952]	149	760		.8306		1.4216	
Sarel and Newman	[1956]	145–146	740					1.4173
Tsuda, Hayatsu, and Kishida	[1959]							
Zweifel, Ayyangar, Munekata, and Brown	[1964]						1.4208	
Selected value	[1967]	^{e} 149±1.5	760		^{b} .8301	^{c} .8255	^{b} 1.4205	^{c} 1.4185
					±.0005	±.0007	±0.0001	±0.0001

Antoine constants: *A* 8.273, *B* 2044., *C* 230.

dt/dp at 760 mmHg, ^{e} 0.040 °C/mmHg

Data for Isomeric Hexanols—Continued

Investigators	Vapor Pressures and Boiling Points		Freezing Point	Density, *d* g cm^{-3}		Refractive Index, n_D	
	°C	mmHg	t_m, °C	20 °C	25 °C	20 °C	25 °C
3,3-Dimethyl-1-butanol, $C_6H_{14}O$, mol wt. 102.178, state at 25 °C liq.							
See also table 139							
Sutter [1936]	140–143	760					
Strating and Backer [1936]	140–143	760					
Whitmore and Heyd [1938]	139–143	760				1.4150– 1.4179	
Whitmore, Whitaker, Mattil, and Popkin [1938]	140–146	739				1.4120– 1.4134	
Huston and Agett [1941]	141–143	740			0.813		1.4152
Whitmore, Whitaker, Mosher, Brevik, Wheeler, Miner, Sutherland, Wagner, Clapper, Lewis, Lux, and Popkin [1941]						1.4140– 1.4150	
Enyeart [1942]	142.4–142.6	741				**1.4143**	
Malinkovskii, Volkova, and Morozova [1949]	140–142	760					
Birch [1950]	143	760					
Ipatieff, Thompson, and Pines [1951]	141–142	760					
Sarel and Newman [1956]	144–145	740			**0.8097**		**1.4115**
Brown and Subba Rao [1959]	140–141	741				**1.4132**	
Botteron and Shulman [1962b]	140–145	760					
Selected value [1967]	[e] 143±1	760		[c] 0.8147 ±0.001	[a] 0.8097 ±0.001	[b] 1.4138 ±0.0005	[a,c] 1.4118 ±0.0007

Antoine constants: *A* 8.271, *B* 2010., *C* 230.

dt/*dp* at 760 mmHg, [e] 0.040 °C/mmHg

Investigators	Vapor Pressures and Boiling Points		Freezing Point	Density, *d* g cm^{-3}		Refractive Index, n_D	
	°C	mmHg	t_m, °C	20 °C	25 °C	20 °C	25 °C
2,3-Dimethyl-2-butanol, $C_6H_{14}O$, mol wt. 102.178, state at 25 °C liq.							
See also table 139							
Pavlov [1879]			−14	0.8224			
Delacre [1906]	120	760					
Delacre [1907]	120	760	−12				
Stevens [1933]	120	760					
Sutter [1938]	117–120	760					
Ginnings and Webb [1938]	**118.0–118.8**	760			0.8118		
Hovorka, Lankelma, and Bishop [1941]	**118.70**	760			.81861		**1.4151**
Enyeart [1942]	118	740				**1.4176**	
Howard, Mears, Fookson, Pomerantz, and Brooks [1947]	**118.4**	760	**−10.4**	**.8236**	**.8193**	**1.4170**	**1.4148**
Pichler, Ziesecke, and Traeger [1950]	**118.0–118.6**	760		.8223		1.4140	
Levina, Tantsyreva, and Fainzel'berg [1952]	117–118	750		.8249		1.4235	
Overberger and Berenbaum [1952]					.8155		**1.4155**
Hickinbottom and Hogg [1954]	116–117	760				**1.4161– 1.4169**	
Russell and Brown [1955]						**1.4182**	
Saunders [1956]	118	760					**1.4157**
Pillar and Pines [1962]	120–121	760				**1.4176**	
Selected value [1967]	[e] 118.6±0.2 [e] 26.8±0.5	760 10	[a] −10.4 ±0.3	[d] 0.8226 ±0.0007	[d] 0.8182 ±0.0007	[b] 1.4173 ±0.0003	[b] 1.4150 ±0.0003

Antoine constants: *A* 7.12924, *B* 1271.40, *C* 180.64

dt/*dp* at 760 mmHg, 0.0402 °C/mmHg

Data for Isomeric Hexanols—Continued

Investigators		Vapor Pressures and Boiling Points		Freezing Point	Density, *d* g cm^{-3}		Refractive Index, n_D	
		°C	mmHg	t_m, °C	20 °C	25 °C	20 °C	25 °C
3,3-Dimethyl-2-butanol, $C_6H_{14}O$, mol wt. 102,178, state at 25 °C liq.								
See also table 140								
Richard	[1910]	121–123	760	+4				
Pickard and Kenyon	[1914]	119–120	760		0.8199		1.4146	
Lowry	[1914]				.8185			
Willcox and Brunel	[1916]	**120.0–120.6**	760					
Van Risseghem	[1921]	**119.5–122**	760	−1				
Whitmore and Rothrock	[1933]	117–121	760	−2±2.5				
Whitmore and Meunier	[1933]	120.4	760	5.3			1.4148	
Whitmore	[1938]	118	738				1.4148	
Ginnings and Webb	[1938]	**119.9–120.9**	760			0.8157		
Baker and Adkins	[1940]	120	746					1.4132
Schmerling and Friedman	[1940]	119–120	760				1.4153	
Enyeart	[1942]	120	740				1.4151	
Mosher and LaCombe	[1950a]	119	760		.8199		1.4153	
Pichler, Ziesecke, and Traeger	[1950]	**119–120**	760		.8167		1.4153	
Ipatieff, Thompson, and Pines	[1951]	118–119	760				1.4148	
Zeiss and Tsutsui	[1953]	120–121	760					1.4138
Saunders	[1956]	119.5	760				1.4160	
Sarel and Newman	[1956]	118.5–120	741			.8122		1.4153
Mislow, O'Brien, and Schaefer	[1962]	118.5–120.5	760					1.4127
Selected value	[1967]	[e] 120±1	760	[a] 5.3 ±0.5	[d] 0.8179 ±0.001	[d] 0.8139 ±0.0015	[b] 1.4151 ±0.0003	[b] 1.4132 ±0.0004

Antoine constants: *A* 8.261, *B* 1883, *C* 230.

dt/dp at 760 mmHg, [e] 0.037 °C/mmHg

Index to the Bibliography

Numbers refer to the Bibliography, page 1–389.

References to data used in the selection of refractive index, density, boiling point, vapor pressure, and melting point are in boldface type.

Numbers in parentheses refer to sources of reviews, or theoretical calculations only.

Reference numbers under each property are listed in the order of date of publication.

References to Properties of 2-Hexanol

Refractive Index
2018, **1378**, 1828, 1748, **1273**, **486**, **1017**, **789**, 1910, **1939**, 731, **706**, **803**, **1377**, 808, **338**, **2016**, **1824**, **505**

Density at 20–30 °C Only
1378, **311**, 1748, 1273, 486, **1017**, **603**, **17**, 1377, **338**

Density at all Temperatures
2018, **1378**, **1380**, **1828**, **486**, **789**, **92**

Normal Boiling Point
1408, 1526, 2018, 1378, **311**, 1828, **1273**, 639, 1024, 1027, **1121**, 215, 1017, **1287**, 1910, 1714, **603**, 92, 17, 731, 706, 1554, 349, **803**, 1377, 808, **338**, 2016, 505

Vapor Pressure and Boiling Points at Other Pressures
486, **789**, **1939**, **1824**, 1823

Critical Temperature
(347)

Normal Melting Point
338

Association in the Liquid Phase
(1755), 1705

References to Properties of 3-Hexanol

Refractive Index
1379, **1018**, **1017**, **789**, 248, **1668**, 238, **738**, **890**, **1377**, 447, **338**, **2016**, 226, **124**, 505

Density at 20–30 °C
1018, 1017, **603**, 1668, **17**, **738**, **1377**, **338**

Density at all Temperatures
1062, 1058, 397, **1019**, **1379**, **789**

Normal Boiling Point
1058, 397, 1379, 1026, 1025, 1027, 448, 1018, 248, 1017, 720, **789**, **603**, 1714, 1923, 1668, 17, 857, **1377**, **338**, 1249, 124, 505

Vapor Pressure and Boiling Points at Other Pressures
789, **738**, **2016**

Normal Melting Point
338

Association in the Liquid Phase
(1755)

References to Properties of 2-Methyl-1-Pentanol

Refractive Index
1425, 1273, 1204, **789**, 731, 1377, 725, **338**, **1823**, 347

Density at 20–30 °C Only
1273, 1287, **1377**, 725, 338, 1823

Density at all Temperatures
1064, 1435, 1746, **789**, **347**

Normal Boiling Point
1064, 657, 1435, 1630, 1983, 1746, **1273**, 1039, 621, 1204, 1803, 1614, **1287**, 1714, 1111, **789**, 929, 1554, 731, 1895, 1260, 1377, 177, **338**, 265, 16, **1823**

Vapor Pressure and Boiling Points at Other Pressures
789, 725, **1823**

Heat of Combustion
2034, (1721)

Association in the Liquid Phase
(1755), 1705

References to Properties of 3-Methyl-1-Pentanol

Refractive Index
1273, **1030**, **787**, 799, **373**, 1214, **1377**, **2005**, **338**, **994**

Density at 20–30 °C Only
917, **826**, 1273, 1030, **1287**, 799, **176**, 1377, 338

Density at all Temperatures
1833, 704, **787**, 175

Normal Boiling Point
917, 1833, 704, 826, 1850, **1273**, **1287**, 1714, 1842, 799, **787**, 373, 1377, 1214, 2005, **338**, 1954, 994

Vapor Pressure and Boiling Points at Other Pressures
1030, **1029**, **787**, **175**, **176**

Association in the Liquid Phase
(1755)

References to Properties of 4-Methyl-1-Pentanol

Refractive Index
123, **1273**, **787**, 799, 1377, **338**

Density at 20-30°C Only
1273, **1287**, 799, 1377, 338

Density at all Temperatures
640, 123, **787**

Normal Boiling Point
640, 246, 1020, **1273**, 1121, 1204, **1287**, 1614, 933, 1714, 1978, 799, **1377**, 1663, 1593, **338**, 247

Vapor Pressure and Boiling Points at Other Pressures
347, **787**

Critical Temperature
347

Normal Melting Point
338

Association in the Liquid Phase
(1755)

References to Properties of 2-Methyl-2-Pentanol

Refractive Index
509, 412, **969**, **786**, **1275**, **1922**, **6**, **804**, **1377**, 1593, 1051, **1824**, **226**

Density at 20–30 °C Only
1275, **603**, 1922, 6, 1377, 1051

Density at all Temperatures
509, 412, 969, **1300**, **786**

Normal Boiling Point
847, 1135, 742, 743, **1960**, 412, 1463, 969, 1829, 786, 350, 1714, **603**, 6, **1377**, 804, 1051, 1311, 1543

Vapor Pressure and Boiling Points at Other Pressures
509, **786**, **1275**, **1922**, **1824**, **226**

Normal Melting Point
786

Association in the Liquid Phase
(1755), 1705

References to Properties of 3-Methyl-2-Pentanol

Refractive Index
2019, **1275**, **1923**, **785**

Density at 20–30 °C
1377, 603

Density at all Temperatures
1976, 2019, **785**

Normal Boiling Point
1976, 350, **1923**, 1714, **603**, 2019, 785, 1377

Vapor Pressure and Boiling Points at Other Pressures
1275, **785**

Association in the Liquid Phase
(1755)

References to Properties of 4-Methyl-2-Pentanol

Refractive Index
1378, 1838, 123, 239, **238**, **1032**, 1829, 472, **789**, **1922**, 1923, 467, 468, 1566, **738**, 1812, **803**, 1893, 1377, 808, **1695**, **2016**, **226**, **1458**, **1193**

Density at 20–30 °C Only
1823, 239, 238, 1922, 603, **738**, **1812**, **1893**, **1377**, **1823**, **1458**

Density at all Temperatures
655, 1378, 656, 123, **1829**, **789**, 467, 468, 891

Normal Boiling Point
655, 656, 1838, 1630, 1960, **239**, **238**, 292, 215, 1614, 1095, 1923, 1714, **789**, **603**, 526, 467, 1566, 857, 738, 1554, 1377, 431, **808**, 1695, 2016, **1823**, **226**, 1612, **1459**, 1823, 1193, 837

Vapor Pressure and Boiling Points at Other Pressures
894, 1378, **1039**, **1032**, 1829, **472**, **1922**, **789**, 1753, 1812, **803**, **891**, **1823**, 226

Normal Melting Point
1823

References to Properties of 2-Methyl-3-Pentanol

Refractive Index
1380, 123, 969, **1275**, **1922**, **784**, 738, **804**, **1377**, 338, **631**

Density at 20–30 °C Only
1275, 1922, 603, 738, 1377

Density at all Temperatures
1380, **123**, **969**, **789**

Normal Boiling Point
1526, 742, 519, 969, 775, 621, 1922, 1714, **603**, **784**, **1377**, 804, **338**, 1852

Vapor Pressure and Boiling Points at Other Pressure
1275, **784**, **738**, **631**

References to Properties of 3-Methyl-3-Pentanol

Refractive Index
509, 1315, **1273**, **1275**, **367**, 784, **790**, 2010, 1377, **2005**, **1650**, **1653**, **993**, 1743

Density at 20–30 °C Only
1315, **1273**, 1548, **1275**, **603**, **790**, 1377, **1830**, **1650**, **1653**

Density at all Temperatures
1468, **509**, **1300**, **784**, **2010**

Normal Boiling Point
1976, 1468, 1960, 1315, 521, 1859, 1638, **1273**, 1548, 1275, 350, 367, **603**, 1714, 784, 1554, 2010, 1377, **2005**, 285, 1311, 1830, 1312, 1650, 993

Vapor Pressure and Boiling Points at Other Pressures
509, 296, **1275**, **784**, **790**, 1653

Normal Melting Point
509, **790**, **1830**, 1743

Association in the Liquid Phase
(1755)

References to Properties of 2-Ethyl-1-Butanol

Refractive Index
1923, 613, 1209, **788**, **1947**, 490, **10**, 1893, **13**, 1377, **560**, **338**, 709

Density at 20–30 °C Only
1923, **613**, **1893**, 1377, **338**, **1823**

Density at all Temperatures
347, **788**

Normal Boiling Point
1614, 1767, 1714, 1923, **613**, **788**, 1554, 10, **1377**, 560, **338**, 1823, 709, 473

Vapor Pressure and Boiling Points at Other Pressures
788, **1823**, 1947, 490

Normal Melting Point
1823

Association in the Liquid Phase
(1755)

References to Properties of 2,2-Dimethyl-1-Butanol

Refractive Index
1476, **788**, **1914**, 1377, 1539, **165**

Density at 20–30 °C Only
333, 603, 1377, 165

Density at all Temperatures
190, **788**

Normal Boiling Point
190, 333, 921, 1714, 1476, 416, **603**, 788, **1377**, 165

Vapor Pressure and Boiling Points at Other Pressures
1914, **788**, 1539, 1148

Normal Melting Point
190, 165

Association in the Liquid Phase
(1755)

References to Properties of 2,3-Dimethyl-1-Butanol

Refractive Index
618, **1377**, **338**, **1539**, **1808**, **2036**, 1128

Density at 20–30 °C Only
618, **333**, 1031, **1377**, **338**, **1808**

Normal Boiling Point
618, 333, 1031, 1714, 1377, 338

Vapor Pressure and Boiling Points at Other Pressures
1539, 1808

References to Properties of 3,3-Dimethyl-1-Butanol

Refractive Index
1917, **1946**, 799, **1947**, **490**, 1119, **1539**, 633, **232**

Density at 20–30 °C Only
799, **1539**

Density at all Temperatures
1119

Normal Boiling Point
1714, 1703, 1917, **490**, 1119, 152, 828, 196, 186

Vapor Pressure and Boiling Points at Other Pressures
1918, 1946, **799**, **1947**, 1592, 1217, **1539**, 232

References to Properties of 2,3-Dimethyl-2-Butanol

Refractive Index
1168, **785**, **490**, **790**, 1377, 1051, **1299**, **753**, **1522**, **1543**, **1385**

Density at 25–30 °C Only
603, **790**, **1377**, 1051, 1299

Density at all Temperatures
567, **1343**, **785**

Normal Boiling Point
567, 1343, 740, 405, 404, 1477, 1691, 1168, 1714, **603**, **785**, 490, **1377**, 753, 1543, 1385

Vapor Pressure and Boiling Points at Other Pressures
1681, 490, **785**, **790**, 1299, 809, **1522**,

Normal Melting Point
1343, 404, **790**

Association in the Liquid Phase
(1755)

References to Properties of 3,3-Dimethyl-2-Butanol

Refractive Index
1382, **1933**, **1910**, **71**, **1566**, **1213**, 1377, **828**, 1805, **490**, 1052, **1543**, 1539, **2016**, **1193**

Density at 20–30 °C Only
1382, 1087, 1691, **603**, **1213**, **1377**, 1539

Normal Boiling Point
1477, 545, 1382, **1960**, 1832, 332, **1933**, 1941, 1910, **603**, 1714, 1566, **1377**, 1213, 828, 184, **1052**, 490, **2016**, 1543, 1193

Vapor Pressure and Boiling Points at Other Pressures
1045, 71, 484, **1539**

Normal Melting Point
446, 1477, 1832, **1933**, 1941

1-Heptanol

Properties of the Liquid Phase at Various Temperatures

Refractive Index

Measurements of the refractive index of 1-heptanol have been frequently reported in the literature, although few of these have been made on samples of known high purity. The data in table 146, which lists the more reliable values, scatters over a range of about 0.003 at 20 and 0.0012 at 25 °C. The selections at 20 and 25 °C were made to coincide as well as possible with what appeared to be the best values and to interpolate smoothly to other temperatures and wavelengths. The uncertainty is about 0.0005 at these two temperatures. Surprisingly, there have been several studies of refractive index over ranges of temperature and wavelengths, so that taken together, a comparatively wide range of conditions has been covered. The selected values in table 145 were taken from smoothed curves of the experimental values plotted against temperature and $1/(\lambda-1000)^{1.6}$. Falk [1909] carried out measurements from 22 to 71.5 °C at a series of wavelengths throughout the visible region, and his data agree favorably with later measurements. Eykman [1919] also measured refractive index over the visible spectrum at 18.7 and 79.9 °C. Other references which contain data used in arriving at table 145 are Sherrill [1930], Deffet [1931], Bilterys and Gisseleire [1935], and Vogel [1948].

Density

As for 1-hexanol, density data extend back for a considerable period. Cross, C. J. [1877] reported values from 0 to 27 °C. More recent values based on careful measurements at 20 and 25 °C have been reported by Norris and Cortese [1927], Sherrill [1930], Ellis and Reid [1932],

TABLE 143. 1-Heptanol. Selected values. Physical and thermodynamic properties

Temp. °C	Refractive Index, n_D	Density g cm^{-3}	Vapor Pressure, mmHg
0		0.8364	
10	1.4277	.8294	
20	1.4242	.8223	
25	1.4223	.8187	
30	1.4203	.8151	
40	1.4164	.8077	
50	1.4125	.8002	
60	1.4087	.7926	
70	1.4048	.7848	7.0
75			9.7
75.4			10
80	1.4009	.7768	13.4
85			18.0
90		.7687	24.0
95			31.6
100		.7603	41.0
105			52.7
110		.7518	67.0
115			84.3
118.9			100
120		.7431	105.1
125			129.8
130		.7342	159.
135			194.
135.9			200
140		.7250	234.
145			280.
150			334.
155			395.
155.4			400
160			465.
165			544.
170			633.
175			733.
176.3			760

Data For Phase Transitions

Initial	Final	Temp. °C	dt/dP deg mm^{-1}	Pressure mmHg	ΔH kcal mol^{-1}	$d\Delta H/dt$ cal deg^{-1} mol^{-1}	ΔS cal deg^{-1} mol^{-1}	ΔC_p cal deg^{-1} mol^{-1}
c	liq	−34.0±0.3		760	3.16±0.05	28.1±0.5	13.2±0.2	14.9±0.5
c	liq	−32.8±0.3						
liq	g	−32.8±0.3						
liq	g	25		0.15±0.05	16.5±0.7	−23.8±0.7	55.3±2	−23.8±0.7
liq	g	176.3±0.3	0.0459	760	11.5±0.5		25.6±1	

Condensed Phase Heat Capacity

State	Temp. °C	C_p cal deg^{-1} mol^{-1}
c	−34.0	41.3±0.5
liq	−34.0	56.2±0.2

Properties of the Saturated Real Gas

Temp. °C	H^r-H^0 kcal mol^{-1}	S^r-S^0 cal deg^{-1} mol^{-1}	$C_p-C_p^0$ cal deg^{-1} mol^{-1}

Data for the Standard States at 25 °C

State	Heat of Combustion ΔH_c^0 kcal mol^{-1}	Heat of Formation ΔH_f^0 kcal mol^{-1}	Entropy S^0 cal deg^{-1} mol^{-1}	Gibbs Energy of Formation ΔG_f^0 kcal mol^{-1}	Heat Capacity, C_p cal deg^{-1} mol^{-1}
liq	−1109.1±0.4	−95.8±0.4	76.5±1	−34.0±0.4	66.5±0.5
g	−1125.6±0.8	−79.3±0.8	114.8±0.7	−28.9±0.8	42.7±0.5

Critical Constants

Temp. 360 °C, 633. K	Pressure atm	Density 0.267 g cm^{-3}

Constants in Vapor Pressure and Density Equation								
Antoine Equation				Francis Equation				
Temp. Range	A	B	C	Temp. Range	A	$B\times10^3$	C	E
60 to 176 °C	6.64767	1140.64	126.56	0 to 140 °C	1.03886	0.3553	121.49	600

Table 144. 1-Heptanol. Selected values. Thermodynamic functions of the ideal gas at one atmosphere

Temperature K	Entropy S^0 cal deg^{-1} mol^{-1}	Heat Capacity C_p^0 cal deg^{-1} mol^{-1}	Enthalpy Function $(H^0-H^0_0)/T$ cal deg^{-1} mol^{-1}	Gibbs Energy Function $(G^0-H^0_0)/T$ cal deg^{-1} mol^{-1}	Heat of Formation ΔH_f^0 kcal mol^{-1}	Gibbs Energy of Formation ΔG_f^0 kcal mol^{-1}
0	0	0	0	0	−68.6	−68.6
273.15	111.26	40.11	26.55	−84.71	−78.5	−33.1
298.15	114.83	42.70	27.80	−87.03	−79.3	−28.9
300	115.07	42.91	27.88	−87.19	−79.4	−28.6
400	128.79	53.62	32.98	−95.81	−82.2	−11.2
500	141.82	63.51	38.12	−103.70	−84.5	6.8
600	154.09	71.92	43.05	−111.03	−86.4	25.3
700	165.69	79.15	47.67	−118.02	−87.8	44.0
800	176.67	85.32	52.02	−124.67	−88.8	62.9
900	187.02	90.65	56.04	−130.98	−89.5	82.0
1000	196.83	95.25	59.72	−137.11	−89.9	101.0

Table 145. 1-Heptanol. Selected values. Refractive index at various temperatures and wavelengths

Symbol	Wavelength, Å	Refractive Index, n								
		15 °C	20 °C	25 °C	30 °C	40 °C	50 °C	60 °C	70 °C	80 °C
$\mathrm{He_{red}}$	6678.2	1.4235	1.4218	1.4200	1.4180	1.4140	1.4101	1.4068	1.4025	1.3986
$\mathrm{H_c}$	6562.8	1.4237	1.4220	1.4202	1.4182	1.4142	1.4103	1.4071	1.4027	1.3988
$\mathrm{Na_D}$	5892.6	1.4260	1.4242	1.4223	1.4203	1.4164	1.4125	1.4087	1.4048	1.4009
$\mathrm{Hg_e}$	5460.7	1.4277	1.4257	1.4239	1.4219	1.4179	1.4141	1.4103	1.4064	1.4023
$\mathrm{He_{blue}}$	5015.7	1.4305	1.4283	1.4266	1.4244	1.4205	1.4166	1.4128	1.4090	1.4048
$\mathrm{H_F}$	4861.3	1.4315	1.4294	1.4276	1.4254	1.4215	1.4176	1.4138	1.4100	1.4057
$\mathrm{Hg_g}$	4358.3	1.4356	1.4335	1.4318	1.4296	1.4256	1.4218	1.4179	1.4143	1.4096
$\mathrm{H_{G'}}$	4340.5	1.4358	1.4337	1.4319	1.4297	1.4258	1.4219	1.4181	1.4145	1.4098

Carter and Jones [1934], Butler, Ramchandani, and Thomson [1935], Jones, Bowden, Yarnold, and Jones [1948], Cook [1952], and Robinson, Edmister, and Dullien [1966]. Except for the value of Butler, Ramchandani, and Thomson at 25 °C, which is 0.0018 g cm^{-3} high, all these data fell within 0.0005 g cm^{-3} of the values calculated from the Francis equation. Data covering the widest temperature range, from 0 to 140 °C, have been obtained by Bingham and Fornwalt [1930]. Most of their values run 0.0005 to 0.0008 g cm^{-3} higher than the calculated ones. Data at various temperatures have also been reported by Carrara and Ferrari [1906], 22 to 85 °C; Falk [1909], 25 to 68 °C; Sherrill [1930], 0 to 20 °C; Deffet [1931], 0 to 30 °C; and Bilterys and Gisseleire [1935], 0 to 30 °C. McKinney, Skinner and Staveley [1959] made an accurate determination at 0 °C, and Sackmann and Sauerwald reported a value of 0.8617 g cm^{-3} at -35.5 °C. Efremov [1966] measured approximate values of density of saturated liquid and vapor from 0 to 360 °C.

Vapor Pressure and Boiling Point

Reported values of the normal boiling point range over several degrees. Table 146 contains a collection of the better values. The selected value of 176.3 °C is near the middle of the range which they represent and the uncertainty is about 0.3 °C. The only two systematic studies of vapor pressure at various temperatures are by Butler, Ramchandani, and Thomson [1935] and Thomas and Meatyard [1963]. The Antoine constants are based on these data and on several additional measurements of the boiling point at various pressures. The observed vapor pressures of Butler, Ramchandani, and Thomson from 60 to 153 °C are within about 2 mm of the calculated ones. The calculated values agree closely with the ones observed by Thomas and Meatyard at the lower end of their range of around 68 °C but diverge at increasing temperatures so that the observed values are 9 to 12 mmHg below the calculated ones from 143 °C to the boiling point. Sample comparisons of observed and calculated boiling points at low pressures are Sherrill [1930], 84.7 °C/20 mmHg observed, 86.8 °C calculated; Verkade and Coops [1927], 68.4–68.6 °C/7.0 mmHg observed, 70.0 °C calculated; and Ellis and Reid [1932], 99.3–99.5 °C/40 mmHg observed, 99.5 °C calculated.

Critical Properties

Critical Temperature

Brown, J. C. [1906] made several observations of the critical temperature. These varied from 363.25 to 366.5 °C. Efremov [1966] obtained 360 °C by observing the disappearance of the meniscus. It is difficult to assign a reason for this difference, since neither investigator gave specific information on sample purity or on details of the measurement. But since Efremov's values on other alcohols were in good agreement with accurate measurements by other investigators, and since his result for 1-heptanol was close to the value obtained by interpolation from the other normal alkanols, his value was selected.

Solid-Liquid Phase Equilibria

Normal Melting Point and Triple Point

A collection of the most reliable melting point data is given in table 146. McKenna, Tartar, and Lingafelter [1949] purified their sample by fractional distillation under nitrogen and protected it from contact with moisture during the measurement. The melting point was determined in a specially designed cryostat containing nitrogen in the gas phase. Temperature was measured with a carefully calibrated thermocouple. It seems unlikely that their value could be in error by more than a few 0.1 °C, and this was selected as the normal melting point. This value is also reasonably close to the other data in table 146. Parks, Kennedy, Gates, Mosley, Moore, and Renquist [1956] determined the melting point in an aneroid calorimeter. They concluded that their sample contained 1.8 mol percent impurity from an analysis of the melting curve. The initial freezing point of this sample was -33.2 °C, and this gives -32.8 °C for the melting point of pure 1-heptanol. Although the authors did not state so explicitly, they apparently sealed the alcohol sample in the calorimeter with a helium atmosphere. Thus their melting point should be close to the triple point for 1-heptanol. They assumed that most of the impurities present were dissolved air and water, initially present in the alcohol before sealing. Again it seems necessary to conclude that there is an unexpectedly large difference between the melting point in equilibrium with air or nitrogen at 1 atm and the triple point. This is similar to the situation for 2-propanol, 1-butanol, and 2-methyl-2-propanol. Since accurate data for the melting point in air and the triple point are available for the same compound in only a few instances, it is difficult to determine how widespread this phenomenon is among the alcohols. If the difference between the melting point in air and the triple point of 1-heptanol is due to dissolved nitrogen, and if it forms an ideal solution, then the alcohol must contain 4.5 mol percent, or 1.13 weight percent, nitrogen at the melting point.

Heat of Fusion

Parks, Kennedy, Gates, Mosley, Moore, and Renquist [1956] obtained 3.182 kcal mol^{-1} at -32.8 °C in the aneroid calorimeter. This is converted to 3.16 kcal mol^{-1} at -34.0 °C. The heat capacity of the solid and liquid at the melting point were obtained by extrapolating their heat capacity data.

TABLE 146. 1-Heptanol. Reported values. Simple physical properties

Investigators		Vapor Pressures and Boiling Points		Freezing Point	Density, *d* g cm^{-3}		Refractive Index, n_D	
		°C	mmHg	t_m, °C	20 °C	25 °C	20 °C	25 °C
1-Heptanol, $C_4H_{16}O$, mol wt. 116.205, state at 25 °C liq								
Carrara and Coppadoro	[1903]	175	760	−36.5				
Carrara and Ferrari	[1906]	175.7	760		0.8187			
Lowry	[1914]				.8237			
Willcox and Brunel	[1916]	172.5–173.5	760					
Levene and Taylor	[1918]	175.5–176.5	760		.8254		1.42463	
Timmermans	[1922a]	174.0	760	−34.6				
Wood and Comley	[1924]	174.8–175.1	760					
Norris and Cortese	[1927]	175.8–176.2	760			0.8187		1.4224
Verkade and Coops	[1927]	174.8	760					
Garner, McKie, and Knight	[1927]	174.8	760					
Harkins	[1928]				.82209			
Malone and Reid	[1929]	176.2	760					
Sherrill	[1930]	176.9						
Errera and Sherrill	[1930]				.8214			
Bingham and Fornwalt	[1930]	174.6–176.0	760		.8218			
Deffet	[1931]	176.35	760	−34.1		.81922		
Ellis and Reid	[1932]	176.3	760			.81915		1.4222
Butler, Thomson, and Maclennan	[1933]	175.6				.81960	1.42337	
Burdick and Adkins	[1934]					.8250		1.4237
Carter and Jones	[1934]					.8184		1.4226
Bilterys and Gisseleire	[1935]	176.81	760	−33.8		.81901	1.4240	
Butler, Ramchandani, and Thomson	[1935]	175.6	760			.82053	1.4257	
Komarewsky and Coley	[1941a]	173.5–175.0	760				1.4245	
Komarewsky and Coley	[1941b]							1.4225
Jones, Bowden, Yarnold, and Jones	[1948]					.8188		
Vogel	[1948]	175	760		.8219		1.42351	
McKenna, Tartar, and Lingafelter	[1949]	175.4	760	−34.03				
Tschamler, Richter, and Wettig	[1949b]	174.0	760	−34.9				
Adkins and Rosenthal	[1950]							1.4230
Mumford and Phillips	[1950]	175.9	760		.8236	.8202	1.4238	
Pichler, Ziesecke, and Traeger	[1950]	176.0	760		.8219		1.4241	
Sackmann and Sauerwald	[1950]			−35.5				
Schiessler, Speck, and Dixon	[1951]	178	760				1.4238	
Oppenheim	[1951]	175.0–175.6	760	−35.0				1.42273
Searles	[1951]	175–177	760				1.4243	
von Errichsen	[1952]	176.0–176.1	760		.8223		1.4249	
Cook	[1952]	176.1	760	−33	.8228		1.4243	
McKenna, Tartar and Lingafelter	[1953]	176.4	760				1.4218	
Brewster	[1954]						1.4242	
Wotiz and Webster	[1956]							1.4221
Thomas and Meatyard	[1963]	176.6	760				1.4248	1.4228
Robinson, Edmister, and Dullien	[1966]						1.42425	
Selected value	[1967]	176.3±0.3	760	−34.0	0.8223	0.8187	1.4242	1.4223
		75.4±0.5	10	±0.3	±0.0003	±0.0005	±0.0003	±0.0003

Antoine constants: A 6.64767, *B* 1140.64, *C* 126.56

dt/*dp* at 760 mmHg, 0.0459 °C/mmHg

Properties of the Liquid at 25 °C

Heat Capacity

The heat capacity at 25 °C was obtained by interpolation of the smoothed values reported by Parks, Kennedy, Gates, Mosley, Moore, and Renquist [1956]. These are the only heat capacity data.

Absolute Entropy

Parks, Kennedy, Gates, Mosley, Moore, and Renquist [1956] report a third law entropy based on observed heat capacity and auxiliary data down to 80 K. This is shown on table 144. The long extrapolation to 0 K gives rise to an appreciable uncertainty in this value, and a somewhat smaller value was selected to achieve internal consistency with the heat of vaporization and the gas phase entropy.

Heat of Combustion

When converted to current units and standard state, Zubov [1898], as reported by Swietoslawski [1920], obtained a heat of combustion of −1106.0 kcal mol^{-1}, Verkade and Coops obtained −1108.1 kcal mol^{-1}, and Chao and Rossini [1965] obtained −1109.6 kcal mol^{-1}. Because of some uncertainty in the purity of the sample used by Chao and Rossini, a compromise of −1109.1 kcal mol^{-1} was selected for ΔHc^0.

Vapor-Liquid Equilibrium at 25 °C

Vapor Pressure

The lowest temperature for direct measurement of vapor pressure was 60 °C by Butler, Ramchandani, and Thomson [1935]. Extrapolation of their data to 25 °C by use of their vapor pressure equation gives 0.22 mm. The selected Antoine constants give 0.13 mm at 25 °C. Both these values have a large uncertainty, and a compromise of 0.15 mm was selected.

Heat of Vaporization

There are no direct measurements of heat of vaporization, or even vapor pressure measurements, at 25 °C. The vapor pressure equation of Butler, Ramchandani, and Thomson [1935], based on measurements at higher temperatures, predicts a heat of vaporization of 16.41 kcal mol^{-1} at 25 °C, assuming an ideal gas. The value of $\Delta H_v = 20.2$ kcal mol^{-1} is obtained from the selected Antoine constants at 25 °C, but little reliance can be placed on this result because of the long extrapolation below the experimental range. At 60 °C, the lower limit of experimental measurements, the Antoine equation gives a heat of vaporization of 16.64 kcal mol^{-1}. If we assume an average temperature coefficient of −25 cal deg^{-1} mol^{-1} between 25 and 60 °C, the heat of vaporization becomes 17.51 kcal mol^{-1} at 25 °C. The third law entropy found by Parks, Kennedy, Gates, Mosley, Moore, and Renquist [1956], the selected ideal gas entropy, and the vapor pressure at 25 °C imply a heat of vaporization of 16.05 kcal mol^{-1}. All of these values contain large uncertainties and the selected value was a compromise among them.

Temperature Derivative of the Heat of Vaporization

At the equilibrium vapor pressure at 25 °C, 1-heptanol should behave as an ideal gas. Therefore, the temperature derivative of the heat of vaporization is equal to the difference between the heat capacities of the ideal gas and of the liquid.

Vapor-Liquid Equilibrium at the Normal Boiling Point

Normal Boiling Point

The value calculated from the Antoine equation was selected.

Heat of Vaporization

The Antoine equation gave 11.03 kcal mol^{-1} using the selected constants and an estimated second virial coefficient of −1.5 liter mol^{-1}. Brown, J. C. [1906] obtained 12.26 kcal mol^{-1} by a calorimetric measurement. Although neither of these values can be considered as accurate, the difference is difficult to reconcile. It is unlikely that the vapor pressure calculation could be more than about 0.5 kcal in error, so a value of 11.5 kcal mol^{-1} was selected. There are no data upon which to base a reliable calculation of the temperature derivative of ΔH_v.

Properties of the Ideal Gas State

Ideal gas thermodynamic functions have been published by Chermin [1961] and by Green [1961]. These are obtained by applying the methylene increment to data for the lower alcohols, as explained in the discussion of 1-pentanol. The entropy and heat capacity listed in these two sets of tables agree within 0.1 cal deg^{-1} mol^{-1} at 298.15 K and within 1 cal deg^{-1} mol^{-1} in the range from 298.15 to 1000 K. The values of Green were selected.

Index to the Bibliography

Numbers refer to the Bibliography, page 1–389.

References to data used in the selection of refractive index, density, boiling point, vapor pressure, and melting point are in boldface type.

Numbers in parentheses refer to sources of reviews, or theoretical calculations only.

Reference numbers under each property are listed in the order of date of publication.

Refractive Index
508, 515, **1043**, 123, 506, 513, **1273**, 1604, 398, **486**, 254, 248, 274, 146, 253, 1112, 1304, 799, **926**, **927**, 1222, **6**, **1856**, 1420, **13**, **1224**, 1246, **1377**, **1293**, **1593**, **1558**, 29, **1865**, **338**, **1152**, **207**, **630**, **1990**, **1758**, **1494**

Density at 20–30 °C Only
1349, 576, **1087**, **1043**, **1273**, **707**, **495**, **486**, **254**, **248**, 274, 1112, **253**, **1288**, 799, 1222, **6**, **853**, **1856**, **1420**, **1224**, 1377, 338, 1865, 1494

Density at all Temperatures
369, 2012, **510, 273, 515, 509,** 123, 513, **1848, 1604, 150, 398, 146,** 1527, **1154,** 481

Normal Boiling Point
643, 1576, 369, 868, 2012, 1349, 2033, 658, 272, 273, 1827, 1395, 1435, 515, 1631, 1284, 1960, 1043, **1294,** 509, 123, 1774, 1595, 1273, **573,** 1121, 150, 1597, **398,** 486, **254,** 1981, **146,** 1288, 1952, 799, 926, 6, 1278, 1856, 1807, **1153,** 1007, 1247, 1377, 1224, 1293, 1593, 1558, **338,** 29, 1865, 1152, 331, 1852

Vapor Pressure and Boiling Points at Other Pressures
1838, 710, **513, 1848, 1604, 486, 248, 253, 1304,** 305, **1899, 207, 630, 1990, 1758**

Critical Temperature
218, 748, 649, 481

Critical Volume and Density
481

Normal Melting Point
555, 272, 1336, **1774, 398,** 146, **1153, 1807,** 1527, 1293, 338, 1328

Heat of Fusion
1328

Heat Capacity of the Liquid
1328

Calorimetric Heat of Vaporization at the Normal Boiling Point
219

Heat of Combustion
2033, (1721), 1848, (1507), (626), 287, 288

Third Law Entropy
1328

Molecular Vibration Frequencies and Spectra
1613, 1012, 456, 797

Thermodynamic Functions of the Ideal Gas
623, 291

Association in the Liquid Phase
182, (1754), 78

Isomeric Heptanols

Refractive Index

Observed and selected values of the refractive index at the sodium D-line are shown at 20 and 25 °C on the unnumbered tables for the isomeric heptanols. Where data exist, values at other temperatures are listed in tables 147 to 152. No measurements have been made above 30 °C. There have been few accurate systematic investigations of this group of compounds. Most of the accurate data have been obtained by Pichler, Ziesecke, and Traeger [1950], Cook [1952], and Thomas and Meatyard [1963]. Pickard and Kenyon and Levene, Huston, Whitmore, and their co-workers, have also published much data over a long period of time.

Selected values of the refractive indices of five heptanols at various wavelengths are listed in table 153. These were obtained by drawing smooth curves through observed data plotted versus $1/(\lambda-1000)^{1.6}$, and where necessary correcting back to the selected value of n_D at 20 °C. These selections were based on the data of Eykman [1919], de Graef [1925 and 1931], Sherrill [1930], and Timmermans and Hennaut-Roland [1955].

Density

Density data at 20 and 25 °C are reported on the unnumbered tables. Most of these data are relatively inaccurate, and consequently there are large discrepancies among different investigators. There are few data of any kind outside the vicinity of room temperature. However, sufficient data are available for seven of these compounds to allow the density to be expressed as a function of temperature by a least squares calculation. The constants in the Francis equation and the densities calculated from this equation for six of these compounds are given in tables 147 to 152. The data for 3-ethyl-3-pentanol did not cover a range large enough to determine the constant *E*, and density was therefore expressed by a linear function of temperature. Thomas and Meatyard [1963] measured the density of 2-heptanol, 3-heptanol, 4-heptanol, and 2,4-dimethyl-3-pentanol from room temperature to around 140 °C. Thus the selected densities for these compounds at higher temperatures are based mostly on their results. Poleteff [1891], Masson [1909], Sherrill [1930], and Malinovskii, Volkova, and Morozova [1949] have reported values below room temperature for these compounds. Owen, Quayle, and Beavers [1930] have reported values at 0 and at around 60 °C. Weissler [1948] has determined densities at 30 °C, and Pickard and Kenyon [1912 and 1913] have obtained values at temperatures up to 120 °C. Owen, Quayle, and Beavers [1930] were the principal source of density data outside room temperature range for 3-methyl-3-hexanol and 3-ethyl-3-pentanol.

Vapor Pressure and Boiling Point

Observed values of boiling points at various pressures are shown in the unnumbered tables. Thomas and Meatyard [1963] have conducted the only systematic measurements of vapor pressure over a range of temperature. They studied 2-heptanol, 3-heptanol, 4-heptanol, 2-methyl-2-hexanol, and 2,4-dimethyl-3-pentanol.

TABLE 147. Isomeric Heptanols. Selected values. Physical properties of the liquid

2-Heptanol				3-Heptanol				4-Heptanol			
Temp. °C	Refractive Index, n_D	Density g cm^{-3}	Vapor Pressure, mmHg	Temp. °C	Refractive Index, n_D	Density g cm^{-3}	Vapor Pressure, mmHg	Temp. °C	Refractive Index, n_D	Density g cm^{-3}	Vapor Pressure, mmHg
0		0.8324		0		0.8374		0		0.8338	
10	1.4249	.8251		10	1.4260	.8293		10		.8264	
20	1.4210	.8177		20	1.4220	.8212		20	1.4200	.8187	
25	1.4190	.8139		25	1.4200	.8170		25	1.418	.8149	
30	1.4171	.8101		30		.8129		30		.8109	
40		.8024		40		.8044		40		.8024	
50		.7944		50		.7958		50		.7947	7.0
59.1			10	58.6			10	55			9.8
60		.7862	10.6	60		.7871	11.0	55.3			10
65			14.6	65			15.3	60		.7862	13.5
70		.7778	19.8	70		.7782	20.8	65			18.3
75			26.5	75			28.0	70		.7775	24.4
80		.7693	35.0	80		.7691	37.0	75			32.1
85			45.5	85			48.2	80		.7686	41.8
90		.7604	58.5	90		.7599	62.1	85			53.7
95			74.3	95			79.1	90		.7593	68.4
100		.7513	93.5	100		.7504	99.6	95			86.2
101.5			100	100.1			100	98.3			100
105			116.3	105			124.	100		.7498	107.6
110		.7420	143.4	110		.7407	153.	105			133.
115			175.	115			187.	110		.7400	163.
118.4			200	116.7			200	115			199.
120		.7324	212.	120		.7309	227.	115.1			200
125			256.	125			274.	120		.7299	240.
130		.7224	305.	130		.7208	327.	125			289.
135			362.	135			388.	130		.7195	344.
138.0			400	136.0			400	134.5			400
140		.7122	427.	140		.7104	457.	135			408.
145			500.	145			535.	140		.7086	480.
150		.7016	582.	150		.700	623.	145			562.
155			675.	155			722.	150			655.
159.2			760	156.8			760	155.5			760
160		.691	777.	160			832.	160			876.

Constants	Temp. Range	A	B	C	E	Constants	Temp. Range	A	B	C	E	Constants	Temp. Range	A	B	C	E
Antoine eq	50 to 159 °C	6.33006	977.8	124.3		Antoine eq	55 to 156 °C	6.33032	948.1	120.2		Antoine eq	47 to 155 °C	6.67161	1140.3	145.8	
Francis eq	0 to 150 °C	1.11013	2.551×10^{-4}	166.64	600	Francis eq	0 to 140 °C	1.05024	4.440×10^{-4}	127.72	600	Francis eq	0 to 140 °C	1.14550	2.169×10^{-4}	186.99	600

Table 148. Isomeric Heptanols. Selected values. Physical properties of the liquid

2-Methyl-1-hexanol				3-Methyl-1-hexanol				4-Methyl-1-hexanol			
Temp. °C	Refractive Index, n_D	Density g cm^{-3}	Vapor Pressure, mmHg	Temp. °C	Refractive Index, n_D	Density g cm^{-3}	Vapor Pressure, mmHg	Temp. °C	Refractive Index, n_D	Density g cm^{-3}	Vapor Pressure, mmHg
10		0.835		10		0.834		10		0.832	
20	1.423	.827		20	1.424	.828		20	1.425	.824	
25	1.421	.823		25	1.422	.824		25	1.423	.820	
30		.819		30	1.420	.820		30		.816	
65.			10	75.			10	75.			10
70			13.	80			13.	80			14.
80			23.	90			23.	90			25.
90			38.	100			38.	100			43.
100			61.	110			62.	110			71.
110			95.	120.			100	117.			100
111.			100	130			150.	120			112.
120			146.	137.			200	130			171.
128.			200	140			228.	134.			200
130			219.	150			338.	140			252.
140			322.	154.			400	150			363.
146.			400	160			493.	153.			400
150			465.	170			707.	160			507.
160			661.	172.			760	170			694.
164.			760					173.			760

Constants	Temp. Range	*A*	*B*	*C*	*E*	Constants	Temp. Range	*A*	*B*	*C*	*E*	Constants	Temp. Range	*A*	*B*	*C*	*E*
Antoine eq	70 to 165 °C	9.273	2794.	273.		Antoine eq	80 to 172 °C	9.622	3000.	273.		Antoine eq	75 to 175 °C	6.7232	1145.	125.	
Francis eq						Francis eq						Francis eq					

TABLE 149. Isomeric Heptanols. Selected values. Physical properties of the liquid

2-Methyl-2-hexanol

Temp. °C	Refractive Index, n_D	Density g cm^{-3}	Vapor Pressure, mmHg
0		0.8308	
10	1.4149	.8227	
20	1.4190	.8144	
25	1.4170	.8103	
30		.8060	
35			4.5
40		.7975	6.5
45			9.1
46.4			10
50		.7888	12.6
55			17.2
60		.7798	23.2
65			30.8
70		.7707	40.4
75			52.4
80		.7613	67.3
85			85.5
88.4			100
90		.7517	107.5
95			134.
100		.7417	166.
104.6			200
105			203.
110		.7315	248.
115			299.
120		.7208	360.
123.0			400
125			428.
130			509.
135			600.
140			704.
142.5			760
145			821.

Constants	Temp. Range	*A*	*B*	*C*	*E*
Antoine eq	38 to 143 °C	6.95661	1240.3	161.8	
Francis eq	0 to 115 °C	0.90535	5.924×10^{-4}	26.09	350

5-Methyl-2-hexanol

Temp. °C	Refractive Index, n_D	Density g cm^{-3}	Vapor Pressure, mmHg
10		0.822	
20	1.419	.814	
25	1.417	.810	
30		.806	
80			45.
90			72.
97.			100
100			112.
110			169.
114.			200
120			251.
130			365.
132.			400
140			522.
150			734.
151.			760

Constants	Temp. Range	*A*	*B*	*C*	*E*
Antoine eq	75 to 155 °C	8.965	2580.	273.	
Francis eq					

2-Methyl-3-hexanol

Temp. °C	Refractive Index, n_D	Density g cm^{-3}	Vapor Pressure, mmHg
10	1.426	0.831	
20	1.422	.824	
25	1.420	.820	
30		.816	
40		.808	
50		.800	10
60			19.
70			35.
80			59.
90			95.
91.			100
100			148.
107.			200
110			220.
120			318.
127.			400
130			446.
140			609.
147.			760

Constants	Temp. Range	*A*	*B*	*C*	*E*
Antoine eq	50 to 147 °C	6.2492	918.	125.	
Francis eq					

TABLE 150. Isomeric Heptanols. Selected values. Physical properties of the liquid

3-Methyl-3-hexanol

Temp. °C	Refractive Index, n_D	Density g cm^{-3}	Vapor Pressure, mmHg
0		0.843	
10		.8342	
20	1.4226	.8250	
25	1.421	.8204	
30		.8158	
40		.807	
45.			10
50		.797	14.
60		.788	25.
70			45.
80			74.
86.			100
90			118.
100			179.
103.			200
110			263.
120			374
122.			400
130			519.
140			701.
142.4			760

Constants	Temp. Range	A	B	C	E
Antoine eq	50 to 143 °C	6.178	883.	125.	
Francis eq	0 to 65 °C	0.8767	8.58×10^{-4}	20.1	600

3,4-Dimethyl-1-pentanol

Temp. °C	Refractive Index, n_D	Density g cm^{-3}	Vapor Pressure, mmHg
10		0.838	
20	1.428	.831	
25	1.426	.827	
30		.823	
40		.815	
50		.806	
109.			100
110			105.
120.			156.
126.			200
130			229.
140			329.
145.			400
150			466.
160			648.
165.			760

Constants	Temp. Range	A	B	C	E
Antoine eq	120 to 165 °C	8.874	2625.	273.	
Francis eq					

2,4-Dimethyl-2-pentanol

Temp. °C	Refractive Index, n_D	Density g cm^{-3}	Vapor Pressure, mmHg
0		0.832	
10		.822	
20	1.417	.8120	
25	1.415	.808	
30		.803	
50			22.
60			40.
70			68.
78.			100
80			110
90			170.
94.			200
100			254.
110			365.
112.			400
120			511.
130			696.
133.			760

Constants	Temp. Range	A	B	C	E
Antoine eq	55 to 135 °C	6.129	838.	125.	
Francis eq					

TABLE 151. Isomeric Heptanols. Selected values. Physical properties of the liquid

3-Ethyl-3-Pentanol			
Temp. °C	Refractive Index, n_D	Density g cm^{-3}	Vapor Pressure, mmHg
0		0.861	
10		.852	
15	1.4327		
20	1.4301	.8445	
25	1.4277	.8400	
30		.835	
35			5.4
40		.826	7.7
43.7			10
45			10.9
50		.817	15.1
55			20.6
60		.807	27.6
65			36.4
70			47.5
75			61.2
80			77.8
85			98.0
85.5			100
90			122.
95			151.
100			184.
102.1			200
105			223.
110			269.
115			321.
120			381
121.5			400
125			449.
130			525.
135			612.
140			708.
142.5			760
145			816.

Constants	Temp. Range	*A*	*B*	*C*	*E*
Antoine eq	35 to 143 °C	6.29473	948.9	135.5	
Francis eq	0 to 45 °C	0.8656	12.18×10^{-4}		

2,2-Dimethyl-3-pentanol			
Temp. °C	Refractive Index, n_D	Density g cm^{-3}	Vapor Pressure, mmHg
0		0.841	
10		.833	
20	1.423	.826	
25	1.421	.822	
30		.818	
39.			10
40			11.
50			21.
60			38.
70			64.
79.			100
80			104.
90			160.
95.			200
100			237.
110			339.
115.			400
120			472.
130			640.
136.			760

Constants	Temp. Range	*A*	*B*	*C*	*E*
Antoine eq	45 to 138 °C	6.050	827.	125.	
Francis eq					

2,3-Dimethyl-3-pentanol			
Temp. °C	Refractive Index, n_D	Density g cm^{-3}	Vapor Pressure, mmHg
0		0.858	
10		.849	
20	1.428	.840	
25	1.426	.836	
30		.831	
42.			10
50			17.
60			31.
70			53.
80			87.
83.			100
90			136.
99.			200
100			204.
110			297.
119.			400
120			418.
130			573.
139.			760
140			767.

Constants	Temp. Range	*A*	*B*	*C*	*E*
Antoine eq	45 to 140 °C	6.115	856.	125.	
Francis eq					

Table 152. Isomeric Heptanols. Selected values. Physical properties of the liquid

2,4-Dimethyl-3-pentanol

Temp. °C	Refractive Index, n_D	Density g cm^{-3}	Vapor Pressure, mmHg
0		0.8464	
10	1.421	.8382	
20	1.425	.8296	
25	1.423	.8253	
30	1.420	.8209	
35			6.4
40		.8119	9.2
41.3			10
45			12.8
50		.8027	17.6
55			23.7
60		.7932	31.6
65			41.4
70		.7834	53.7
75			68.9
80		.7733	87.3
83.0			100
85			109.5
90		.7629	136.1
95			168.
99.4			200
100		.7521	205.
105			248.
110		.741	298.
115			356.
118.4			400
120		.729	422.
125			497.
130			583.
135			679.
138.8			760
140			787.

Constants	Temp. Range	*A*	*B*	*C*	*E*
Antoine eq	35 to 139 °C	6.49430	1029.6	146.1	
Francis eq	0 to 120 °C	1.22429	1.878×10^{-4}	226.71	600

2-Methyl-2-Ethyl-1-butanol

Temp. °C	Refractive Index, n_D	Density g cm^{-3}	Vapor Pressure, mmHg
0		0.841	
10		.834	
20	1.426	.828	
25	1.424	.824	
30		.820	
80			30.
90			53.
100			87.
103.			100
110			137.
119.			200
120			210.
130			309.
137.			400
140			443.
150			619.
156.			760

Constants	Temp. Range	*A*	*B*	*C*	*E*
Antoine eq	85 to 155 °C	6.632	1056.	125.	
Francis eq					

Constants	Temp. Range	*A*	*B*	*C*	*E*
Antoine eq					
Francis eq					

TABLE 153. Isomeric heptanols. Selected values refractive index at various wavelengths at 25 °C

Symbol	Wavelength, angstroms	2-Heptanol	4-Heptanol	3-Methyl-3-hexanol	3-Ethyl-3-pentanol	2,4-Dimethyl-2-pentanol
He_{red}	6678.2	1.4184	1.4176	1.4203	1.4277	1.4151
H_c	6562.8	1.4186	1.4179	1.4205	1.4279	1.4153
Na_D	5892.6	1.4210	1.4200	1.4226	1.4301	1.4170
Hg_e	5015.7	1.4224	1.4218	1.4244	1.4319	1.4187
He_{blue}	4861.3	1.4251	1.4242	1.4267	1.4343	1.4213
H_F	4358.3	1.4262	1.4251	1.4277	1.4354	1.4224
Hg_g	4340.5		1.4293	1.4318	1.4394	1.4271
$H_{G'}$			1.4294	1.4319	1.4395	1.4273

The Antoine constants calculated from the experimental data for these compounds, and also for 3-ethyl-3-pentanol, are given in tables 147 to 152. A nonlinear least-quares procedure, as explained in appendix B, was used to fit the data for 2-heptanol. The constants for the other five compounds were calculated by a linear least squares procedure after converting the Antoine equation to a form which is linear in the constants. This procedure is also described in appendix B.

For the other heptanols, there is insufficient data to carry out least square calculations or to fix the magnitude of the Antoine C constant with any confidence. In most cases there were no more than about three boiling points outside the vicinity of 1 atm. For these compounds, plots of log P versus $1/(t+273)$ and $1/(t+125)$ were prepared. The Antoine constants were calculated from the plot which gave the straightest line. Constants obtained in this way have value only for making rough interpolations of boiling points or vapor pressures between the experimental points. Selected normal boiling points were calculated from the Antoine equation wherever the constants could be evaluated. In the other cases, selection was based on what were considered the best directly measured values.

Vapor pressures and boiling points calculated from the Antoine constants detailed for the six compounds for which are given in numbered tables 147 to 152 least squares calculations were completed. Such tables were also prepared for several additional isomeric heptanols for which density or refractive index measurements have been reported at temperatures other than 20 or 25 °C. A short table of boiling points is given for these compounds also.

Heat of Vaporization

Grubb and Osthoff [1953] report ΔHv for 3-ethyl-3-pentanol of 12.3 kcal mol^{-1}, although no source is given for it. Heats of vaporization are listed for six heptanols at their boiling points in table 154. These were calculated from the Antoine constants with the assumption that the second virial coefficient is -1 liter mol^{-1} at this temperature. These are the six compounds whose Antoine constants were obtained by a least-squares fit to the experimental data. The uncertainty in the ΔHv obtained in this way is in the range of 0.5 to 1 kcal mol^{-1}.

TABLE 154. Isomeric Heptanols. Heat of vaporization at the normal boiling point calculated from the Antoine constants

	t_b, °C	ΔH_v kcal mol^{-1}
2-Heptanol	159.2	10.11
3-Heptanol	156.8	10.15
4-Heptanol	155.0	10.27
2-Methyl-2-hexanol	142.5	10.28
3-Ethyl-3-pentanol	142.5	9.42
2,4-Dimethyl-3-pentanol	138.8	9.56

Melting Point

The few melting point values which have been reported in the literature are included in the unnumbered tables. Cook [1952] found that 2-heptanol forms a glass in the range of -90 to -75 °C, and the data for 3-heptanol may represent glass formation rather than crystallization. The tendency for glass formation is common among these compounds and hinders crystallization. Edgar, Calingaert, and Marker [1929] have reported that 2,3,3-trimethyl-2-butanol forms a hydrate which melts at 80 °C. Pillai and Pines [1961] also prepared this hydrate and found that it melted at 82 °C.

Data for Isomeric Heptanols

Investigators		Vapor Pressures and Boiling Points		Freezing Point	Density, d g cm^{-3}		Refractive Index, n_D	
		°C	mmHg	t_m, °C	20 °C	25 °C	20 °C	25 °C
2-Heptanol, $C_4H_{16}O$, mol wt. 116.205, state at 25 °C liq.								
See also table 147								
Schorlemmer	[1873]	160–162	760					
Henry	[1909]	156–157	762		0.8193		**1.42131**	
Masson	[1909]	157–158	760					
Pickard and Kenyon	[1911]	158–160	760		.8185			
		73.5	20					
Thole	[1913]					0.8155		
Malone and Reid	[1929]	158.5	754					
Whitmore and Otterbacher	[1930]	155–157.5	760					
Sherrill	[1930]	158.7	760			0.81340		1.4190
Errera and Sherrill	[1930]				.8153			
Ellis and Reid	[1932]	158.7	760			0.81340		**1.4190**
Dubois	[1947]							
Huston and Bostwick	[1948]	77	24				**1.4214**	
Malinovskii, Volkova, and Morozova	[1949]	155–158	760					
Pichler, Ziesecke, and Traeger	[1950]	161.0	760		.8190		**1.4209**	
Adkins and Rosenthal	[1950]							**1.4184**
Huston and Tiefenthal	[1951]	158.8	745				1.4218	
Cook	[1952]	160.4	760		.8179		**1.4209**	
Pomerantz	[1952]	159.7	760		.8167	0.8129	**1.4203**	**1.4182**
Zeiss and Tsutsui	[1953]	159–160	760					1.4197
Wiley and Davis	[1954]	149–150	760				1.4204	
Williams and Mosher	[1954]	149–150	760			0.815	1.4203	
Evans and Huston	[1959]	157–159	760					1.4217
Prout and Spikner	[1962]	157–159.5	760			0.835		1.4178
Cuvigny and Normant	[1962]	64	12		.823		1.4240	
Thomas and Meatyard	[1963]	158.2	760		.820		**1.4210**	
Selected value	[1967]	^{e} 159.2±0.7	760		.8177	0.8139	1.4210	1.4190
		^{e} 59.1±1	10		±.0005	±0.0005	±0.0004	±0.0005
Antoine constants: *A* 6.33006, *B* 977.8, *C* 124.3.								*dt/dp* at 760 mmHg, 0.0470 °C/mmHg
3-Heptanol, $C_4H_{16}O$, mol wt. 116.205, state at 25 °C liq.								
Pickard and Kenyon	[1913]	66	18		0.8227	0.8187	1.4206	
Dillion and Lucas	[1928]	152.7–154	745			.8159	1.4201	1.4185
Levene and Haller	[1929b]	66–7	20					1.4198
Sherrill	[1930]	155.9	740.5		**.8210**	.8169		
		65.8	20					
Errera and Sherrill	[1930]				.8194	.8159		
Levene and Walti	[1931]	66	18					
Adams and VanderWerf	[1950]	155–157	736			.8165	1.4228	1.4208
Nazarov and Fisher	[1950]	152–154	760				1.4230	
Pichler, Ziesecke, and Traeger	[1950]	153–154	760		.8204	.8163	1.4201	
Cook	[1952]	156.4	760	−80 to −75	**.8211**	**.8170**	**1.4219**	1.4197
Protiva, Exner, Borovicka, and Pliml	[1952]	150–157						1.4200
Zeiss and Tsutsui	[1953]	78–78.5	56					
Union Carbide Corporation	[1953]	156.2	760	**−70**	.8209			
Union Carbide Corporation	[1955]	156.4	760					
Tishchenko and Stanishevskii	[1961]	66	18		.8237		1.4140	
Botteron and Shulman	[1962a]	152	760					
Thomas and Meatyard	[1963]	**156.6**	760				**1.4218**	**1.4198**
Selected value	[1967]	^{e} 156.8±0.5	760	^{a} −70.±2.	^{b} .8212	^{a} 0.8170	^{b} 1.4220	^{c} 1.4200
		^{e} 58.6±0.5	10		±0.0010	±0.0010	±0.0010	±0.0010
Antoine constants: *A* 6.30332, *B* 948.1, *C* 120.2.								*dt/dp* at 760 mmHg, °C/mmHg ^{e} 0.046

Data for Isomeric Heptanols—Continued

Investigators		Vapor Pressures and Boiling Points		Freezing Point	Density, d g cm^{-3}		Refractive Index, n_D	
		°C	mmHg	t_m, °C	20 °C	25 °C	20 °C	25 °C
4-Heptanol		4-Heptanol, $C_4H_{16}O$, mol wt. 116.205, state at 25 °C liq.						
See also table 147								
Vavon	[1914]	153	760					
Willcox and Brunel	[1916]	154–155	760					
Eykman	[1919]	154.5–155.5	763					
Behal	[1919]				0.8200		1.41657	
Brunel	[1923]	155.42	760			0.8129		1.4178
Norris and Cortese	[1927]	155.9–156.0	760			.8156		1.4184
Dillon and Lucas	[1928]	153.4–154.4	745	−37.2– 41.5		.8175	1.4199	1.4173
Errera and Sherrill	[1930]				.8170			
Sherrill	[1930]	155.4	755.2	−41.5	.8183			
		63.8	16					
Suknevich and Chilingaryan	[1936]	154–156	760					
Tuot	[1936]	70	25		.8113		1.4184	
Goldwasser and Taylor	[1939]	155.4	760		.820		1.4325	
Böeseken and Hanegraaff	[1942]				.816		1.4222	
Rust, Seubold, and Vaughan	[1948]						1.4193	
Pichler, Ziesecke, and Traeger	[1950]	155.2–155.4	760		.8220		1.4199	
Cook	[1952]	155.1	760	−33±2	.8172		1.4202	
Zeiss and Tsutsui	[1953]	74–75	30					1.4186
Haszeldine	[1953]	155	760					
Kornblum, Smiley, Ungnade, White,		155	760				1.4200	
Taub, and Herbert	[1955]						1.4202	
Thomas and Meatyard	[1963]	154.2	760		.820		1.4199	1.4178
Selected value	[1967]	[e] 155.0±0.5	760	[a] −42.± 0.5	[b] .8187	[c] 0.8149	[b] 1.4200	[c] 1.418
		[e] 55.3±0.5	10		±.002	±0.003	±0.0010	±0.002

Antoine constants: *A* 6.67161, *B* 1140.3, *C* 145.8. *dt/dp* at 760 mmHg, [e]0.045 °C/mmHg

2-Methyl-1-hexanol, $C_4H_{16}O$, mol wt. 116.205, state at 25 °C liq

See also table 148

Investigators		°C	mmHg	t_m, °C	20 °C	25 °C	20 °C	25 °C
Zelinskiĭ and Przheval'skiĭ	[1908]	162–164	750		0.8270		1.4226	
Levene and Mikeska	[1929]	71–72	15					
Morgan, Hardy, and Procter	[1932]	164–165	760					
Wender, Levine, and Orchin	[1950]	112–113.5	100					
Pichler, Ziesecke, and Traeger	[1950]	163–164.4	760		.8257		1.4226	
Nazarov and Kakhniashvili	[1954a]	162–164	760		.8290		1.429	
Selected value	[1967]	[e] 164.±2.	760		[b] 0.827	[c] 0.823	[b] 1.423	[c] 1.421
		[e] 65.±2.	10		±0.002	±0.003	±0.003	±0.003

Antoine constants: *A* 9.273, *B* 2794, *C* 273. *dt/dp* at 760 mmHg, [e] 0.04 °C/mmHg

Data for Isomeric Heptanols—Continued

Investigators		Vapor Pressures and Boiling Points		Freezing Point	Density, *d* g cm^{-3}		Refractive Index, n_D	
		°C	mmHg	t_m, °C	20 °C	25 °C	20 °C	25 °C
3-Methyl-1-hexanol, $C_7H_{16}O$, mol. wt. 116.205, state at 25 °C liq								
See also table 148								
Dewael and Weckering	[1924]	168–169	754		0.8258		1.4245	
Norris and Cortese	[1927]	171.7–172.7	760			0.8245		1.4246
Levene and Marker	[1931b]	80	25			0.824		1.422
Huston and Agett	[1941]	161–162	740			0.816		1.420
Zeile and Meyer	[1949]	91	13					
Pichler, Ziesecke, and Traeger	[1950]	171.7–172.7	760		.8258		1.4245	
Selected value	[1967]	^{e}172.±2	760		^{b,c}.828	^{b}0.824	^{b}1.424	^{b}1.422
		^{e}75.±3.	10		±.002	±0.002	±0.002	±0.003
Antoine constants: *A* 9.622, *B* 3000., *C* 273.								*dt/dp* at 760 mmHg, ^{e} 0.04 °C/mmHg
4-Methyl-1-hexanol, $C_7H_{16}O$, mol wt. 116.205, state at 25 °C liq								
Dewael and Weckering	[1924]	173	760		0.8239		1.4219	
Levene and Marker	[1931b]	77	20					1.4233
Graves	[1931]	162–164	760					
Huston and Agett	[1941]	168–169	740			0.820		1.4225
Cason, Brewer, and Pippen	[1948]	83–84	23.5					1.4231
Pichler, Ziesecke, and Traeger	[1950]	173	760		.8239		1.4219	
Milburn and Truter	[1954]	172	760				1.4256	
Djerassi and Geller	[1959]	74.6	10					1.4138
Dauben and Liang	[1959]	85–88	30					1.4235
Lardicci and Pino	[1961]	81–82	19					1.4242
Pino, Lardicci, and Centoni	[1961]	126	140					1.4241
Julia, Julia, and Stalla-Bourdillon	[1961]	84–85	18				1.4249	
Baston and Morgan	[1962]	83–84	23					
Kurtz	[1962]	75–76	14				1.4250	
Julia, Julia, Tchen, and Graffin	[1964]	83	23					1.4239
Selected value	[1967]	^{e}173.±1.	760		^{b}.824	^{a,c}0.820	^{b}1.425	^{b,c}1.423
		^{e}75.±1.	10		±.002	±0.002	±0.002	±0.002
Antoine constants: *A* 6.7232, *B* 1145., *C* 125.								*dt/dp* at 760 mmHg, ^{e} 0.044 °C/mmHg
5-Methyl-1-hexanol, $C_7H_{16}O$, mol wt. 116.205, state at 25 °C liq								
Levene and Allen	[1916]	170.5	755			0.8192		
Malone and Reid	[1929]	169.5	735					
Huston and Agett	[1941]	168–169	740			.818		1.424
Sorm and Arient	[1950]	167–169	760					
Cook	[1952]	172	760		0.8157		1.4222	1.4202
Nazarov, Kakhniashvili, and Ryabchenko	[1954]	167–168	760		.8226		1.4247	
Kurtz	[1962]	74–78	14				1.4268	
Selected value	[1967]	^{a}172.±1	760		^{a,c}.816	^{b}.812	^{b}1.424	^{b,c}1.422
					±.002	±.002	±0.002	±0.002
								dt/dp at 760 mmHg, ^{f} 0.04 °C/mmHg

Isomeric Heptanols—Continued

Investigators		Vapor Pressures and Boiling Points		Freezing Point	Density, *d* g cm^{-3}		Refractive Index, n_D	
		°C	mmHg	t_m, °C	20 °C	25 °C	20 °C	25 °C
2-Methyl-2-hexanol, $C_7H_{16}O$, mol wt. 116.205, state at 25 °C liq								
See also table 149								
Henry	[1906]	141–142	760					
Muset	[1906b]	141–142	755					
Henry	[1909]	141–142	755		0.8155		1.41592	
Edgar, Calingaert, and Marker	[1929]	137–141	760		.814			
Owen, Quayle, and Beavers	[1930]				.8141	0.8097		
Whitmore and Church	[1933]	139–142	740				1.4176	1.41515
		59–61	25					
Whitmore and Badertscher	[1933]	65.	35					
		63.	29				1.4179	
Whitmore and Woodburn	[1933]	139.4–140.4	735		.8119	.8094	1.4175	
Church, Whitmore, and McGrew	[1934]	141–143	730				1.4186	
Whitmore and Johnston	[1938]	139.5–140.5	741		.813		1.4173	
		110	250					
Whitmore and Orem	[1938]				.8146		1.4186	
Ginnings and Hauser	[1938]	143.0–143.2	760			.8093		
Petrov and Kurbskii	[1944]	65	30					
Nazarov and Fisher	[1948]	137–138	760					
Pichler, Ziesecke, and Traeger	[1950]	143.1	760		.8142		1.4187	
Huston and Brault	[1950]	139–140	740				1.4175	
Pansevich-Kolyada and Prilezhaev	[1951]	141.5–142.5	760					
Cook	[1952]	94	120				1.4181	
Levina, Tantsyreva, and Faĭnzil'berg	[1952]	138–139	742		.8136		1.4185	
Protiva, Exner, Borovicka, and Pliml	[1952]	51–51	7					
Sutherland	[1953]	142.5–143.	760			.8098		1.4161
Nazarov, Kakhniashvili, and Ryabchenko	[1954]	140–142	760		.8150	and	1.4176	and
					.8146		1.4180	
Urry, Stacey, Huyser, and Juveland	[1954]	82	80				1.4180	
Foster, Larchar, Lipscomb, and McKusick	[1956]	43–46	9					1.4196
Petrov, Sushchinskii, Zakharov, and Rogozhnikova	[1957]	69–70	42.5		.8150		1.4168	
Petrov, Zakharov, and Krasnova	[1959]	60–61	35		.8153		1.4170	
Thomas and Meatyard	[1963]	142.8	760		.815		1.4193	1.4173
Selected value	[1967]	^{e} 142.5±0.5	760		^{b} .8144	^{b} 0.8103	^{b} 1.4190	^{b} 1.4170
		^{e} 46.4±0.5	10		±.001	±0.001	±0.0010	±0.001

Antoine constants: *A* 6.95661, *B* 1240.3, *C* 161.8

dt/dp at 760 mmHg, ^{e} 0.0427 °C/mmHg

Investigators		°C	mmHg	t_m, °C	20 °C	25 °C	20 °C	25 °C
3-Methyl-2-hexanol, C_7H_{16}, mol wt. 116.205, state at 25 °C								
Bjelous	[1912]	79–81	52			0.8220		1.42066
Montagne	[1930]	151–152	760					
Selected value	[1967]	^{e} 152.±2.	760					
		^{e} 49.±5.	10					

Antoine constants: *A* 8.728, *B* 2485., *C* 273.

dt/dp at 760 mmHg, ^{e} 0.04 °C/mmHg

Isomeric Heptanols—Continued

Investigators		Vapor Pressures and Boiling Points		Freezing Point	Density, d g cm^{-3}		Refractive Index, n_D	
		°C	mmHg	t_m, °C	20 °C	25 °C	20 °C	25 °C
4-Methyl-2-hexanol, $C_7H_{16}O$, mol. wt. 116.205, state at 25 °C liq								
Davies, Dixon and Jones	[1930]	95–97	50			**0.8177**		**1.4251**
Levene and Marker	[1931d]	146–147	760			**.816**		
Cymerman, Heilbron and Jones	[1945]	(149)	760				1.4290	1.4270
Huston and Bostwick	[1948]	85.5	44				1.4223	
Gordon and Burwell	[1949]	**150–151**	760					
Huston and Tiefenthal	[1951]	152.2	744				**1.4236**	
Nerdel and Henkel	[1953]	58–60	16		0.810			
Evans and Huston	[1959]	**151–153**	760				1.426	
Woo, Dion and Bartz	[1961]	148	760					1.420
Selected value	[1967]	^{e}151. ±2. ^{e}60. ±5.	760 10		^{c}.821 ±.003	^{b}0.817 ±.002	^{a}1.424 ±0.003	^{c}1.422 ±0.003
Antoine constants: A 9.791, B 2930., C 273.								dt/dp at 760 mmHg, ^{e}0.04 °C/mmHg
5-Methyl-2-hexanol, C_7H_{16}, mol wt. 116.205, state at 25 °C liq								
See also table 149								
Rohn	[1878]	148–150	760		0.815			
Tuot	[1936]	74	28		.8131		**1.4192**	
Whitmore and Johnston	[1938]	**152–153**	760		**.814**		1.4180	
Huston and Bostwick	[1948]	73	32				1.4227	
Malinovskii, Volkova, and Morozova	[1949]	148–150	760		.809		1.420	
Huston and Tiefenthal	[1951]	**150.4**	744				**1.4194**	
Cook	[1952]	154	739				**1.4191**	
Selected value	[1967]	^{e}151. ±4. ^{e}51. ±2.	760 10		^{a}.814 ±.002	^{c}0.810 ±0.003	^{b}1.419 ±0.001	^{c}1.417 ±0.002
Antoine constants: A 8.965, B 2580., C 273.								dt/dp at 760 mmHg, ^{e}0.04 °C/mmHg
2-Methyl-3-hexanol, C_7H_{16}, mol wt. 116.205, state at 25 °C liq								
See also table 149								
Henry	[1906a]	141–142	760					
Muset	[1906]	141–145	760				1.4137	
Pickard and Kenyon	[1912]				0.8250	0.8226	**1.4215**	
Conant, Webb, and Mendum	[1929]	151–157	760					
Bartlett, Kuno, and Levene	[1937]	52	12					
Whitmore and Johnston	[1938]	144–145	734		.822		1.4213	
George	[1943]	146.0 107.4	730 200		.8228		**1.4215**	
Malinovskii and Konevichev	[1948]	140–143	760		.8231			
Pichler, Ziesecke, and Traeger	[1950]	145–146	760		.8239		**1.4215**	
Huston and Brault	[1950]	142–145	740				1.4178	
Nazarov and Kakhniashvili	[1954b]	143–144	760		.8226			
Bailey and King	[1955]	141–145	752					1.4160
Fleischacker and Woods	[1956]	140–141.5	760					
Dzotsenidze	[1958]	86–87	13		.8407		1.444	
Selected value	[1967]	^{e}147. ±1. ^{e}50. ±2.	760 10		^{a}.824 ±.002	^{c}.820 ±.003	^{b}1.422 ±0.002	^{c}1.420 ±0.003
Antoine constants: A 6.2492, B 918., C 125.								dt/dp at 760 mmHg, ^{e}0.046 °C/mmHg

Isomeric Heptanols—Continued

3-Methyl-3-hexanol, $C_7H_{16}O$, mol wt. 116.205, state at 25 °C liq

See also table 150

Investigators		Vapor Pressures and Boiling Points °C	Vapor Pressures and Boiling Points mmHg	Freezing Point t_m, °C	Density, d g cm^{-3} 20 °C	Density, d g cm^{-3} 25 °C	Refractive Index, n_D 20 °C	Refractive Index, n_D 25 °C
Fourneau and Tiffeneau	[1907]	139–141	760					
Guerbet	[1912a]	139–140	760					
Halse	[1914]	142–144	760		0.8267			
Eykman	[1919]	141.5–142.5	770			0.8188		
de Graef	[1925]	142–143	760		.8254	.8212	1.4227	
Edgar, Calingaert, and Marker	[1929]	137–139	760		.822			
Owen, Quayle, and Beavers	[1930]					.8198		
Whitmore and Badertscher	[1933]	56.	20				1.4231	
		52.	16					
Ginnings and Hauser	[1938]	142.7–142.9	760			.8202		
Shikheev	[1946]	139–142	760		.8270			
Zeile and Meyer	[1949]	53	16					
Pichler, Ziesecke, and Traeger	[1950]	142.8	760		.8254		1.4224	
Soehring, Frey, and Endres	[1955]	140–141	760		.8254		1.4287	
Fleischacker and Woods	[1956]	140	760				1.423	
Davies, Kenyon, and Salamé	[1957]	58–59	25				1.4224	
Selected value	[1967]	[e] 142.4±1	760		[b] .8250	[b,c] .8204	[b] 1.4226	[c] 1.421
		[e] 45.±2.	10		±.001	±.001	±0.001	±0.002

Antoine constants: *A* 6.178, *B* 883., *C* 125. *dt/dp* at 760 mmHg, [e] 0.046 °C/mmHg

4-Methyl-3-hexanol, $C_7H_{16}O$, mol wt. 116.205, state at 25 °C liq

Investigators		Vapor Pressures and Boiling Points °C	Vapor Pressures and Boiling Points mmHg	Freezing Point t_m, °C	Density, d g cm^{-3} 20 °C	Density, d g cm^{-3} 25 °C	Refractive Index, n_D 20 °C	Refractive Index, n_D 25 °C
Fourneau and Tiffeneau	[1907]	149–150	760					

5-Methyl-3-hexanol, $C_7H_{16}O$, mol wt. 116.205, state at 25 °C liq

Investigators		Vapor Pressures and Boiling Points °C	Vapor Pressures and Boiling Points mmHg	Freezing Point t_m, °C	Density, d g cm^{-3} 20 °C	Density, d g cm^{-3} 25 °C	Refractive Index, n_D 20 °C	Refractive Index, n_D 25 °C
Wagner	[1884]	147–148	756.5					
Levene and Mikeska	[1929]	63–64	19					
		66	18					
Levene and Marker	[1931c]	81	60					1.4171
Jones and McCombie	[1942]	93–96	105				1.4128	
Shuikin and Bel'skii	[1957]	135–135.5	758		0.8331		1.4220	
Benkeser, Hyzdra and Burrous	[1959]	146–148	760				1.4171	
Selected value	[1967]	[e] 148.±2.	760		[a] 0.833	[c] 0.829	[b] 1.419	[a] 1.417
		[c] 45.±2.	10		±0.002	±0.003	±0.004	±0.002

Antoine constants: *A* 8.700, *B* 2450., *C* 273. *dt/dp* at 760 mmHg, [e] 0.04 °C/mmHg

2-Ethyl-1-pentanol, $C_7H_{16}O$, mol wt. 116.205, state at 25 °C liq

Investigators		Vapor Pressures and Boiling Points °C	Vapor Pressures and Boiling Points mmHg	Freezing Point t_m, °C	Density, d g cm^{-3} 20 °C	Density, d g cm^{-3} 25 °C	Refractive Index, n_D 20 °C	Refractive Index, n_D 25 °C
Morgan, Hardy, and Procter	[1932]	164–166	760			0.832		
Levene, Rothen, and Meyer	[1936]	107	100			.8280		1.4250
Adams and VanderWerf	[1950]	164–166	760			.8296		1.4251
Protiva, Exner, Borovicka, and Pliml	[1952]	150–157	?					
Meakin, Mumford, and Ward	[1959]	165–167	760					
Selected value	[1967]	[e] 166.±3.	760		[c] 0.833	[b] .829	[c] 1.427	[b] 1.425
		[e] 57.±5.	10		±.003	±.002	±0.003	±0.002

Antoine constants: *A* 8.578, *B* 2501., *C* 273. *dt/dp* at 760 mmHg, [e] 0.04 °C/mmHg

Isomeric Heptanols—Continued

Investigators	Vapor Pressures and Boiling Points		Freezing Point	Density, *d* g cm^{-3}		Refractive Index, n_D	
	°C	mmHg	t_m, °C	20 °C	25 °C	20 °C	25 °C
2,2-Dimethyl-1-pentanol, $C_7H_{16}O$, mol wt. 116.205, state at 25 °C liq							
Brannock [1959]	**152.5–153.**	760				**1.4251**	
McElrath, Fritz, Brown, LeGall, and Duke [1960]	154	760					
Selected value [1967]	^{a}153. ±2.	760				^{a} 1.425 ±0.002	^{c} 1.423 ±0.003
dt/*dp* at 760 mmHg, ^{f} 0.04 °C/mmHg							
2,3-Dimethyl-1-pentanol, $C_7H_{16}O$, mol wt. 116.205, state at 25 °C liq							
Levene and Marker [1931a]	75	17			**0.834**		
Colonge and Dreux [1953]	**162–164**	745				**1.4314**	
Dreux [1955]	**162–164**	742					1.428
Selected value [1967]	^{e} 164. ±3. ^{e} 66. ±5.	760 10		^{c} 0.838 ±.002	^{a} .834 ±.002	^{a} 1.431 ±0.002	^{a,c} 1.429 ±0.003
Antoine constants: *A* 9.380, *B* 2840., *C* 273.					*dt*/*dp* at 760 mmHg, ^{e} 0.04 °C/mmHg		
2,4-Dimethyl-1-pentanol, $C_7H_{16}O$, mol wt. 116.205, state at 25 °C							
Chu and Marvel [1931]	160–162	760		0.793		**1.427**	
Graves [1931]	153–158	760					
Morgan, Hardy, and Procter [1932]	158–159	760			0.821	1.421	
Levene and Marker [1935]	157	760			**.816**		
Shonle, Waldo, Keltch and Coles [1936]	159.65–159.9	760					
Goldwasser and Taylor [1939]	**157**	760		**.819**			
Dirscherl and Nahm [1943]	52–55	7					
Pichler, Ziesecke, and Traeger [1950]	157–158	760					
Selected value [1967]	^{a} 159. ±1.	760		^{a} .819 ±.003	^{a,c} .815 ±.003	^{a} 1.427 ±0.003	^{c} 1.425
3,3-Dimethyl-1-pentanol, $C_7H_{16}O$, mol wt. 116.205, state at 25 °C liq							
Schmerling [1945]	163–164 78–79	745 20		0.8320		1.4275	
Birch [1949]	167	760					
Selected value [1967]	^{e} 165. ±3. ^{e} 67. ±4.	760 10					
Antoine constants: *A* 9.445, *B* 2875., *C* 273.					*dt*/*dp* at 760 mmHg, ^{e} 0.04 °C/mmHg		

Isomeric Heptanols—Continued

3,4-Dimethyl-1-pentanol, $C_7H_{16}O$, mol wt. 116.205, state at 25 °C liq

See also table 150

Investigators		Vapor Pressures and Boiling Points °C	Vapor Pressures and Boiling Points mmHg	Freezing Point t_m, °C	Density, d g cm^{-3} 20 °C	Density, d g cm^{-3} 25 °C	Refractive Index, n_D 20 °C	Refractive Index, n_D 25 °C
Wojcik and Adkins	[1933]	159–162	760					1.4261
Levene and Marker	[1935]	164	760			0.828		
Huston and Agett	[1941]	160–162	740			0.818	1.427	
Detling, Crawford, Yabroff, and Peterson	[1947]	170.3	760		0.8345		1.4280	
Wender, Metlin, and Orchin	[1951]	164.5–166.0	760					1.4290
Adkins and Williams	[1952]	163–170	760				1.4288	
Tsuda, Kishida, and Hayatsu	[1960]	165	760			0.825		1.4270
		118–119	150					
Selected value	[1967]	[e] 165. ±3.	760		[c] 0.831	[b] 0.827	[b] 1.428	[b,c] 1.426
		[e] 60. ±4.	10		±0.003	±0.002	±0.002	±0.003

Antoine constants: A 8.874, B 2625., C 273.

dt/dp at 760 mmHg, [e] 0.04 °C/mmHg

4,4-Dimethyl-1-pentanol, $C_7H_{16}O$, mol wt. 116.205, state at 25 °C

Investigators		Vapor Pressures and Boiling Points °C	Vapor Pressures and Boiling Points mmHg	Freezing Point t_m, °C	Density, d g cm^{-3} 20 °C	Density, d g cm^{-3} 25 °C	Refractive Index, n_D 20 °C	Refractive Index, n_D 25 °C
Homeyer	[1931]				0.8152			
Whitmore and Homeyer	[1933a]	158	737		0.815		1.4202	
Whitmore, Whitaker, Mosher, Breivik, Wheeler, Miner, Sutherland, Wagner, Clapper, Lewis, Lux, and Popkin	[1941]	160	728					
Haggard	[1946]						1.4200	
Malinovskii, Volkova, and Morozova	[1949]	158–162	760		0.82		1.430	
Searles	[1951]	144–145	745					
Selected value	[1967]	[b] 160. ±3.	760		[a] 0.815	[c] 0.811	[b] 1.420	[c] 1.418
			10		±0.002	±0.003	±0.002	±0.003

dt/dp at 760 mmHg,[f] 0.04 °C/mmHg

3-Ethyl-2-pentanol, $C_7H_{16}O$, mol wt. 116.205, state at 25 °C lig

Investigators		Vapor Pressures and Boiling Points °C	Vapor Pressures and Boiling Points mmHg	Freezing Point t_m, °C	Density, d g cm^{-3} 20 °C	Density, d g cm^{-3} 25 °C	Refractive Index, n_D 20 °C	Refractive Index, n_D 25 °C
Fourneau and Tiffeneau	[1907]	148–152	760					
Colonge	[1927]	148–150	760					
Lucas	[1929]	151.0–151.5	743			0.8335	1.4284	1.4264
Selected value	[1967]	[b] 152. ±3.	760		[c] 0.838	[a] .834	[a] 1.428	[a,c] 1.426
					±.003	±.002	±0.002	±0.002

dt/dp at 760 mmHg, [f] 0.04 °C/mmHg

Isomeric Heptanols—Continued

Investigators	Vapor Pressures and Boiling Points		Freezing Point	Density, *d* g cm^{-3}		Refractive Index, n_D	
	°C	mmHg	t_m, °C	20 °C	25 °C	20 °C	25 °C
2,3-Dimethyl-2-pentanol, $C_7H_{16}O$, mol wt. 116.205, state at 25 °C liq							
Edgar, Calingaert, and Marker [1929]	129.–130.5	760		0.804			
Levene and Marker [1931a]				.838			
Norton and Hass [1936]	139.0–139.7	744			0.8285 and .8276		1.4234 and 1.4231
Ginnings and Hauser [1938]	138.5–139.5	760			.8307		
James [1943]				.8324		1.4252	
Pichler, Ziesecke, and Traeger [1950]	138.2–139.5	760		.8307			
Huston and Van Dyke [1953]	129–131	730					
Schotta and Veibel [1953]							
Schmerling and Meisinger [1953]	137–138	760				1.4276 to 1.4304	
Freudenberg, Lwowski, ahd Hohmann [1955]	49.7	15			.8287		1.4240
Brown and Nakagawa [1955]	54	28				1.4162	
Lukes and Langthaler [1957]	137–139	760		.8360		1.4251	
Pillai and Pines [1961]	139.9–140.	750				1.4268	
Selected value [1967]	^{e} 139.7±1.	760		^{a} .832 ±.003	^{c} .828 ±.003	^{b} 1.425 ±0.003	^{b,c} 1.423 ±0.003
	^{e} 44. ±2.	10					
Antoine constants: *A* 6.186, *B* 875., *C* 125.							*dt/dp* at 760 mmHg, ^{e} 0.046 °C/mmHg
2,4-Dimethyl-2-pentanol, $C_7H_{16}O$, mol wt. 116.205, state at 25 °C liq							
See also table 150							
Khonin [1909]	133	749				1.4172	
Barbier and Locquin [1913]	120–130	760					
Willcox and Brunel [1916]	132–133	760					
Edgar, Calingaert, and Marker [1929]	127–129	760					
de Graef [1931]	133.1–133.2	760		0.8103	0.8002	1.4165	
Ginnings and Hauser [1938]	132.5–133.5	760			.8100		
Whitmore and Johnston [1938]	130–131	738		.811		1.4166	
Pichler, Ziesecke, and Traeger [1950]	132.8–133.4	760		.8122		1.4172	
Hickinbottom, Peters, and Wood [1955]	130–132	760				1.4140	
Brown and Nakagawa [1955]	54	28				1.4162	
Petrov, Sushchinskii, Zakharov, and Rogozhnikova [1957]	59.5	42.5		.8119		1.4170	
Petrov, Zakharov, and Krasnova [1959]	59.5	42.5		.8119		1.4170	
Esso Research and Eng. Co. [1959]	133–134	760					
Selected value [1967]	^{e} 133. ±1.	760		^{b} .812 ±.002	^{c} .808 ±.003	^{b} 1.417 ±0.001	^{c} 1.415 ±0.002
	^{e} 38. ±2.	10					
Antoine constants: *A* 6.129, *B* 838., *C* 125.							*dt/dp* at 760 mmHg, ^{e} 0.045 °C/mmHg

Isomeric Heptanols—Continued

3-Ethyl-3-pentanol, $C_7H_{16}O$, mol wt. 116.205, state at 25 °C liq.

See also table 151

Investigators		Vapor Pressures and Boiling Points		Freezing Point	Density, *d* g cm^{-3}		Refractive Index, n_D	
		°C	mmHg	t_m, °C	20 °C	25 °C	20 °C	25 °C
Davies and Kipping	[1911]	140–142	760					
Eykman	[1919]	62	30	−10.5	0.8441			
Edgar, Calingaert, and Marker	[1929]	140–142	760		.838			
Lucas	[1929]	140.5–141.5	743			0.8413	1.4305	1.4281
Owen, Quayle, and Beavers	[1930]					.8367		
Moyer and Marvel	[1931]	139–142	760					
Böeseken and Wildschut	[1932]	138–142	760		.8426		1.4275	
Whitmore and Badertscher	[1933]	72–73	52				1.4294	
Church, Whitmore, and McGrew	[1934]	138–140	742					
Ginnings and Hauser	[1938]	143.1–143.2	760			.8402		
Milas and Perry	[1946]	141–142	760					
Pichler, Ziesecke, and Traeger	[1950]	142.1	760		.8412		1.4305	
Cook	[1952]	87	100				1.4300	
Timmermans	[1952]			−14.2				
Grubb and Osthoff	[1953]	35	5		.842		1.4330	
Soehring, Frey, and Endres	[1955]	140.5–141.5	760		.8412		1.4298	
Timmermans and Hennaut-Roland	[1955]	55.88	22	−12.34	.84402	0.83972		
Hauser and Chambers	[1956]	53–54	20					1.4276
Sager and Bradley	[1956]	142–143	760					
Sager	[1956]	141–142	760					
Liberman, Lapshina, and Kazanskii	[1956]	84.7–84.8	92	−12.55	.84511		1.43018	
Dashkevich and Bratchanskii	[1957]	142	760					
Searles, Pollart, and Lutz	[1957]	136–138	760				1.4265	
Lanning and Moore	[1958]	142–143	760					
Zook, March, and Smith	[1959]	141–142	731				to	1.4272 1.4278
Desgrandchamps, Deluzarche, and and Maillard	[1961]	50	20					
Hamelin	[1961]	143	760					
Viehe and Reinstein	[1962]	140–142	760					
Hillman	[1962]	140–145	760					
Andreev and Kukharskaya	[1962]	140–144	760		0.8390		1.4344	
Selected value	[1967]	[e] 142.5±1.0 [e] 43.7±1.0	760 10	[b] −12.4±1.	[b] .8445 ±.0010	[b,c] 0.8400 ±.0010	[b] 1.4301 ±0.0010	[b] 1.4277 ±0.0010

Antoine constants: *A* 6.29473, *B* 948.9, *C* 135.5 *dt*/*dp* at 760 mmHg, [e] 0.047 °C/mmHg

3,3-Dimethyl-2-pentanol, $C_7H_{16}O$, mol wt. 116.205, state at 25 °C liq.

Investigators		°C	mmHg	t_m, °C	20 °C	25 °C	20 °C	25 °C
Edgar, Calingaert, and Marker	[1929]	147–148	760		0.828			
Mosher	[1940]	145	737				1.4300	
Mosher and Whitmore	[1948]						1.4300	
Pillai and Pines	[1961]	146.8–147.2	750				1.4301	
Selected value	[1967]	[e] 147.±2. [e] 36.±3.	760 10				[b] 1.4300 ±0.001	[c] 1.428 ±0.002

Antoine constants: *A* 8.143, *B* 2210., *C* 273. *dt*/*dp* at 760 mmHg, [e] 0.046 °C/mmHg

Isomeric Heptanols—Continued

Investigators	Vapor Pressures and Boiling Points		Freezing Point	Density, *d* g cm^{-3}		Refractive Index, n_D	
	°C	mmHg	t_m, °C	20 °C	25 °C	20 °C	25 °C
3,4-Dimethyl-2-pentanol, $C_7H_{16}O$, mol wt. 116.205, state at 25 °C liq.							
Willstätter and Holt [1919]	149–150.5	719		0.837			
Sassiver and English [1960]	75–80	49					
Selected value [1967]	^{f} 153.±3. ^{f} 49.±4.	760 10					
4,4-Dimethyl-2-pentanol, $C_7H_{16}O$, mol wt. 116.205, state at 25 °C liq.							
Whitmore and Homeyer [1933b]	137–137.5	736		**0.8115**		1.4188	
Whitmore and Homeyer [1933a]	136–137	741		.812		1.4185 to 1.4190	
Whitmore and Homeyer [1933c]	137–137.5	736		**.8115**		1.4188	
Whitmore, Popkin, Whitaker, Matill,	132–140	741				1.4194	
and Zech [1938]	137	739				**1.4185**	
Whitmore and Johnston [1938]	136.5	738				1.4180	
Huston and Bostwick [1948]	65	40				1.4248	
Huston and Tiefenthal [1951]	135.4	742				1.4241	
Cook [1952]	138	760		**.8113**	(0.8070)	**1.4186**	(1.4162)
Gasson, Millidge, Robson, and Wild [1953]	136–138	740					
Shiner, Boskin, and Smith [1955]	137–138	751					**1.4168**
Brown and Nakagawa [1955]	137–137.5	736				1.4180	
Gaylord and Caul [1955]	50.5–57.5	25	**−60.**	**.8133**		**1.4188**	
Kornblum, Smiley, Ungnade, White, Taub, and Herbert [1955]	72	8				1.4262	
Selected value [1967]	^{e} 138.±1. ^{e} 43.±2.	760 10	^{a} −60.±2.	^{b} .811 ±.001	^{c} .807 ±.002	^{b} 1.4187 ±0.0010	^{a,c} 1.417 ±0.002
Antoine constants: *A* 6.207, *B* 875., *C* 125.							*dt/dp* at 760 mmHg, ^{e} 0.045 °C/mmHg
2,2-Dimethyl-3-pentanol, $C_7H_{16}O$, mol wt. 116.205, state at 25 °C liq.							
See also table 151							
Favorskiĭ [1913]				0.82462	0.82058		
Leroide [1921]	140–148	760					
Edgar, Calingaert and Marker [1929]	136–137	760		.825			
Levene and Walti [1931]	63–64	19					
Ginnings and Hauser [1938]	134.7–135.1	760			**.8224**		
Whitmore, Meyer, Pedlow and Popkin [1938]	133.4	732				1.4223 to 1.4225	
Stevens and McCoubrey [1941]	137–138	760					
Whitmore and Forster [1942]	67	55				1.4223 to 1.4232	
James [1943]	136.5	760		**.8254**		**1.4229**	
Zook, McAleer and Horwin [1946]	44–45	15				1.4215 to 1.4218	
Pichler, Ziesecke and Traeger [1950]	134.7–135.1	760		**.8264**			1.4180
Mosher, Cox and Kreitzer [1953]	135	757					
Gaylord and Caul [1955]			5.	.8281		1.4238	
Foley, Welch, La Combe and Mosher [1959]	136	760				**1.4230 to** 1.4235	
Selected value [1967]	^{e} 136.±1. ^{e} 39.±2.	760 10	^{a} +5.±2.	^{a,c} .826 ±.002	^{a} .822 ±.002	^{a} 1.423 ±0.001	^{c} 1.421 ±0.002
Antoine constants: *A* 6.050, *B* 827., *C* 125.							*dt/dp* at 760 mmHg, ^{e} 0.047 °C/mmHg

Isomeric Heptanols—Continued

Investigators		Vapor Pressures and Boiling Points		Freezing Point	Density, *d* g cm^{-3}		Refractive Index, n_D	
		°C	mmHg	t_m, °C	20 °C	25 °C	20 °C	25 °C

2,3-Dimethyl-3-pentanol, $C_7H_{16}O$, mol wt. 116.205, state at 25 °C liq.

See also table 151

Investigators		°C	mmHg	t_m, °C	d 20 °C	d 25 °C	n_D 20 °C	n_D 25 °C
Pariselle and Simon	[1921]	136	760		0.8415	0.8372	1.427	
Whitmore and Evers	[1933]	136–137	740		.833		1.4287	
Norton and Hass	[1936]	137.7–138.5	743			**.8366**		**1.4263**
					and	**.8382**		
Ginnings and Hauser	[1938]	139.6–139.8	760			**.8365**		
James	[1943]				.8324			
Pichler, Ziesecke, and Traeger	[1950]	139.6–139.8	760		**.8402**		**1.4280**	
Cook	[1952]	71	58				1.4294	
Schmerling and Meisinger	[1953]	137–138	760				1.4295 to	
							1.4309	
Sokolova and Fedotov	[1956]	68–68.5	50		.8320		1.4270	
Selected value	[1967]	[e] 139.±1.	760		[a,c] .840	[a] .836	[a] 1.428	[a,c] 1.426
		[e] 42.±2.	10		±.003	±.001	±0.002	±0.002

Antoine constants: *A* 6.115, *B* 856., *C* 125. *dt/dp* at 760 mmHg, [e] 0.047 °C/mmHg

2,4-Dimethyl-3-pentanol, $C_7H_{16}O$, mol wt. 116.205, state at 25 °C liq.

See also table 152

Investigators		°C	mmHg	t_m, °C	d 20 °C	d 25 °C	n_D 20 °C	n_D 25 °C
Munch	[1876]	131–132	760		0.8300			
Poletaeff	[1891]	140	760		.8288	**0.8249**	1.42259	
Conant, Webb, and Mendum	[1929]	140–150	760					
Conant and Blatt	[1929]	134–138	760					
		137–140	760					
Graves	[1931]	139	760					
Whitmore and Johnston	[1938]	137–138	738		.831		1.4246	
Ginnings and Hauser	[1938]	138.4–138.9	760		.8254			
Wibaut and Pelt	[1938]	66.9	50				1.4188	
Goldwasser and Taylor	[1939]	140	760		**.8288**		1.4226	
Whitmore and George	[1942]	87.5	125				1.4246	
Huston and Auvapara	[1944]	136–137	745		.8157		1.4159	
Scattergood, Miller, and Gammon	[1945]	136–137	760					
Weissler	[1948]				.8272			1.4169
Nazarov and Pinkira	[1949]	78	9		.8859		1.4778	
Huston and Brault	[1950]	137.8	740				**1.4250**	
Pichler, Ziesecke, and Traeger	[1950]	138.9	760		**.8294**		**1.4250**	
Swain and Boyles	[1951]	139–140	760				1.4229	1.4209
Cook	[1952]	138.6±0.1	760	**−8.±2.**	**.8304**	0.8259	**1.4250**	
Razuvaev and O'ldekop	[1953]	137–141	760		.8302		1.418	
Zeiss and Tsutsui	[1953]	137–138	760					**1.4222**
Tarbell and Price	[1957]	133–137	760				1.43235	
Maddock and Goble	[1962]	139–140	760					
Thomas and Meatyard	[1963]	139.0	760		.829		**1.4248 to**	
							1.4250	
Selected value	[1967]	[e] 138.8±1.	760	[a] −8.±2.	[b] .8296	[b,c] 0.8253	[b] 1.425	[a,c] 1.423
		[e] 41.3±1.	10		±.001	±0.001	±0.002	±0.002

Antoine constants: *A* 6.49430, *B* 1029.6, *C* 146.1. *dt/dp* at 760 mmHg, [e] 0.047 °C/mmHg

Isomeric Heptanols—Continued

2-Methyl-2-ethyl-1-butanol, $C_7H_{16}O$, mol wt. 116.205, state at 25 °C

See also table 152

Investigators		Vapor Pressures and Boiling Points °C	mmHg	Freezing Point t_m, °C	Density, d g cm^{-3} 20 °C	25 °C	Refractive Index, n_D 20 °C	25 °C
Favorskiĭ and Zalesskiĭ-Kibardine	[1925]	111	145					
		155	738		0.8282	0.8251	1.425336	
Rice, Jenkins, and Harden	[1938]	150–151	760				1.4261	
Sokolova	[1953]	86–90	50				1.4328	
Sarel and Newman	[1956]	152	740					1.4288
Searles, Pollart, and Lutz	[1957]	156.5	760					
Selected value	[1967]	[e] 156. ±2.	760		[a] .828 ±.002	[c] .824 ±.003	[a] 1.426 ±0.003	[c] 1.424 ±0.004
		[e] 62. ±2.	10					

Antoine constants: A 6.632, B 1056., C 125.

dt/dp at 760 mmHg, [e] 0.043 °C/mmHg

3-Methyl-2-ethyl-1-butanol, $C_7H_{16}O$, mol wt. 116.205,

Investigators		Vapor Pressures and Boiling Points °C	mmHg	Freezing Point t_m, °C	Density, d g cm^{-3} 20 °C	25 °C	Refractive Index, n_D 20 °C	25 °C
Dirscherl and Nahm	[1943]	65–66.5	14					
Sarel and Newman	[1956]	84–85	38			0.8327		1.4234
Tsuda, Hayatsu, and Kishida	[1959]	91.5	50			.8326		1.4286
Tsuda, Kishida, and Hayatzu	[1960]	91.5	50			.8326		
Selected value	[1967]	[e] 60. ±3.	10		[c] .837 ±.003	[b] 0.833 ±0.002	[c] 1.428 ±0.004	[b] 1.426 ±0.003

Antoine constants: A 9.023, B 2671., C 273. 7

2,2,3-Trimethyl-1-butanol, $C_7H_{16}O$, mol wt. 116.205

Investigators		Vapor Pressures and Boiling Points °C	mmHg	Freezing Point t_m, °C	Density, d g cm^{-3} 20 °C	25 °C	Refractive Index, n_D 20 °C	25 °C
Gleim	[1941]				0.8466		1.4331	
Ford, Jacobson, and McGrew	[1948]	157–158	760				1.4320	
Hickinbottom, Peters, and Wood	[1955]	55–60	15				1.4346	
McElrath, Fritz, Brown, LeGall, and Duke	[1960]	156–157	760					
Farina and Peronaci	[1966]	161–162	760		0.8372		1.4296	
Selected value	[1967]	[b] 157. ±3.	760		[a] 0.847 ±0.002	[c] 0.843 ±.003	[b] 1.433 ±0.002	[c] 1.431 ±0.003

2,3,3-Trimethyl-1-butanol, $C_7H_{16}O$, mol wt. 116.205

Investigators		Vapor Pressures and Boiling Points °C	mmHg	Freezing Point t_m, °C	Density, d g cm^{-3} 20 °C	25 °C	Refractive Index, n_D 20 °C	25 °C
Stevens and McCoubrey	[1941]	159.5–162	761					1.4288
Sarel and Newman	[1956]	158–159	740			0.8238		1.4230
Zweifel, Ayyangar, Munekata, and Brown	[1964]						1.4294	
Selected value	[1967]	[b] 160. ±3.	760				[c] 1.431 ±0.003	[a] 1.429 ±0.002

Isomeric Heptanols—Continued

Investigators		Vapor Pressures and Boiling Points		Freezing Point	Density, *d* g cm^{-3}		Refractive Index, n_D	
		°C	mmHg	t_m, °C	20 °C	25 °C	20 °C	25 °C
2,3,3-Trimethyl-2-butanol, $C_7H_{16}O$, mol wt. 116.205, state at 25 °C liq.								
Butlerov	[1875]	131–132	760	17.				
Richard	[1910]	125–130	760	17.				
Willcox and Brunel	[1916]	132–133	760					
Edgar, Calingaert, and Marker	[1929]	130	760	17.				
Ginnings and Hauser	[1938]	130.3–130.8	760			0.8380		
Schmerling, Friedman, and Ipatieff	[1940]	128–129	760					
Stevens and McCoubrey	[1941]	130	760					
Huston and Barrett	[1946]	128–130	760					
Lewis and Wright	[1952]	130–132	760					1.4278
Huston and Van Dyke	[1953]	129–130	750					
Huisgen and Zirngibl	[1958]	131–133	760					
Selected value	[1967]	^{b}131.±2.	760	^{b}+17.±2.	^{c}0.842 ±0.003	^{a}0.838 ±0.002	^{c}1.430 ±0.003	^{a}1.428 ±0.002

dt/dp at 760 mmHg, ^{f} 0.04 °C/mmHg

Index to the Bibliography

Numbers refer to the Bibliography, page 1–389.

References to data used in the selection of refractive index, density, boiling point, vapor pressure, and melting point are in boldface type.

Numbers in parentheses refer to sources of reviews, or theoretical calculations only.

Reference numbers under each property are listed in the order of date of publication.

References to Properties of 2-Heptanol

Refractive Index
741, **1604**, **486**, **803**, **1893**, **1119**, **13**, **1377**, 808, **338**, **1406**, 2016, 1958, 1962, 505, 482, 1193, **1758**

Density at 20–30 °C Only
741, **1378**, **1752**, **495**, **486**, **1377**, **338**, **1406**, 1962, 373, 1432

Density at all Temperatures
1136, **1380**, **1604**, **1893**, **1119**, **1758**

Normal Boiling Point
1577, 741, 1136, 1121, 1938, 457, 1119, 1377, **808**, **338**, **1406**, 2016, 1958, 1962, 505, 1432, 1193

Vapor Pressure and Boiling Points at Other Pressures
1378, **1604**, **486**, **803**, **1758**

Normal Melting Point
338

Molecular Vibration Frequencies and Spectra
1613

References to Properties of 3-Heptanol

Refractive Index
1379, 422, 1023, **1604**, 5, 1246, 1377, **338**, 2016, **1758**, 1787

Density at 20–30 °C Only
1379, 422, 495, 1377, 5, **338**, 1823, 1787

Density at all Temperatures
1758, **1604**

Normal Boiling Point
1377, 1246, 1429, **338**, 185

Vapor Pressure and Boiling Points at Other Pressures
1379, 422, 1023, 1604, **1045**, 5, 1823, 2016, **1787**, **1758**

Normal Melting Point
338, **1823**

Molecular Vibration Frequencies and Spectra
1613

References to Properties of 4-Heptanol

Refractive Index
1838, 123, 509, 238, 1273, **422**, 1604, 1811, 613, 171, 1524, **1377**, **338**, 2016, **949**, **1758**

Density at 20–30 °C Only
123, 238, 1273, 422, 495, 1811, 613, 171, 1377, **338**

Density at all Temperatures
1838, 509, **1604**, **1758**

Normal Boiling Point
1838, 1960, 509, 1273, 1711, 613, 171, 1524, 1377, 338, 720

Vapor Pressure and Boiling Points at Other Pressures
238, 422, 1604, 1811, 2016, 949, 1758

Normal Melting Point
422, 1604, 338

References to Properties of 2-Methyl-1-Hexanol

Refractive Index
2018, 1204, 1377, 1250

Density at 20–30 °C Only
1377, 1250

Density at all Temperatures
2018

Normal Boiling Point
1204, 1377, 1250

Vapor Pressure and Boiling Points at Other Pressures
2018, 1039, 1899

Association in the Liquid Phase
1705

References to Properties of 3-Methyl-1-Hexanol

Refractive Index
420, 1273, 1030, 799, 1377

Density at 20–30 °C Only
420, 1273, 1030, 1377

Normal Boiling Point
420, 1273, 1377

Vapor Pressure and Boiling Points at Other Pressures
1030, 799, 2015

References to Properties of 4-Methyl-1-Hexanol

Refractive Index
420, 1030, 799, 276, 1377, 1182, 384, 428, 994, 1389, 859, 977, 860, 861

Density at 20–30 °C Only
420, 1030, 799, 1377

Normal Boiling Point
420, 621, 1377, 1182, 428

Vapor Pressure and Boiling Points at Other Pressures
1030, 799, 276, 384, 944, 977, 1389, 428, 96, 860, 861

References to Properties of 5-Methyl-1-Hexanol

Refractive Index
799, 338, 977, 1252

Density at 20–30 °C Only
1020, 799, 338, 1252

Normal Boiling Point
1663, 338, 1252

Vapor Pressure and Boiling Points at Other Pressures
1020, 1121, 799, 977

Association in the Liquid Phase
1705

References to Properties of 2-Methyl-2-Hexanol

Refractive Index
741, 1911, 1912, 296, 1922, 1937, 1951, 804, 1377, 338, 1051, 1712, 1252, 1824, 549, 1365, 1368, 1758

Density at 20–30 °C Only
741, 480, 601, 1937, 1922, 1951, 1377, 1051, 1712, 1252, 1365, 1368

Density at all Temperatures
1300, 1758

Normal Boiling Point
742, 741, 480, 601, 1247, 804, 1377, 1311, 1712, 1252

Vapor Pressure and Boiling Points at Other Pressures
1912, 1911, 1951, 296, 1922, 1358, 804, 338, 1051, 1429, 1712, 1824, 549, 1365, 1368, 1758

Association in the Liquid Phase
1705

References to Properties of 3-Methyl-2-Hexanol

Refractive Index
154

Density at 20–30 °C Only
154

Normal Boiling Point
1202

Vapor Pressure and Boiling Points at Other Pressures
154

References to Properties of 4-Methyl-2-Hexanol

Refractive Index
386, 373, 803, 808, 505, 1980

Density at 20–30 °C Only
386, 1034, 1259

Normal Boiling Point
1034, 616, 505, 1980

Vapor Pressure and Boiling Points at Other Pressures
386, 373, 803, 808, 1259

References to Properties of 5-Methyl-2-Hexanol

Refractive Index
1811, 1922, 803, 1119, 808, 338

Density at 20–30 °C Only
1811, 1922

Density at all Temperatures
1495, 1119

Normal Boiling Point
1495, 1119

Vapor Pressure and Boiling Points at Other Pressures
1811, 1922, 803, 808, 338

References to Properties of 2-Methyl-3-Hexanol

Refractive Index
1235, 1380, 1922, 588, 1118, 804, 1377, 1250, 67, 539, 476

Density at 20–30 °C Only
1380, 1922, 588, 1377, 476

Density at all Temperatures
1235, 1250, 1118

Normal Boiling Point
1235, 332, 1377, 1250, 539

Vapor Pressure and Boiling Points at Other Pressures
93, 1922, 588, 1118, 804, 67, 476

References to Properties of 3-Methyl-3-Hexanol

Refractive Index
509, 401, 1911, 1377, 1650, 539, 387

Density at 20–30 °C Only
509, 480, 601, 1377, 1650

Density at all Temperatures
695, 401, 1300, 1607

Normal Boiling Point
551, 652, 695, 509, 401, 480, 601, 1607, 1377, 1537, 539

Vapor Pressure and Boiling Points at Other Pressures
1911, 2015, 387

Normal Melting Point
1772

References to Properties of 4-Methyl-3-Hexanol

Density at 20–30 °C Only
551

Normal Boiling Point
551

References to Properties of 5-Methyl-3-Hexanol

Refractive Index
1032, 857, 1619, 124

Density at 20–30 °C Only
1619

Normal Boiling Point
1873, 1619, 124

Vapor Pressure and Boiling Points at Other Pressures
1039, 1032, 857

References to Properties of 2-Ethyl-1-Pentanol

Refractive Index
1204, 1040, 5

Density at 20–30 °C Only
1204, 1040, 5

Normal Boiling Point
1204, 5, 1429, 1157

Vapor Pressure and Boiling Points at Other Pressures
1040

References to Properties of 2,2-Dimethyl-1-Pentanol

Refractive Index
197

Normal Boiling Point
197, 1148

References to Properties of 2,3-Dimethyl-1-Pentanol

Refractive Index
326, 455

Density at 20–30 °C Only
1029

Normal Boiling Point
326, 455

Vapor Pressure and Boiling Points at Other Pressures
1029

References to Properties of 2,4-Dimethyl-1-Pentanol

Refractive Index
292, 1204

Density at 20–30 °C Only
292, 1204, 1031, 613

Normal Boiling Point
621, 1204, 1031, 1614, 613, 1377

Vapor Pressure and Boiling Points at Other Pressures
292, 424

References to Properties of 3,3-Dimethyl-1-Pentanol

Refractive Index
1565

Density at 20–30 °C Only
1565

Normal Boiling Point
152

Vapor Pressure and Boiling Points at Other Pressures
1565, 196

References to Properties of 3,4-Dimethyl-1-Pentanol

Refractive Index
1978, 799, 415, 1900, 14, 1809,

Density at 20–30 °C Only
799, 415, 1031

Density at all Temperatures
1809

Normal Boiling Point
1031, 1978, 415, 1900, 14

Vapor Pressure and Boiling Points at Other Pressures
1809, 799

References to Properties of 4,4-Dimethyl-1-Pentanol

Refractive Index
1918, 1947, 680, 1229

Density at 20–30 °C Only
772, 1918

Density at all Temperatures
1119

Normal Boiling Point
1119

Vapor Pressure and Boiling Points at Other Pressures
1918, 1947, 1593

References to Properties of 3-Ethyl-2-Pentanol

Refractive Index
1088

Density at ^{2}*0–30 °C Only*
1088

Density at all Temperatures
551

Normal Boiling Point
551, 320

Vapor Pressure and Boiling Points at Other Pressures
1088

References to Properties of 2,3-Dimethyl-2-Pentanol

Refractive Index
1275, 841, 1567, 563, 1092, 1385, 226

Density at 20–30 °C Only
480, 1029, 1275, 601, 841, 1377, 563, 1092

Normal Boiling Point
480, 601, 1377, 231, 1092, 1385

Vapor Pressure and Boiling Points at Other Pressures
1029, 1275, 809, 1567, 563, 226, 1308

Normal Melting Point
1578

References to Properties of 2,4-Dimethyl-2-Pentanol

Refractive Index
903, 402, 1922, 1377, 755, 1365, 1368

Density at 20–30 °C Only
1922, 601, 1377, 1365, 1368

Density at all Temperatures
903, 402

Normal Boiling Point
1960, 480, 402, 601, 1377, 755, 498

Vapor Pressure and Boiling Points at Other Pressures
903, 1922, 226, 1365, 1368

References to Properties of 3,3-Dimethyl-2-Pentanol

Refractive Index
1209, 1215, 1385

Density at 20–30 °C Only
480

Normal Boiling Point
480

Vapor Pressure and Boiling Points at Other Pressures
1209, 1385

References to Properties of 3,4-Dimethyl-2-Pentanol

Density at all Temperatures
1965

Normal Boiling Point
1965, 1541

References to Properties of 4,4-Dimethyl-2-Pentanol

Refractive Index
1918, 1919, 1920, 1922, 1939, 803, 808, 338, 226, 584, 1612, 949

Density at 20–30 °C Only
1920, 1919, 1918, 338, 584

Normal Boiling Point
338

Vapor Pressure and Boiling Points at Other Pressures
1920, **1919**, 1918, 1922, 1939, **803**, **808**, 581, 1581, **226**, **584**, **949**

Normal Melting Point
226, **584**

References to Properties of 3-Ethyl-3-Pentanol

Refractive Index
484, **1088**, 172, **1911**, 1377, 338, 648, **1650**, 1782, **724**, **1054**, 1594, 993, 2030, 32

Density at 20–30 °C Only
1088, 480, **172**, **601**, 1377, 648, 1650, 1054, 32

Density at all Temperatures
509, **1300**, **1782**

Heat of Combustion
2034, (1721)

Normal Boiling Point
388, 480, 1218, 172, **601**, 1181, 1377, 1650, 1531, 1530, 382, 1594, 993, 696, 32, 761

Vapor Pressure and Boiling Points at Other Pressures
509, **1088**, **1911**, **296**, **338**, **648**, 1782, 1054, **724**, **2030**, **413**

Normal Melting Point
509, 1777, **1782**, **1054**

References to Properties of 2,2-Dimethyl-3-Pentanol

Refractive Index
1934, 1914, **841**, 2031, 1212, 584, **543**

Density at 20–30 °C Only
519, 480, **601**, **841**, 1377, 584

Density at all Temperatures
519

Normal Boiling Point
1014, 480, **601**, 1693, **841**, 1377, 1212, 543

Vapor Pressure and Boiling Points at Other Pressures
1914, 519, **2031**, 584, 1934, 1045

Normal Melting Point
584

References to Properties of 2,3-Dimethyl-3-Pentanol

Refractive Index
1315, 1913, **1275**, 1377, **338**, 1567, 1653

Density at 20–30 °C Only
1315, 1913, 1275, **601**, **841**, 1377, 1653

Normal Boiling Point
601, **1377**

Vapor Pressure and Boiling Points at Other Pressures
1913, 1315, **1275**, **338**, 1567, **1653**

References to Properties of 2,4-Dimethyl-3-Pentanol

Refractive Index
1401, 1922, 1952, 613, 800, 1893, 1255, **804**, 1377, 1716, **338**, 1462, **2016**, 1739, **1758**, 1915

Density at 20–30 °C Only
1401, 1922, 601, 613, 800, 1893, 1255, 1377, 338, 1462, **1758**

Density at all Temperatures
1228

Normal Boiling Point
1228, 1401, 332, **601**, 613, 1554, 1377, **804**, 1716, **338**, 1462, 2016, 331, 1739, 1110

Vapor Pressure and Boiling Points at Other Pressures
1922, 1952, **1915**, 800, 1255, 804, **1758**

Normal Melting Point
338

References to Properties of 2-Methyl-2-Ethyl-1-Butanol

Refractive Index
521, **1476**, 1652, 1539, 1594

Density at 20–30 °C Only
520, 1652

Normal Boiling Point
1476, **1594**

Vapor Pressure and Boiling Points at Other Pressures
521, **1652**, **1539**

References to Properties of 3-Methyl-2-Ethyl-1-Butanol

Refractive Index
1539, **1808**, **1809**

Density at 20–30 °C Only
1539, **1808**, **1809**

Vapor Pressure and Boiling Points at Other Pressures
424, **1539**, **1808**, **1809**

References to Properties of 2,2,3-Trimethyl-1-Butanol

Refractive Index
609, 546, 755

Density at 20–30 °C Only
609, **802**

Normal Boiling Point
546, **1148**

Vapor Pressure and Boiling Points at Other Pressures
755

References to Properties of 2,3,3-Trimethyl-1-Butanol

Refractive Index
1693, 1539, 2036

Density at 20–30 °C Only
1539

Normal Boiling Point
1693

Vapor Pressure and Boiling Points at Other Pressures
1539

References to Properties of 2,3,3-Trimethyl-2-Butanol

Refractive Index
1052

Density at 20–30 °C Only
601

Normal Boiling Point
256, 1477, 1960, 480, **601**, 1566, 1693, 802, 1052, 1428

Vapor Pressure and Boiling Points at Other Pressures
809

Normal Melting Point
256, 1477, 480, 1385

Molecular Vibration Frequencies and Spectra
379

1-Octanol

Properties of the Liquid Phase at Various Temperatures

Refractive Index

The more reliable refractive index data at 20 and 25 °C are shown in table 158. Most of these scatter over a range of about 0.001. Butler, Ramchandani, and Thomson [1935], Dorough, Glass, Gresham, Malone, and Reid [1941] and Driesbach and Martin [1949] all used carefully purified samples so the selected values were close to their results. The values of Komarewsky and Coley [1941a,b] were high. Eykman [1919] reported refractive index data throughout the visible spectrum at 18.4 and 79.8 °C, and Deffet [1931] made similar measurements at 15 °C. Nevgi and Jatkar [1934] and Weissler [1948] measured n_D at 30 °C. Bonauguri, Bicelli, and Spiller [1951] have reported values at 13.5 °C, and Thomas and Meatyard [1963] worked at 15 °C. Vogel [1948] measured the refractive indices at several wavelengths at 20 °C, but they are high compared to the other reported values and were not used in the selection. Selected values of n_D from 15 to 80 °C based on these values are listed in table 155. The refractive indices at other wavelengths, in table 157, were taken from plots of observed data against $1/(\lambda-1000)^{1.6}$. The values at 20, 25, and 30 °C were obtained by interpolation.

Density

The Index to the Bibliography for 1-octanol indicates an extensive amount of density data, and some of the reported data are given in table 158. Ellis and Reid [1932], Butler, Thomson, and Maclennan [1933], Butler, Ramchandani and Thomson [1935], Oliver [1937], Dorough, Glass, Gresham, Malone, and Reid [1941], Jones, Bowden, Yarnold, and Jones [1948], Dreisbach and Martin [1949], Cook [1952], von Erichsen [1952], Brown and Smith [1962], and Paraskevopoulos and Missen [1962] have made accurate density measurements. The selected values at 20 and 25 °C as calculated from the Francis equation are within about 0.0005 g cm^{-3} of most of these. The principal sources of data at other temperatures are Carrara and Ferrari [1906], Bingham and Darrall [1930], and Costello and Bowden [1958]. Below 60 °C the values of Costello and Bowden ran 0.003 to 0.002 g cm^{-1} below most other values, and these were not used in evaluating the constants in the Francis equation. Since there were not many other data at higher temperatures, their data were used in that region, and the calculated values were within about 0.001 g cm^{-3} of Costello and Bowden's. Densities measured by Bingham and Darrall agreed well with other data at the low temperature end but were higher than those of Costello and Bowden by about 0.002 g cm^{-3}. Calculated values fell in between these two extremes above 60 °C. Carrara and Ferrari's values scattered quite a bit above and below the calculated ones and most of these were not used in establishing the curve. Deffet [1931] reported data from 0 to 30 °C, and McKinney, Skinner, and Staveley [1959] made an accurate measurement at 0 °C. A few additional points at different temperatures were used to help establish the constants. Sackmann and Sauerwald [1950] obtained 0.8492 g cm^{-3} at −14 °C. Efremov [1966] measured the saturated liquid and vapor densities from 0 to 385 °C. These were less accurate than the data used to determine the selected values but were within about 0.004 g cm^{-3} of them in the range from 0 to 120 °C.

TABLE 155. 1-Octanol. Selected values. Physical and thermodynamic properties

Temp. °C	Refractive Index, n_D	Density g cm^{-3}	Vapor Pressure, mmHg
−10		0.8460	
0		.8394	0.0096
10		.8327	.0256
15	1.4316		
20	1.4296	.8258	.0645
25	1.4276	.8223	.100
30	1.4257	.8188	.154
40	1.4218	.8117	.352
50	1.4179	.8044	.77
60	1.4140	.7970	1.61
70	1.4102	.7893	3.2
80	1.4063	.7815	7.7
85			8.1
88.5			10
90		.7735	10.9
95			14.6
100		.7653	19.3
105			25.2
110		.7568	32.5
115			41.4
120		.7480	52.4
125			65.7
130		.7390	81.6
134.9			100
135			100.6
140			123.1
145			149.5
150			180.
152.8			200
155			216.
160			257.
165			305.
170			359.
173.4			400
175			421.
180			491.
185			570.
190			658.
195			757.
195.2			760
200			867.

Data For Phase Transitions

Initial	Final	Temp. °C	dt/dP deg mm^{-1}	Pressure mmHg	ΔH kcal mol^{-1}	$d\Delta H/dt$	ΔS	ΔC_p
						cal deg^{-1} mol^{-1}		
c	liq	−15.5±0.5		760	10.1±1		39.2±4	
liq	g	25	115.	0.100±0.01	15.6±0.5	−29.5±2	51.7±1.5	−29.5±2
liq	g	195.2±0.2	0.0478	760	11.2±0.8	−33.7±4	23.9±2	−29.7±3

Condensed Phase Heat Capacity

State	Temp. °C	C_p
		cal deg^{-1} mol^{-1}
liq	195.2	99.4±3

Properties of the Saturated Real Gas

Temp. °C	H^r-H^0	S^r-S^0	$C_p{}^r-C_p{}^0$
	kcal mol^{-1}	cal deg^{-1} mol^{-1}	
195.2	−0.16±0.05	−0.25±0.1	+1.0±0.3

Data for the Standard States at 25 °C

State	Heat of Combustion $\Delta H_c{}^0$ kcal mol^{-1}	Heat of Formation $\Delta H_f{}^0$ kcal mol^{-1}	Entropy S^0 cal deg^{-1} mol^{-1}	Gibbs Energy of Formation $\Delta G_f{}^0$ kcal mol^{-1}	Heat Capacity, C_p cal deg^{-1} mol^{-1}
liq	−1265.7±0.4	−101.6±0.4	90.2±1.5	−34.2±0.6	77.7±2
g	−1281.3±0.6	−86.0±0.6	124.1±0.7	−28.7±0.6	48.2±0.5

Critical Constants

Temp. 385 °C, 658. K	Pressure atm,	Density 0.266 g cm^{-3}

Constants in Vapor Pressure and Density Equation

Antoine Equation

Temp. Range	A	B	C
70 to 195 °C	6.83790	1310.62	136.05
0 to 80 °C	12.0701	4506.8	319.9

Francis Equation

Temp. Range	A	$B\times10^3$	C	E
−15 to 140 °C	0.99077	0.3627	75.70	500

TABLE 156. 1-Octanol. Selected values. Thermodynamic functions of the ideal gas at one atmosphere

Temperature	Entropy S^0 cal deg^{-1} mol^{-1}	Heat Capacity C_p^0 cal deg^{-1} mol^{-1}	Enthalpy Function $(H^0-H^0_0)/T$ cal deg^{-1} mol^{-1}	Gibbs Energy Function $(G^0-H^0_0)/T$ cal deg^{-1} mol^{-1}	Heat of Formation ΔHf^0 kcal mol^{-1}	Gibbs Energy of Formation ΔGf^0 kcal mol^{-1}
0	0	0	0	0	−74.0	−74.0
273.15	120.11	45.22	29.70	−90.41	−85.1	−33.5
298.15	124.14	48.17	31.13	−93.01	−86.0	−28.7
300	124.41	48.41	31.22	−93.19	−86.1	−28.3
400	139.91	60.56	37.04	−102.87	−89.2	−8.6
500	154.64	71.76	42.89	−111.75	−91.8	11.9
600	168.49	81.26	48.49	−120.00	−93.8	32.9
700	181.61	89.43	53.73	−127.88	−95.4	54.1
800	194.04	96.39	58.66	−135.38	−96.5	75.6
900	205.71	102.40	63.22	−142.49	−97.2	97.2
1000	216.79	107.58	67.38	−149.41	−97.7	118.8

TABLE 157. 1-Octanol. Selected values refractive index at various temperatures and wavelengths

Symbol	Wavelength, Å	Refractive Index, n				
		15 °C	20 °C	25 °C	30 °C	80 °C
He_{red}	6678.2	1.4291	1.4271	1.4251	1.4231	1.4039
H_c	6562.8	1.4294	1.4274	1.4254	1.4235	1.4043
Na_D	5892.6	1.4316	1.4296	1.4276	1.4257	1.4063
Hg_e	5460.7	1.4334	1.4315	1.4295	1.4275	1.4081
He_{blue}	5015.7	1.4359	1.4339	1.4320	1.4299	1.4104
H_F	4861.3	1.4369	1.4350	1.4330	1.4309	1.4114
Hg_g	4358.3	1.4411	1.4391	1.4371	1.4351	1.4154
$H_{G'}$	4340.5	1.4412	1.4392	1.4372	1.4353	1.4156

Vapor Pressure and Boiling Point

The literature on boiling points is fairly extensive. Table 158 lists those values which have resulted from precision measurements. The selected normal boiling point is 195.2 °C, which is within about 0.2 °C of most of the better values. No measurements have been made above one atmosphere, but there have been several series of studies of vapor pressure over a range of temperatures below one atmosphere. Butler, Ramchandani, and Thomson [1935] carried out the first such measurements over the range from 60 to 153 °C; Dorough, Glass, Gresham, Malone, and Reid [1941] measured the vapor pressure at four temperatures from 100 to 195 °C; Dreisbach and Shrader [1949] carried a series of precise measurements from 122 to 195 °C; Thomas and Meatyard [1963] reported values from 82 to 195 °C; and Rose, Papahronis, and Williams [1958] made accurate measurements from 92 to 154 °C. In addition there have been scattered measurements of boiling points at various pressures. These data were used in fitting the Antoine constants shown in table 155. Below the normal boiling point, the calculated vapor pressures are within about 2 mm of the observed ones. Thus the values reported by the various investigators are in relatively good agreement.

There are three sets of measurements of vapor pressure in the region below 10 mm. Besides the data of Butler, Ramchandani and Thomson [1935], Quitzsch, Hüttig, Vogel, Gesemann and Geiseler [1953] have measured the vapor pressure from 20 to 80 °C by use of an isoteniscope. Their estimated uncertainty in pressure is 0.1 mm. Finally, Davies and Kybett [1965] have measured the vapor pressure of the solid phase from −35 to −22 °C and of the liquid from −6 to +9 °C in a Knudsen effusion cell. They express their results as $\log P(\text{mmHg}) = 18.889 - 5507/T$ for the solid, and $\log P(\text{mmHg}) = 10.217 - 3343/T$ for the liquid. Paraskevopoulos and Missen [1962] estimated a vapor pressure of 2.35 mm at 60 °C by extrapolating vapor liquid equilibrium measurements in the system carbon tetrachloride-octanol. However, this result is definitely too high.

Although not in the same range, the data of Quitzsch, Hüttig, Vogel, Gesemann and Geiseler are not compatible with those of Davies and Kybett. Extrapolation of either set shows that those of Quitzsch et al. are too

TABLE 158. 1-Octanol. Reported values. Simple physical properties

Investigators		Vapor Pressures and Boiling Points		Freezing Point	Density, *d* g cm^{-3}		Refractive Index, n_D	
		°C	mmHg	t_m, °C	20 °C	25 °C	20 °C	25 °C
1-Octanol, $C_8H_{18}O$, mol wt. 130.232, state at 25 °C, liq.								
Zander	[1884]	195.5	760					
Carrara and Ferrari	[1906]	195.5	760		0.8272			
Lespieau	[1914]	193.5	760	−14				
Lowry	[1914]				.8270			
Timmermans	[1922a]	194.0	760	−16.3				
Wood and Comley	[1924]	195.6–195.9	760					
Lecat	[1926]	195.15	760					
Malone and Reid	[1929]	195.1	760					
Smyth and Stoops	[1929]				.8253	0.8220		
Bingham and Darrall	[1930]				.82570			
Deffet	[1931]	194.45	760	−16.7		.82529	1.4302	
Ellis and Reid	[1932]	194.7	760			.82137		1.4274
Kailan and Raff	[1932]	195.0	760					
Butler, Thomson, and Maclennan	[1933]	194.5	760			.82238	1.42937	
Harkins and Grafton	[1933]				.8252			
Butler, Ramchandani, and Thomson	[1935]	194.5	760			.82322	1.42957	
Olivier	[1937]	194.9–195.2	760		.8249			
Komarewsky and Coley	[1941a]	194.0–195.0	760				1.4315	
Komarewsky and Coley	[1941b]							1.4295
Dorough, Glass, Gresham, Malone, and Reid	[1941]	195.0	760	−15.0		.8224		1.4275
Muller	[1942]				0.8256		1.4320	
Fischer and Reichel	[1943]						1.4295	
Ralston, Hoerr, and DuBrew	[1944]			−13.10				
Addison	[1945]	194.5	760		.8244		1.4291	
Vogel	[1948]	193.3	760		.8273		1.43325	
Jones, Bowden, Yarnold, and Jones	[1948]					.8221		
Dreisbach and Martin	[1949]	195.28	760	−14.97	.82555	.82209	1.42913	1.42749
Tschamler, Richter, and Wettig	[1949b]			−16.8				
Dreisbach and Shrader	[1949]	195.28	760					
Mumford and Phillips	[1950]	194.6	760		.8265	.8232	1.4237	
Adkins and Rosenthal	[1950]							1.4284
Winsor	[1950]						1.4304	
Ziegler and Gellert	[1950]			−15.9				
Sackmann and Sauerwald	[1950]			−14				
Bonauguri, Bicelli, and Spiller	[1951]	194.5	760					
Cook	[1952]	195.0	760	−15	0.8255		1.4295	
von Errichsen	[1952]	195.7–195.8	760		.8254		1.4292	
Stavely and Spice	[1952]	193.2	760		0.8254			
McKenna, Tartar, and Lingafelter	[1953]	194.2	760					1.4274
Jacobson	[1955]							1.4290
Rathmann, Curtis, McGreer, and Smyth	[1956]						1.43018	
Costello and Bowden	[1958]	195.2	760	−16.9	.8227			
Lawesson and Yang	[1959]						1.4296	
Brown and Smith	[1962b]	195.2	760			0.82247		1.42741
Geiseler, Fruwert, and Stockel	[1962]	195			.8255		1.4296	
Paraskevopoulos and Missen	[1962]					.82205		
Thomas and Meatyard	[1963]	194.7	760					1.4277
Blood and Hagemeyer	[1964]				.8265			
Davies and Kybett	[1965a]			−16.7– −17.2				
Rose, Paphronis, and Williams	[1958]	91.9	12.2					1.42727
Selected value	[1967]	195.2±0.2 88.5±1	760 10	−15.5 ±0.5	.8258 ±.0005	.8223 ±.001	1.4296 ±0.001	1.4276 ±0.001

Antoine constants: *A* 6.83790, *B* 1310.62, *C* 136.05. *dt/dp* at 760 mmHg, 0.0471 °C/mmHg low, at least at the low temperature end. In view of the uncertainty in pressure measurement estimated by Quitzsch et al. and the difficulty in using an isoteniscope for very low pressures, the data of Davies and Kybett are judged to be more reliable. A reasonable set of Antoine constants for the range from about 0 to 80 °C can be fit to the data of Davies and Kybett, Quitzsch et al. at 50 °C and above, Butler, Ramchandani, and Thomson from 60 to 80 °C, and one value from Verkade and Coops [1927] at 82.8 °C. These constants are also shown in table 155. Although these constants differ appreciably from those for the higher temperature range, the two sets of constants predict vapor pressures which are the same to within 0.1 mm in the region of overlap, from 60 to 80 °C, which is within the experimental uncertainties.

Critical Properties

Critical Temperature

Brown, J. C. [1906] made several measurements with the results varying from 383.5 to 387.3 °C. Fischer and Reichel [1943] obtained 384.6 °C. Little information was given concerning the purity of these samples. Efremov [1966] obtained 385 °C for "chemically pure grade" alcohol. The average of 385 °C was selected, with an estimated uncertainty of 1 °C.

Critical Density

Efremov [1966] has made the only measurement, and his value was selected. No measurements of critical pressure have been reported.

Solid-Liquid Phase Equilibria

Normal Melting Point

Significant melting point measurements range from about −18 to −13 °C. Table 158 lists the more reliable values. The solid and liquid vapor pressure curves of Davies and Kybett [1965] meet at −23.7 °C, which is too low for the triple point. Dreisbach and Martin made a careful determination, although it is difficult to reconcile their result with more recent ones. They claimed a purity of 99.7 percent. The selected value is a compromise among these, and the uncertainty is at least 0.5 °C and possibly more.

Heat of Fusion

The heat of fusion is taken as the difference between the heat of sublimation of the solid and the heat of vaporization of the liquid, as derived from the vapor pressure measurements of Davies and Kybett [1965].

Properties of the Liquid at 25 °C

Heat Capacity

von Reis [1881] has measured enthalpy changes in a drop calorimeter with upper temperatures from 64 to 195 °C, and lower temperatures at around 25 °C. These data can be represented by a heat capacity which is a linear function of temperature. The equation is $C_p = 74.53 + 0.1276\ t$ cal deg^{-1} mol^{-1}, in which t is the Celsius temperature. It is difficult to estimate the accuracy of these measurements, but they cannot be considered very reliable because of the general state of instrumentation at that time. The heat capacity of the liquid was calculated from this equation.

Heat of Combustion

There have been only two determinations of the heat of combustion. When converted to current units and standard state, Verkade and Coops [1927] obtained $\Delta H_c^0 = -1264.6$ kcal mol^{-1} at 25 °C. Chao and Rossini [1965] reported −1265.65 kcal mol^{-1}. Since this difference is within the uncertainty in the calorimetric measurements in 1927 Chao and Rossini's was selected.

Absolute Entropy

The entropy of the liquid was calculated from the entropy of the gas, the heat of vaporization, and the vapor pressure at 25 °C.

Properties of the Real Gas

No real gas properties have been measured. Ideal gas corrections at the normal boiling point were estimated from the critical temperature, an estimated critical pressure, and an acentric factor of 0.48.

Vapor-Liquid Equilibrium at 25 °C

Vapor Pressure

The selected value was calculated from the Antoine constants derived for the 0–80 °C temperature range as recorded in table 155.

Heat of Vaporization

There are no direct calorimetric measurements. Davies and Kybett [1965] calculated 15.3 kcal mol^{-1} from their vapor pressure data in the range of −6 to 9 °C. The Antoine constants for the 0–80 °C listed in table 155 gives 15.4 kcal mol^{-1}. Antoine constants fitted to the vapor pressure data of Quitzsch, Hüttig, Vogel, Gesemann, and Geiseler [1953] alone give 17.0 kcal mol^{-1} at 25 °C. The selected value was based on the one calculated from the Antoine constants with a slight adjustment for internal consistency.

Vapor-Liquid Equilibrium at the Normal Boiling Point

At the pressure of the equilibrium vapor at 25 °C, the gas may be considered ideal. Thus $d\Delta H/dT$ may be assumed equal to ΔC_p, the difference between the heat capacity of the gas and the liquid.

Vapor-Liquid Equilibrium at the Normal Boiling Point

Normal Boiling Point

This was calculated from the Antoine constants for the corresponding temperature range.

Heat of Vaporization

Brown, J. C. [1903] obtained a value of 12.7 kcal mol^{-1} by calorimetric measurement with electric heating. Using an estimated second virial coefficient of −1.7 liters mol^{-1} with the Antoine constants in table 155 gave a heat of vaporization of 11.6 kcal mol^{-1}. Considerable uncertainty must be attached to each of these results, however. They both seem high to other data on 1-octanol, and a slightly lower value than either was selected.

Heat Capacity of the Liquid

The heat capacity at 195.2 °C was calculated from the equation derived from the measurements of von Reis [1881]. It can be considered only as highly approximate.

Temperature Derivative of the Heat of Vaporization

The total derivative of ΔH with respect to temperature was calculated from the heat capacities of the liquid and saturated vapor, the heat of vaporization, and the estimated second virial coefficient, using the formula given in the corresponding section of the discussion on 1-pentanol.

Properties of the Ideal Gas State

Ideal gas thermodynamic functions have been published by Chermin [1961] and Green [1961]. Both of these have used the methylene increment derived from hydrocarbons to predict the data for the higher alcohols. Additional details are given in the section on 1-pentanol. The values tabulated by Green were selected and listed in table 156.

Test of Internal Consistency

Internal consistency among the vapor-liquid equilibrium properties is shown in the table below.

	ΔH kcal mol^{-1}	ΔS cal deg^{-1} mol^{-1}
liquid (25 °C)→real gas (25 °C, 0.10 mmHg)	15.6±0.5	52.3±1.5
real gas (25 °C)→ideal gas (25 °C)	0.0	0.0
ideal gas (25 °C)→ideal gas (195.2 °C)	9.97±0.2	25.9±0.6
ideal gas (0.10 mmHg)→ideal gas (760 mmHg)	0.0	−17.76±0.1
ideal gas (195.2 °C, 760 mmHg)→real gas (195.2 °C, 760 mmHg)	−0.16±0.05	−0.25±0.1
real gas (195.2 °C)→liquid (195.2 °C)	−11.2±0.8	−23.9±2
liquid (195.2 °C)→liquid (25 °C)	−15.1±1.5	−39.9±3
Sum	−0.9±1.8	−3.6±3.9

In order to obtain a sum of zero for the cycle, the difference between the heat of vaporization at 25 °C and at the boiling point would have to be 5.3 kcal mol^{-1}. The temperature coefficients calculated for the heat of vaporization lead to about this same conclusion. The data from either direct calorimetry or from vapor pressure values predict a difference of around 3.6 kcal mol^{-1}. The values selected were obtained by adjusting ΔH_v for both temperatures slightly so as to bring the sum of these contributions to within the experimental uncertainties of zero.

Index to the Bibliography

Numbers refer to the Bibliography, page 1–389.

References to data used in the selection of refractive index, density, boiling point, vapor pressure, and melting point are in boldface type.

Numbers in parentheses refer to sources of reviews or theoretical calculations only.

Reference numbers under each property are listed in the order of date of publication.

Refractive Index
123, 509, 1113, 398, **486**, **254**, 1262, **253**, **444**, 799, 926, 927, 1222, **532**, 6, 1856, 1893, **452**, 13, 1224, 1246, **1971**, 180, 1865, **338**, 345, **1152**, **836**, 610, **943**, **1460**, **1003**, 231, **586**, 1758, **165**, **1498**

Density at 20–30 °C Only
1349, 576, **1087**, **123**, 1113, **1646**, **486**, 931, **254**, 708, 1549, **253**, **1288**, 799, **444**, 1222, **6**, **853**, **1856**, 1810, **452**, 1224, **338**, 1682, 1865, 610, 586, **1313**, 165, **230**

Density at all temperatures
2028, 2012, **273**, 705, **509**, **1848**, **149**, **398**, 1262, 1893, **1527**, **347**, **1154**

Normal Boiling Point
2028, 1349, 2012, **272**, 1395, **273**, 656, 1016, 123, **1774**, 1009, 1121, 1580, **398**, **486**, 870, 1981, 1549, 1288, 799, 926, 6, 1972, **1856**, **452**, 1895, 195, 1224, 180, 338, 345, 1865, **1682**, 1152, 377, 836, **347**, **231**, 586, 165

Vapor Pressure and Boiling Points at Other Pressures
953, 937, 189, 509, 1133, **1848**, 148, **486**, 1837, **253**, **254**, 1262, **444**, 10, **453**, 1807, 1246, 610, 943, 1003, 232, 1313, 1758, 5, **1498**, **1442**, **1758**

Critical Temperature
218, 748, 532, 649, (347), 481

Critical Volume and Density
481

Normal Melting Point
256, 555, 272, 1016, 1774, **398**, **444**, 1450, **1807**, **452**, 2027, 1527, 463, 338, 345, 377, 347, 165, **389**

Heat of Fusion
389

Heat Capacity of the Liquid at 25 °C
1866

Calorimetric Heat of Vaporization at the Normal Boiling Point
219

Heat of Combustion
1848, (1501), (626), 287, 288

Molecular Vibration Frequencies and Spectra
1440, 1190, 1012, 456, 797

Thermodynamic Functions of the Ideal Gas
623, 291

Association in the Liquid Phase
1754, 1683, 182, 1460, 78

Isomeric Octanols

A complete list of reported values of simple physical properties is given in the following unnumbered tables for all of the isomeric octanols except 2-octanol. The less significant data have not been included in the table for 2-octanol, but a complete list of references is identified in the Index to the Bibliography on page 1–250. Where possible the constants in the Antoine and Francis equations for the isomeric octanols were calculated by a least squares fit to the observed vapor pressure and density data. These constants, as well as the densities and vapor pressures calculated from them, have been given in numbered tables (159–167). Vapor pressures are given at five degree intervals and boiling points at several standard pressures. The least squares calculation of the Antoine constants was based on a form of the equation which was linear in the constants, as described in appendix B. In some other cases a few scattered boiling points have been reported in the literature, but they are not suitable for establishing the *C* constant in the Antoine equation. The following procedure was adopted to obtain sets of constants which can be used for approximate interpolations of boiling points. Graphs of log P versus $1/(t+273)$ and $1/(t+125)$ were prepared for each compound and the values of the A and B constants were calculated for the graph which was most nearly a straight line. Constants obtained in this way are listed at the end of the unnumbered table for each such compound. In a few cases where there was a sufficient amount of data, numbered tables showing vapor pressures at intervals of 10 degrees were prepared.

Most of the precise physical property data for the isomeric octanols stem from the work of Dorough et al. during the decade from 1930 to 1940. During this time they synthesized and carefully purified the four straight chain isomers and the 18 methyl heptanols. They then conducted a detailed study of the physical properties of this group of compounds, in order to obtain some information about the effect of molecular structure on physical properties of isomers. In addition, they furnished samples of these compounds to other investigators for additional measurements. Using their samples Bingham and Darrall [1930] measured the density and viscosity from 0 to 100 °C; Cline and Andrews [1931] measured the heat capacities from 102 K to around 25 °C; Maass and Wyman measured the surface tension, and Smyth measured the dielectric constant. In addition, Dorough et al. determined the boiling points at 20, 100, 300, and 760 mmHg, densities at 0 and 25 °C, refractive index at 25 °C, melting point, and solubility in water. All of this work has been summarized by Dorough, Glass, Gresham,

Table 159. Isomeric Octanols. Selected values. Physical properties of the liquid

2-Octanol				3-Octanol				4-Octanol			
Temp. °C	Refractive Index, n_D	Density g cm^{-3}	Vapor Pressure, mmHg	Temp. °C	Refractive Index, n_D	Density g cm^{-3}	Vapor Pressure, mmHg	Temp. °C	Refractive Index, n_D	Density g cm^{-3}	Vapor Pressure, mmHg
0		0.8347		0		0.8370		0		0.8344	
10	1.4301	.8278		10		.8293		10		.8269	
20	1.4261	.8207		20	1.423	.8216		20	1.425	.8192	
25	1.4241	.8171		25	1.421	.8176		25	1.4227	.8154	
30	1.4221	.8135		30		.8136		30		.8115	
40	1.4181	.8061		40		.8056		40		.8036	
50		.7984		50		.7973		50		.7956	
60		.7906		60		.7889		60		.7874	
70		.7825	7.6	68.1			10	70		.7790	9.4
74.3			10	70		.7802	11.5	71.			10
75			10.5	75			16.2	75			13.0
80		.7741	14.2	80		.7714	22.3	80		.7704	17.9
85			19.0	85			30.1	85			24.0
90		.7654	25.0	90		.7624	39.7	90		.7616	31.8
95			32.6	95			52.	95			41.4
100		.7563	42.0	100		.7532	66.	100		.7525	53.1
105			53.4	105			83.	105			67.4
110		.747	67.3	109.			100	110			84.5
115			83.9	110		.744	103.	113.9			100
119.1			100	115			127.	115			105.
120			104.	120			154.	120			128.
125			127.	125			185.	125			156.
130			155.	127.			200	130			188.
135			186.	130			220.	131.7			200
136.9			200	135			260.	135			225.
140			223.	140			305.	140			266.
145			266.	145			354.	145			313.
150			314.	149.			400	150			366.
155			369.	150			409.	153.0			400
157.6			400	155			469.	155			425.
160			432.	160			534.	160			491.
165			502.	165			605.	165			563.
170			580.	170			682.	170			643.
175			667.	174.7			760	175			731.
179.8			760	175			765.	176.6			760
180			764.								

Constants	Temp. Range	*A*	*B*	*C*	*E*	Constants	Temp. Range	*A*	*B*	*C*	*E*	Constants	Temp. Range	*A*	*B*	*C*	*E*
Antoine eq	72 to 180 °C	6.3888	1060.4	122.5		Antoine eq	76 to 176 °C	5.2215	560.3	64.7		Antoine eq	71 to 176 °C	5.7396	760.5	89.5	
Francis eq	0 to 100 °C	0.92303	4.298×10^{-4}	30.93	350	Francis eq	0 to 125 °C	1.08199	3.483×10^{-4}	147.01	600	Francis eq	0 to 100 °C	0.89722	5.675×10^{-4}	21.98	350

TABLE 160. Isomeric Octanols. Selected values. Physical properties of the liquid

2-Methyl-1-heptanol

Temp. °C	Refractive Index, n_D	Density g cm^{-3}	Vapor Pressure, mmHg
0		0.8168	
10		.8096	
20	1.424	.8022	
25	1.4219	.7986	
30		.7948	
40		.7873	
50		.7796	
60		.7717	
65.7			10
70		.7636	13.0
75			17.4
80		.7554	22.8
85			29.7
90		.7470	38.1
95			48.3
100		.7384	60.7
105			75.4
110			92.9
111.8			100
115			114.
120			138.
125			165.
130			198.
130.3			200
135			234.
140			276.
145			323.
150			377.
152.0			400
155			436.
160			503.
165			577.
170			659.
175			749
175.6			760

Constants	Temp. Range	A	B	C	E
Antoine eq	77 to 175 °C	6.1860	1002.1	127.6	
Francis eq	0 to 100 °C	1.03201	3.527×10^{-4}	129.15	600

3-Methyl-1-heptanol

Temp. °C	Refractive Index, n_D	Density g cm^{-3}	Vapor Pressure, mmHg
0		.8027	
10		.7955	
20	1.425	.7881	
25	1.4225	.7844	
30		.7807	
40		.7732	
50		.7656	
60		.7579	
70		.7501	
74.6			10
80		.7422	13.5
85			17.5
90		.7342	22.5
95			28.7
100		.7260	36.3
105			45.6
110			56.7
115			70.1
120			86.0
123.8			100
125			104.8
130			127.
135			153.
140			183.
142.5			200
145			218.
150			258.
155			304.
160			356.
163.8			400
165			416.
170			483.
175			559.
180			644.
185			740.
186.0			760

Constants	Temp. Range	A	B	C	E
Antoine eq	87 to 185 °C	7.1977	1584.6	181.1	
Francis eq	0 to 100 °C	0.93672	4.993×10^{-4}	80.39	600

4-Methyl-1-heptanol

Temp. °C	Refractive Index, n_D	Density g cm^{-3}	Vapor Pressure, mmHg
0		0.8247	
10		.8174	
20	1.427	.8101	
25	1.4253	.8064	
30		.8026	
40		.7951	
50		.7874	
60		.7796	
70		.7717	
72.5			10
80		.7637	15.9
85			21.3
90		.7555	28.0
95			36.3
100		.7471	46.4
105			58.6
110			73.1
115			90.4
117.			100
120			111.
125			134.
130			161.
135			192.
136.			200
140			228.
145			268.
150			312.
155			363.
158.			400
160			418.
165			480.
170			548.
175			623.
180			704.
183.2			760

Constants	Temp. Range	A	B	C	E
Antoine eq	81 to 183 °C	5.7368	796.3	95.6	
Francis eq	0 to 100 °C	0.86942	5.980×10^{-4}	15.64	350

TABLE 161. Isomeric Octanols. Selected values. Physical properties of the liquid

5-Methyl-1-heptanol

Temp. °C	Refractive Index, n_D	Density g cm^{-3}	Vapor Pressure, mmHg
0		0.8330	
10		.8260	
20	1.420	.8189	
25	1.4272	.8153	
30		.8117	
40		.8043	
50		.7969	
60		.7893	
70		.7816	
79.1			10
80		.7737	10.6
85			14.2
90		.7656	18.9
95			24.7
100		.7574	32.0
105			41.0
110			51.9
115			65.1
120			81.0
125			99.8
125.1			100
130			122.
135			148.
140			178.
143.2			200
145			213.
150			254.
155			300.
160			352.
164.1			400
165			411.
170			478.
175			553.
180			636.
185			729.
186.6			760
190			831.

Constants	Temp. Range	*A*	*B*	*C*	*E*
Antoine eq	91 to 186 °C	6.4894	1131.9	127.1	
Francis eq	0 to 100 °C	0.88467	5.497×10^{-4}	18.08	350

6-Methyl-1-heptanol

Temp. °C	Refractive Index, n_D	Density g cm^{-3}	Vapor Pressure, mmHg
0		0.8346	
10		.8278	
20	1.427	.8210	
25	1.4255	.8175	
30		.8140	
40		.8069	
50		.7997	
60		.7924	
70		.7849	
80		.7772	
84.1			10
90		.7693	14.3
95			19.2
100		.7613	25.3
105			32.9
110			42.4
115			54.0
120			68.1
125			85.1
128.7			100
130			105.
135			130.
140			158.
145			191.
146.2			200
150			230.
155			274.
160			325.
165			384.
166.3			400
170			450.
175			525.
180			609.
185			704.
187.7			760
190			809.

Constants	Temp. Range	*A*	*B*	*C*	*E*
Antoine eq	95 to 188 °C	6.6443	1170.6	123.3	
Francis eq	0 to 100 °C	0.90988	4.820×10^{-4}	30.12	400

2-Methyl-2-heptanol

Temp. °C	Refractive Index, n_D	Density g cm^{-3}	Vapor Pressure, mmHg
0		0.8237	
10		.8174	
20	1.4221	.8107	
25	1.4201	.8072	
30		.8035	
40		.7957	
50		.7873	
59.5			10
60		.7782	10.3
65			14.0
70		.7684	18.7
75			24.8
80		.7578	32.5
85			42.2
90		.7476	54.2
95			69.0
100		.7340	87.1
103.0			100
105			109.1
110			136.
115			167.
119.4			200
120			205.
125			250.
130			302.
135			363.
137.7			400
140			434.
145			516.
150			611.
155			719.
156.7			760
160			842.

Constants	Temp. Range	*A*	*B*	*C*	*E*
Antoine eq	66 to 156 °C	7.5668	1590.6	182.7	
Francis eq	0 to 100 °C	1.17862	-2.861×10^{-4}	141.98	400

TABLE 162. Isomeric Octanols. Selected values. Physical properties of the liquid

3-Methyl-2-heptanol			
Temp. °C	Refractive Index, n_D	Density g cm^{-3}	Vapor Pressure, mmHg
20	1.422	0.8217	
25	1.4199	.8177	
55.1			10
60			13.1
65			17.0
70			22.0
75			28.1
80			35.6
85			44.7
90			55.7
95			68.9
100			84.6
104.2			100
105			103.
110			125.
115			151.
120			181.
122.8			200
125			215.
130			255.
135			301.
140			354.
144.0			400
145			413.
150			480.
155			557.
160			642.
165			738.
166.1			760

Constants	Temp. Range	A	B	C	E
Antoine eq	68 to 166 °C	7.2335	1601.4	201.8	
Francis eq					

4-Methyl-2-heptanol			
Temp. °C	Refractive Index, n_D	Density g cm^{-3}	Vapor Pressure, mmHg
0		0.8172	
10		.8100	
20	1.424	.8027	
25	1.4225	.7989	
30		.7952	
40		.7875	
50		.7796	
60		.7715	
66.4			10
70		.7632	12.4
75			16.6
80		.7546	21.9
85			28.5
90		.7457	36.8
95			46.9
100		.7365	59.3
105			74.3
110			92.1
112.0			100
115			113.
120			139.
125			168.
129.7			200
130			202.
135			242.
140			288.
145			340.
150.0			400
155			468.
160			544.
165			630.
170			726.
171.6			760
175			833.

Constants	Temp. Range	A	B	C	E
Antoine eq	78 to 172 °C	6.7364	1237.5	149.3	
Francis eq	0 to 100 °C	0.89962	4.768×10^{-4}	28.85	350

5-Methyl-2-heptanol			
Temp. °C	Refractive Index, n_D	Density g cm^{-3}	Vapor Pressure, mmHg
0		0.8283	
10		.8211	
20	1.424	.8137	
25	1.4218	.8098	
30		.8059	
40		.7979	
50		.7896	
60		.7809	
63.5			10
70		.7718	14.5
75			19.0
80		.7623	24.7
85			31.8
90		.7522	40.4
95			50.9
100		.7414	63.7
105			78.9
110			97.1
110.7			100
115			119.
120			144.
125			173.
129.0			200
130			207.
135			247.
140			292.
145			344.
149.8			400
150			402.
155			469.
160			544.
165			628.
170			722.
171.9			760

Constants	Temp. Range	A	B	C	E
Antoine eq	75 to 172 °C	6.8882	1359.8	167.5	
Francis eq	0 to 100 °C	0.92286	3.965×10^{-4}	28.35	300

TABLE 163. Isomeric Octanols. Selected values. Physical properties of the liquid

6-Methyl-2-heptanol

Temp. °C	Refractive Index, n_D	Density g cm^{-3}	Vapor Pressure, mmHg
0		0.8221	
10		.8146	
20	1.423	.8071	
25	1.4209	.8033	
30		.7994	
40		.7916	
50		.7836	
60		.7755	
68.9			10
70		.7672	10.7
75			14.3
80		.7586	18.9
85			24.8
90		.7499	32.1
95			41.3
100		.7409	52.5
105			66.2
110			82.7
114.4			100
115			103.
120			126.
125			154.
130			187.
131.7			200
135			226.
140			271.
145			323.
150			383.
151.3			400
155			452.
160			530.
165			619.
170			719.
171.9			760
175			832.

Constants	Temp. Range	A	B	C	E
Antoine eq	81 to 172 °C	7.2176	1476.0	168.5	
Francis eq	0 to 100 °C	0.88587	5.570×10^{-4}	22.32	350

2-Methyl-3-heptanol

Temp. °C	Refractive Index, n_D	Density g cm^{-3}	Vapor Pressure, mmHg
0		0.8399	
10		.8323	
20	1.4266	.8245	
25	1.4246	.8205	
30		.8165	
40		.8082	
50		.7998	
60		.7912	
64.2			10
70		.7823	14.3
75			19.1
80		.7732	25.2
85			32.9
90		.7638	42.4
95			54.0
100		.7542	68.
105			85.3
108.7			100
110			106.
115			130.
120			158.
125			192.
126.1			200
130			231.
135			275.
140			327.
145			385.
146.2			400
150			452.
155			527.
160			611.
165			706.
167.6			760
170			812.

Constants	Temp. Range	A	B	C	E
Antoine eq	75 to 168 °C	6.6097	1150.1	140.8	
Francis eq	0 to 150 °C	1.27658	1.293×10^{-4}	305.69	700

3-Methyl-3-heptanol

Temp. °C	Refractive Index, n_D	Density g cm^{-3}	Vapor Pressure, mmHg
0		0.8455	
10		.8375	
15	1.4306		
20	1.4283	.8293	
25	1.4263	.8251	
30		.8210	
35	1.4214		
40		.8125	
50		.8038	
59.2			10
60		.7949	10.6
65			14.4
70		.7859	19.4
75			25.7
80		.7766	33.6
85			43.5
90		.7766	56.
95			71.
100		.7671	89.
102.8			100
105		.7573	110.
110			135.
115			165.
120.0			200
125			241.
130			288.
135			342.
139.7			400
140			404.
145			474.
150			553.
155			642.
160			742.
161.			760
165			853.

Constants	Temp. Range	A	B	C	E
Antoine eq	65 to 160 °C	6.5807	1116.2	140.9	
Francis eq	0 to 100 °C	1.01732	4.523×10^{-4}	85.91	500

TABLE 164. Isomeric Octanols. Selected values. Physical properties of the liquid

4-Methyl-3-heptanol

Temp. °C	Refractive Index, n_D	Density g cm^{-3}	Vapor Pressure, mmHg
0		0.8143	
10		.8062	
20	1.420	.7981	
25	1.4179	.7940	
30		.7899	
40		.7816	
44.9			10
45			10.6
50		.7732	13.7
55			17.6
60		.7647	22.3
65			28.2
70		.7561	35.5
75			44.2
80		.7473	54.8
85			67.5
90		.7384	82.7
94.8			100
95			100.7
100		.7293	122.
105			147.
110			176.
113.5			200
115			211.
120			250.
125			296.
130			349.
134.2			400
135			410.
140			479.
145			558.
150			648.
155			750.
155.4			760

Constants	Temp. Range	*A*	*B*	*C*	*E*
Antoine eq	57 to 155 °C	8.2151	2282.9	272.5	
Francis eq	0 to 100 °C	0.85659	6.807×10^{-4}	14.81	350

5-Methyl-3-heptanol

Temp. °C	Refractive Index, n_D	Density g cm^{-3}	Vapor Pressure, mmHg
0		0.8354	
10		.8270	
20	1.418	.8185	
25	1.4156	.8143	
30		.8100	
40		.8014	
44.6			10
45			10.3
50		.7927	13.7
55			18.0
60		.7840	23.5
65			30.2
70		.7751	38.5
75			48.6
80		.7662	60.9
85			75.6
90		.7571	93.0
91.8			100
95			114.
100		.7480	138.
105			166.
110			199.
110.1			200
115			237.
120			280
125			329.
130			386.
131.2			400
135			449.
140			520.
145			600.
150			690.
153.6			760
155			789.

Constants	Temp. Range	*A*	*B*	*C*	*E*
Antoine eq	57 to 153 °C	6.7551	1292.6	180.1	
Francis eq	0 to 100 °C	0.87829	7.316×10^{-4}	17.15	400

2-Methyl-4-heptanol

Temp. °C	Refractive Index, n_D	Density g cm^{-3}	Vapor Pressure, mmHg
0		0.8282	
10		.8210	
20	1.4216	.8136	
25	1.4196	.8098	
30		.8060	
40		.7982	
50		.7903	
60		.7820	
65.			10
70		.7735	14.0
75			18.9
80		.7647	25.1
85			32.9
90		.7556	42.6
95			54.7
100		.7462	69.3
105			87.0
108.2			100
110			108.
115			133.
120			163.
125			198.
125.3			200
130			238.
135			285.
140			339.
145.0			400
150			470.
155			549.
160			637.
165			737.
166.1			760
170			847.

Constants	Temp. Range	*A*	*B*	*C*	*E*
Antoine eq	72 to 164 °C	6.5565	1101.6	133.6	
Francis eq	0 to 100 °C	0.95736	3.889×10^{-4}	51.68	400

TABLE 165. Isomeric Octanols. Selected values. Physical properties of the liquid

3-Methyl-4-heptanol

Temp. °C	Refractive Index, n_D	Density g cm^{-3}	Vapor Pressure, mmHg
0		0.8535	
10		.8453	
20	1.423	.8371	
25	1.4211	.8329	
30		.8287	
40		.8203	
50		.8117	
54.4			10
55			10.4
60		.8031	13.6
65			17.8
70		.7944	22.9
75			29.3
80		.7855	37.0
85			46.5
90		.7765	58.0
95			71.7
100		.7674	88.1
103.2			100
105			108
110			130.
115			157.
120			188.
121.7			200
125			224.
130			266.
135			313.
140			368.
142.7			400
145			430.
150			500.
155			579.
160			667.
164.7			760
165			767.

Constants	Temp. Range	*A*	*B*	*C*	*E*
Antoine eq	67 to 165 °C	7.2456	1599.2	201.7	
Francis eq	0 to 100 °C	0.90767	6.801×10^{-4}	21.66	400

4-Methyl-4-heptanol

Temp. °C	Refractive Index, n_D	Density g cm^{-3}	Vapor Pressure, mmHg
0		0.8397	
10		.8317	
20	1.426	.8235	
25	1.4240	.8194	
30		.8152	
40		.8068	
50		.7981	
59.0			10
60		.7893	10.6
65			14.3
70		.7802	19.1
75			25.2
80		.7709	32.7
85			42.2
90		.7614	53.8
95			67.9
100		.7517	85.1
103.7			100
105			106.
110			130.
115			159.
120			193.
120.9			200
125			233.
130			279.
135			333.
140			394.
140.5			400
145			464.
150			544.
155			634.
160			736.
161.1			760

Constants	Temp. Range	*A*	*B*	*C*	*E*
Antoine eq	58 to 161 °C	6.9920	1337.0	164.1	
Francis eq	0 to 100 °C	1.10806	3.429×10^{-4}	161.04	600

2-Ethyl-1-hexanol

Temp. °C	Refractive Index, n_D	Density g cm^{-3}	Vapor Pressure, mmHg
0		0.8475	
10		.8402	
20	1.4316	.8327	
25	1.4290	.8290	
30		.8252	
40		.8176	
50		.8099	
60		.8021	
70		.7942	5.5
79.3			10
80		.7863	10.5
85			14.1
90		.7782	18.8
95			24.6
100		.7700	32.0
105			41.1
110			52.2
115			65.7
120			81.9
124.7			100
125			101.2
130			124.2
135			151.1
140			183.
142.5			200
145			219.
150			261.
155			310.
160			365.
162.9			400
165			428.
170			499.
175			579.
180			668.
184.6			760
185			768.

Constants	Temp. Range	*A*	*B*	*C*	*E*
Antoine eq	75 to 185 °C	6.67138	1204.50	133.14	
Francis eq	0 to 100 °C	0.97581	5.194×10^{-4}	76.96	600

Table 166. Isomeric Octanols. Selected values. Physical properties of the liquid

3-Ethyl-3-hexanol

Temp. °C	Refractive Index, n_D	Density g cm^{-3}	Vapor Pressure, mmHg
0		0.8558	
10		.8469	
20	1.427	.8381	
25	1.425	.8337	
30		.8293	
40		.8204	
50		.812	
55.			10
60		.803	12.9
70			21.7
80			35.4
90			56.
100			87.
103.			100
110			131.
120			195.
121.			200
130			283.
140.			400
150			566.
159.			760
160			783.

Constants	Temp. Range	A	B	C	E
Antoine eq	58 to 160 °C	8.8289	2570.	273.	
Francis eq	0 to 65 °C	0.8558	8.826×10^{-4}		

2,5-Dimethyl-3-hexanol

Temp. °C	Refractive Index, n_D	Density g cm^{-3}	Vapor Pressure, mmHg
0		0.8355	
10		.8272	
20	1.424	.8188	
25	1.422	.8146	
30		.8104	
40		.8021	
50		.7937	
58.			10
60			11.6
70			21.4
80			37.3
90			62.
100			98.
101.			100
110			148.
118.			200
120			218.
130			311.
138.			400
140			432.
150			586.
159.			760
160			777.

Constants	Temp. Range	A	B	C	E
Antoine eq	64 to 158 °C	6.2694	963.	125.	
Francis eq	0 to 50 °C	0.8355	8.369×10^{-4}		

4-Methyl-2-ethyl-1-pentanol

Temp. °C	Refractive Index, n_D	Density g cm^{-3}	Vapor Pressure, mmHg
20	1.4358		
25	1.434		
70			8.2
73.2			10
75			11.2
80			15.0
85			19.9
90			26.0
95			33.7
100			43.2
105			54.9
110			69.0
115			86.0
118.5			100
120			106.4
125			131.
130			159.
135			193.
136.0			200
140			231.
145			277.
150			328.
155			388.
156.0			400
160			455.
165			532.
170			619.
175			717.
177.1			760

Constants	Temp. Range	A	B	C	E
Antoine eq	69 to 177 °C	6.9292	1326.1	150.5	
Francis eq					

TABLE 167. Isomeric Octanols. Selected values. Physical properties of the liquid

2,2,4-Trimethyl-1-pentanol				2,2,3-Trimethyl-3-pentanol				2,2,4-Trimethyl-3-pentanol			
Temp. °C	Refractive Index, n_D	Density g cm^{-3}	Vapor Pressure, mmHg	Temp. °C	Refractive Index, n_D	Density g cm^{-3}	Vapor Pressure, mmHg	Temp. °C	Refractive Index, n_D	Density g cm^{-3}	Vapor Pressure, mmHg
20	1.4300	0.838		20	1.4355	0.846		20	1.4286	0.8324	
25	1.428	.834		25	1.433	.842		25	1.427	.828	
60			8.2	45			9.8	50			9.9
63.4			10	45.4			10	50.2			10
65			11.0	50			13.0	55			14.4
70			14.7	55			17.0	60			20.5
75			19.4	60			22.1	65			28.4
80			25.3	65			28.4	70			38.3
85			32.7	70			36.2	75			50.8
90			41.8	75			45.7	80			66.0
95			52.9	80			57.3	85			84.
100			66.5	85			71.3	88.7			100
105			82.8	90			88.1	90			106.
109.5			100	93.1			100	95			132.
110			102.3	95			108.	100			161.
115			125.4	100			132.	105			196.
120			152.8	105			160.	105.6			200
125			185.	110			192.	110			234.
127.1			200	111.			200	115			278.
130			222.	115			230.	120			327.
135			266.	120			274.	125			382.
140			315.	125			324.	126.6			400
145			373.	130			382.	130			442.
147.2			400	131.			400	135			508.
150			438.	135			449.	140			580.
155			513.	140			524.	145			658.
160			597.	145			604.	150			743.
165			692.	150			705.	151.0			760
168.3			760	152.6			760	155			834.
170			798.								

Constants	Temp. Range	A	B	C	E	Constants	Temp. Range	A	B	C	E	Constants	Temp. Range	A	B	C	E
Antoine eq Francis eq	60 to 168 °C	7.07819	1423.10	170.78		Antoine eq Francis eq	45 to 153 °C	7.3891	1642.0	211.6		Antoine eq Francis eq	55 to 155 °C	5.1306	498.1	70.4	

Malone, and Reid [1941]. They also reported values of the derived properties such as molar refraction, coefficient of expansion, and parachor, as well as certain chemical and toxicological properties. These data are the principal source of the selected values of refractive index, density, and melting and boiling points for the 21 isomeric octanols which are included.

However, there are reasons for questioning the reliability of the data for several of these compounds. 5-Methyl-3-heptanol was synthesized by the Grignard reaction from 2-methyl-1-bromobutane and propanal, and 4-methyl-2-heptanol was prepared in a similar manner from 2-methyl-1-bromopentane and ethanal. In each case the bromo intermediate was prepared by reacting the corresponding primary alcohol with a $HBr-H_2SO_4$ mixture. It seems very likely that this reagent would yield the tertiary bromo derivatives, 2-methyl-2-bromobutane and 2-methyl-2-bromopentane, rather than the primary bromo derivatives which they indicated. 2-methyl-1-bromobutane boils at 120.5 °C, while 2-methyl-2-bromobutane boils at 108 °C. They reported a boiling point of 117.5 °C (this compound is listed as 1-bromo-3-methylbutane in their paper, apparently as the result of a misprint). They listed the boiling point of 2-methyl-1-bromopentane as 83.8 °C at 100 mmHg, but this cannot be readily compared to other measurements. If the tertiary bromo compounds were actually produced rather than the primary ones, they would have synthesized 4,4-dimethyl-2-hexanol instead of 5-methyl-3-heptanol, and 3,3-dimethyl-2-hexanol instead of 4-methyl-2-heptanol. While the properties obtained by Dorough et al. and by Bingham and Darrall do not seem to correspond to the values for the dimethyl derivatives reported by other investigators, the uncertainties are such that this possibility cannot be entirely ruled out.

The properties obtained by Dorough et al. and Bingham and Darrall for 6-methyl-3-heptanol are quite different from those reported by others. In fact these differences are so large that except for the melting point, it seems unlikely that it could result only from errors in experimental measurements. Although there is considerable uncertainty connected with the earlier work, the boiling point, density, and refractive index of Henne and Matuszak [1944], which appears reliable, agrees reasonably well with these earlier reports. It is necessary to conclude that Dorough et al., or all the other investigators, had either prepared the wrong compound or had used highly impure samples. However, in all cases the methods used for synthesis should have produced the expected product. Until this question is resolved, no selection of properties is possible for this compound.

Dorough et al. and Bingham and Darrall report values of the normal boiling point, density, and refractive index of 2-methyl-2-heptanol, which are consistently lower than those of most of the other investigators. Most of the other density and boiling point data are fairly old, and so are not very dependable. However, the refractive indices of Dorough et al. are definitely around 0.002, or more, lower than all of the other values. Although the values reported by Dorough et al. were given the greatest weight in the selection, they may contain an appreciable error.

Bingham and Darrall reported a density of 3-methyl-2-heptanol, which was considerably lower than that of Dorough et al. and Powell [1924], although supposedly they used the same sample as Dorough et al. The selected densities at 20 and 25 °C are derived from those of Dorough et al. No selection was made for higher temperatures.

Besides the compounds studied by Dorough et al., sufficient vapor pressure data was located for five other octanols to permit a least squares calculation of the Antoine constants. The constants published for 2,2,4-trimethyl-1-pentanol by the Union Carbide Corporation [1958] were adopted and used to calculate vapor pressures and boiling points listed in table 167. Antoine constants reported by Dykyj, Seprakova, and Paulech [1961] were chosen for 4-methyl-2-ethyl-1-pentanol. Both Union Carbide and Dykyj, Seprakova, and Paulech published sets of Antoine constants for 2-ethyl-1-hexanol. The agreement was within a few 0.1 °C from 90 °C to the boiling point. The final selected constants were derived by combining these two sets of data along with a few additional values included on the unnumbered table. The Antoine constants for 2,2,4-trimethyl-3-pentanol and 2,2,3-trimethyl-3-pentanol were calculated by fitting a selection of the boiling point data listed for compounds on the corresponding unnumbered tables.

The heat of vaporization at the normal boiling point was calculated from the Antoine constants for all those isomeric octanols for which the Antoine constants were calculated by a least squares fit to experimental vapor pressures. The results are listed in table 169. In all cases a second virial coefficient of -1 liter mol^{-1} was assumed. Table 169 also includes heat capacity data taken from Cline and Andrews [1931]. The uncertainty in these heat of vaporization values is in the range of 0.2 to 0.5 kcal mol^{-1}.

TABLE 168. Isomeric Octanols. Selected values. Refractive index at various wavelengths at 25 °C

Symbol	Wavelength, Å	Refractive Index		
		2-Octanol	3-Methyl-3-heptanol	4-Methyl-4-heptanol
He_{red}	6678.1	1.4236	1.4260	1.4236
H_C	6562.8	1.4239	1.4262	1.4240
Na_D	5892.6	1.4261	1.4283	1.4260
Hg_e	5460.7	1.4279	1.4301	1.4278
He_{blue}	5015.7	1.4303	1.4325	1.4302
H_F	4861.3	1.4314	1.4335	1.4312
Hg_g	4358.3	1.4355	1.4377	1.4353
$H_{G'}$	4340.5	1.4357	1.4379	1.4355

TABLE 169. Isomeric Octanols. Heat capacity at 25 °C and calculated heat of vaporization at the normal boiling point

Name	Heat Capacity at 25 °C cal deg^{-1} mol^{-1}	Normal Boiling Point, t_b °C	Heat of Vaporization, ΔHv,* at t_b, kcal mol^{-1}
2-Octanol	78.9	179.8	10.60
3-Octanol	80.9	174.7	8.73
4-Octanol	80.7	176.7	9.67
2-Methyl-1-heptanol	74.8	175.6	9.77
3-Methyl-1-heptanol		186.0	11.04
4-Methyl-1-heptanol		183.2	9.49
5-Methyl-1-heptanol	72.7	186.6	10.83
6-Methyl-1-heptanol		187.7	11.45
2-Methyl-2-heptanol	80.7	156.7	11.34
3-Methyl-2-heptanol	71.1	166.1	10.16
4-Methyl-2-heptanol	74.7	171.6	10.58
5-Methyl-2-heptanol	70.8	171.9	10.41
6-Methyl-2-heptanol	75.3	171.9	11.23
2-Methyl-3-heptanol		167.6	10.45
3-Methyl-3-heptanol		161.	10.3
4-Methyl-3-heptanol	73.9	155.4	10.19
5-Methyl-3-heptanol		153.6	9.40
2-Methyl-4-heptanol	79.3	166.1	10.53
3-Methyl-4-heptanol		164.7	10.16
4-Methyl-4-heptanol	87.8	161.1	10.60
2-Ethyl-1-hexanol		184.6	11.13
2-Methyl-2-ethyl-1-pentanol		177.1	11.15
2,2,4-Trimethyl-1-pentanol		168.3	10.73
2,2,3-Trimethyl-3-pentanol		152.5	9.97
2,2,4-Trimethyl-3-pentanol		151.0	8.12

* Calculated from the Antoine Constants.

TABLE 170. Isomeric Octanols. Reported values. Heats of combustion of the liquid at 25 °C

Investigator	Compound	$-\Delta Hc^{\circ}(1)$ kcal mol^{-1}
Louguinine [1882a]	2-Octanol	1262.0
Louguinine [1882b]	2-Octanol	1261.2
Zubov (1913) (recalculated by Swietoslawski [1920]	4-Methyl-4-heptanol	1234.0
Union Carbide Corporation [1958]	2,2,4-Trimethyl-1-pentanol	1260
Tjebbes [1960]	2-Ethyl-1-hexanol	1263.81

Density of 2-ethyl-1-hexanol is based on data listed in the unnumbered table at higher temperatures on values of Kenyon and Platt [1939] and Bingham and Darrall [1930]. The density of 3-ethyl-3-hexanol was calculated from a linear function of temperature from 0 to 60 °C. The only data outside the vicinity of room temperature are those of Owen, Quayle, and Beavers [1930] at 0 and 65 °C. The density of 2,5-dimethyl-3-hexanol outside the 20–25 °C region is based primarily on the data of Carleton-Williams [1879] and Favorskii [1913] and therefore is less certain than those values based on more recent measurements.

There are very few values of refractive index of these compounds outside the range of 20 to 25 °C and the wavelength of the sodium D-line. A few values at other temperatures have been listed in the numbered tables. Refractive indices of three compounds at other wavelengths have been listed in table 168. These were taken from smooth curves of n versus $1/(\lambda-1000)^{1.6}$, after correcting the data to 20 °C when necessary. These selections were derived from the data of Eykman [1919], van Risseghem [1930], and Waterman and teNuyl [1932]. Gladstone and Dale [1863] and Bruhl [1880] also gave values for 2-octanol, but they were not considered in the final selection.

Union Carbide Corporation [1958] has reported the heat capacity of 2-ethyl-1-hexanol as 73.5 cal deg^{-1} mol^{-1} at 25 °C and the heat of vaporization at the boiling point as 12.1 kcal mol^{-1}. Heats of combustion of a few of the isomeric octanols are listed in table 170. The older data have been converted to modern units and conventions. Tjebbes [1960] used modern techniques and instruments with a carefully purified sample. This is the only value which can be used to derive a reliable heat of formation. Thus for 2-ethyl-1-hexanol, $\Delta Hf^{0}(1) = -103.44$ kcal mol^{-1} is obtained at 25 °C.

Isomeric Octanols

Investigators		Vapor Pressures and Boiling Points		Freezing Point	Density, d g cm^{-3}		Refractive Index, n_D	
		°C	mmHg	t_m, °C	20 °C	25 °C	20 °C	25 °C
2-Octanol, $C_8H_{18}O$, mol wt. 130.232, state at 25 °C liq.								
See also table 159								
Dale and Gladstone	[1853]	181	760					
Gladstone and Dale	[1863]							1.4210
Schorlemmer	[1875]	179.5	755					
Bruhl	[1880b]	177.6–177.8	744		0.8193		1.42444	
Schiff	[1883]	179–179.2	762					
Perkin	[1884]	179.5	760			0.8154		
Pickard and Kenyon	[1907]	86	20		.8221		1.424	
Pickard and Kenyon	[1911]				.8214	0.8170	1.4256	
Pickard and Kenyon	[1912]	179	760					
Smith, Clarence	[1914]	110	120			0.8186		
Eykman	[1919]	81	12.5					
Behal	[1919]				.8193		1.42025	
Timmermans	[1921]	179.0		−38.6				
Kenyon	[1926]	86	20					
Malone and Reid	[1929]	180.3	765					
Bingham and Darrall	[1930]				.82082			
Ellis and Reid	[1932]	179.0	760					
Waterman and teNuyl	[1932]	177.2–177.5	760				1.42375	
Whitmore and Herndon	[1933]	177.3	731		0.817		1.4260	
Whitmore and Krueger	[1933]	177.2–177.4	740				1.4260	
Zepalova-Mikhailova	[1937]	179.1	760		0.81984		1.4265	
Kenyon and Young	[1938]	83–85	20					
Coppock and Goss	[1939]	86 93	20 26		.8202		1.4263	
Dorough, Glass, Gresham, Malone, and Reid	[1941]	180.0	760	−31.6		0.8170		1.4238
Kornblum, Lichtin, Patton, and Iffland	[1947]	77 87	15 20		0.8202		1.4264	1.4244
Doughty and Kenyon	[1947]	82	18					
Garwin and Hixson	[1949]						1.4260	
Kornblum and Oliveto	[1949]						1.4262	
Nazarov and Fisher	[1950]	72–73	9		0.8180		1.4260	

Isomeric Octanols—Continued

Investigators	Vapor Pressures and Boiling Points		Freezing Point	Density, *d* g cm^{-3}		Refractive Index, n_D	
	°C	mmHg	t_m, °C	20 °C	25 °C	20 °C	25 °C
2-Octanol, C_8H_{18}, mol wt. 130.232, state at 25 °C liq.							
Adkins and Rosenthal [1950]							1.4252
O'Goremane and Lucas [1950]	73	10					
Cook [1952]	179.6	760	−32	0.8208		1.4260	
Zeiss and Tsutsui [1953]	178–179						1.4248
Dalbert [1953]	178.2–179.2	767	−37– −37.5			1.4253	
Corey and Wechter [1954]	88–89	23				1.4256	
Urry, Stacey, Huyser, and Juveland [1954]	97–98	38				1.4289	
Kornblum, Fishbein, and Smiley [1955]	65	4			0.8151	1.4264	
Kornblum, Larson, Blackwood, Mooberry, Oliveto, and Graham [1956]	45	1				1.4262	
Goering and McCarron [1956]	72–73 83–83.5	9 18			.817		1.4238– 1.4247
Esso Research and Engineering Co. [1957]	176–177					1.4247	
Rikovski and Carich [1957]						1.4259	1.4239
LeGoff, Ulrich, and Penney [1958]						1.4235	
Brown and Subba Rao [1959]	179–140	740					
Kallina and Kuffner [1960]	180	760					
Mislow, O'Brien, and Schaefer [1962]						1.4258	
Geiseler, Fruwert, and Stockel [1962]	180	760		.8206		1.4260	
Thewalt and Rudolph [1964]	85	20				1.4270	
Selected value [1967]	[e] 179.8±0.3 74.3±0.3	760 10	[a] −32±2	[d] .8207 ±.0005	[d] 0.8171 ±0.0005	[b] 1.4261 ±0.0003	[b,c] 1.4241 ±0.0003
Antoine constants: *A* 6.3888, *B* 1060.4, *C* 122.5.				*dt/dp* at 760 mmHg, [e] 0.0492 °C/mmHg			
3-Octanol, $C_8H_{18}O$, mol wt. 130.232, state at 25 °C liq.							
See also table 159							
Pickard and Kenyon [1913]	76	16		0.8247		1.4252	
Bingham and Darrall [1930]				.8209			
Levene and Walti [1931]	82	24					
Dorough, Glass, Gresham, Malone, and Reid [1941]	173.0	760	−45.0		0.8169		1.4209
Zeiss and Tsutsui [1953]	89.5–90	25					1.4250
Sparks and Knobloch [1954]	76	16				1.4252	
Beringer and Schultz [1955]	80–83	20					1.4237 1.4258
Woods and Viola [1956]	172–174	760			.8223		1.421
Shuikin and Bel'skii [1957]	175–176	745		.8344		1.4270	
Kallina and Kuffner [1960]	173	760					
Geiseler, Fruwert, and Stöckel [1962]	177	760		.8258		1.4271	
Lamparsky [1963]	84	20		.8300(+)		1.4282(+)	
Selected value [1967]	[e] 174.7±1 [e] 68.1±1	760 10	[a] −45.0± 0.5	[d] .8216 ±.001	[d] .8176 ±.001	[c] 1.423 ±0.003	[a] 1.421 ±0.002
Antoine constants: *A* 5.2215, *B* 560.3, *C* 64.7.				*dt/dp* at 760 mmHg, [e] 0.0585 °C/mmHg			

Isomeric Octanols—Continued

Investigators		Vapor Pressures and Boiling Points		Freezing Point	Density, *d* g cm^{-3}		Refractive Index, n_D	
		°C	mmHg	t_m, °C	20 °C	25 °C	20 °C	25 °C
4-Octanol, $C_8H_{18}O$, mol wt. 130.232, state at 25 °C liq.								
See also table 159								
Bouveault and Locquin	[1906]	**71**	10					
Levene and Haller	[1929b]	**79**	20					
Bingham and Darrall	[1930]				**0.8199**			
Levene and Marker	[1931a]	79	16		0.820			
Tuot	[1936]	**81**	17		**0.8178**		**1.4248**	
Dorough, Glass, Gresham, Malone, and Reid	[1941]	**176.3**	760	**−40.7**		**0.8159**		**1.4227**
Hargreaves and Owen	[1947]	**77–78**					1.4245	
Winsor	[1948]	173–175	760					
Woods and Schwartzman	[1949]	79	20					1.3886
Nazarov and Fisher	[1950]	162–163	760		**0.8186**		1.4140	
Drahovzal	[1951]	69.5–72.5	9				1.4256	
Zeiss and Tsutsui	[1953]	87	21					1.4232
Kallina and Kuffner	[1960]	**176**	760					
Geiseler, Fruwert, and Stöckel	[1962]	**176**	760		0.8243		**1.4250**	
Selected value	[1967]	[e] 176.6±0.5	760	[a] −40.7±0.5	[d] 0.8192	[d] 0.8154	[b,c] 1.425	[a] 1.4227
		[e] 71.±0.5	10		±0.001	±0.0007	±0.002	±0.0010
Antoine constants: *A* 5.7396, *B* 760.5, *C* 89.5.								*dt/dp* at 760 mmHg, [e] 0.0532 °C/mmHg
2-Methyl-1-heptanol, $C_8H_{18}O$, mol wt. 130.232, state at 25 °C liq.								
See also table 160								
Bingham and Darrall	[1930]				**0.8020**			
Dorough, Glass, Gresham, Malone, and Reid	[1941]	**175.4**	760	−112.0		**0.7987**		**1.4219**
Kallina and Kuffner	[1960]	175	760					
Selected value	[1967]	[b,e] 175.6±0.5	760	[a] −112.0±0.5	[d] 0.8022	[b] 0.7986	[c] 1.424	[a] 1.4219
		[e] 65.7±0.5	10		±0.0005	±0.0005	±0.002	±0.0010
Antoine constants: *A* 6.1860, *B* 1002.1, *C* 127.6.								*dt/dp* at 760 mmHg, [e] 0.0524 °C/mmHg
3-Methyl-1-heptanol, $C_8H_{18}O$, mol wt. 130.232, state at 25 °C liq.								
Bingham and Darrall	[1930]				**0.7881**			
Levene and Marker	[1931b]	99	25			0.823		1.4295
Huston and Agett	[1941]	101	26			.820		1.4285
Dorough, Glass, Gresham, Malone, and Reid	[1941]	**185.8**	760	−90.0		**.7845**		**1.4225**
Lichtenberger and Dürr	[1956]	80	20		.823		1.4285	
Wiemann, Thsai, and Weisbuch	[1964]	84	22					
Selected value	[1967]	[e] 186.0±0.5	760	[a] −90.0±0.5	[d] .7881	[d] .7844	[c] 1.425	[a] 1.4225
		[e] 74.6±0.5	10		±.0005	±.0005	±0.002	±0.0010
Antoine constants: *A* 7.1977, *B* 1584.6, *C* 181.1.								*dt/dp* at 760 mmHg, [e] 0.0486 °C/mmHg

Isomeric Octanols—Continued

Investigators		Vapor Pressures and Boiling Points		Freezing Point	Density, *d* g cm^{-3}		Refractive Index, n_D	
		°C	mmHg	t_m, °C	20 °C	25 °C	20 °C	25 °C
4-Methyl-1-heptanol, $C_8H_{18}O$, mol wt. 130.232, state at 25 °C liq.								
See also table 160								
Bingham and Darrall	[1930]				0.8102			
Koller and Kandler	[1931]	188–193	760					
Levene and Marker	[1933]	81	18					
Shonle, Waldo, Keltch, and Coles	[1936]	181–183	760					
Dorough, Glass, Greshem, Malone, and Reid	[1941]	182.7	760			0.8065		1.4253
Julia, Julia, Tchen, and Graffin	[1964]	55–56	1				1.4282	
Selected value	[1967]	^{e}183.2±0.5	760		^{d}.8101	^{d}0.8064	^{c}1.427	^{a}1.4253
		^{e}72.5±0.5	10		±.0005	±0.0005	±0.002	±0.0010
Antoine constants: *A* 5.7368, *B* 796.3, *C* 95.6.								*dt/dp* at 760 mmHg, ^{e}0.0558 °C/mmHg
5-Methyl-1-heptanol, $C_8H_{18}O$, mol wt. 130.232, state at 25 °C liq.								
See also table 161								
Bingham and Darrall	[1930]				0.8188			
Levene and Marker	[1933]	87	20					
Dorough, Glass, Gresham, Malone, and Reid	[1941]	186.5	760	−104.0		0.8152		1.4272
Wichterle and Vogel	[1954]	180–185	760					
Lardicci, Salvadori, and Pino	[1962]	91–92	17			.8259		1.4290
Pino, Lardicci, Salvadori, and Natta	[1962]	92	16–17					1.4292
Selected value	[1967]	^{e}186.6±0.05	760	^{a}−104.0±	^{d}.8189	^{d}.8153	^{c}1.429	^{a}1.4272
		^{e}79.1±0.5	10	0.5	±.0005	±.0005	±0.002	±0.0010
Antoine constants: *A* 6.4894, *B* 1131.9, *C* 127.1.								*dt/dp* at 760 mmHg, ^{e}0.0497 °C/mmHg
6-Methyl-1-heptanol, $C_8H_{18}O$, mol wt. 130.232, state at 25 °C liq.								
See also table 161								
Levene and Allen	[1916]	188.5	764			0.8230		
Malone and Reid	[1929]	188.0	767					
Bingham and Darrall	[1930]				0.8209			
Dorough, Glass, Gresham, Malone, and Reid	[1941]	187.6	760	−106.0		.8176		1.4255
Milburn and Truter	[1954]	187	760				1.4268	
Selected value	[1967]	^{e}187.7±0.5	760	−106.0±	^{d}.8210	^{d}.8175	^{a,c}1.427	^{a}1.4255
		^{e}84.1±0.5	10	0.5	±.0005	±.0005	±0.001	±0.0010
Antoine constants: *A* 6.6443, *B* 1170.6, *C* 123.3.								*dt/dp* at 760 mmHg, ^{e}0.0472 °C/mmHg

Isomeric Octanols—Continued

Investigators		Vapor Pressures and Boiling Points		Freezing Point	Density, *d* g cm^{-3}		Refractive Index, n_D	
		°C	mmHg	t_m, °C	20 °C	25 °C	20 °C	25 °C
2-Methyl-2-heptanol, $C_8H_{18}O$, mol wt. 130.232, state at 25 °C liq.								
See also table 161								
Masson	[1901]	162	760					
Henry	[1906a]	162	760					
Muset	[1906]	161–162	760		0.819		1.43031	
Bingham and Darrall	[1930]				**0.8073**			
Whitmore and Williams	[1933]	**162–164**	?			**0.8136**	1.4240	
Whitmore and Badertscher	[1933]	**65–66**	15				1.4235	
Whitmore and Church	[1933]	**155–156**	740				1.4240	
Church, Whitmore, and McGrew	[1934]	155–156	760				1.4243	
Dorough, Glass, Gresham, Malone, and Reid	[1941]	**156.1**	760	−50.4		**0.8050**		**1.4201**
Huston, Guile, Sculati, and Wasson	[1941]	161.2	748		**0.8142**		1.4250	
Quayle and Smart	[1944]					**0.8133**	1.4238	1.4218
Prevost and Singer	[1950]	**87**	50					
Huston and Brault	[1950]	**65**	15				1.4248	
Cook	[1952]	**105**	95				1.4241	
Colonge and Falcotet	[1957]	**68**	17		0.818		1.4238	
Selected value	[1967]	^{e} 156.7±0.5	760	^{a} −50.4±	^{d} 0.8107	^{d} 0.8072	^{c} 1.4221	^{a} 1.4201
		^{e} 59.5±0.5	10	0.5	±0.0015	±0.0015	±0.0020	±0.0010
Antoine constants: *A* 7.5668, *B* 1590.6, *C* 182.7.								*dt/dp* at 760 mmHg, ^{e} 0.0414 °C/mmHg
3-Methyl-2-heptanol, $C_8H_{18}O$, mol wt. 130.232, state at 25 °C liq.								
See also table 162								
Powell	[1924]	172–173	760		0.8216		1.433	
Bingham and Darrall	[1930]				0.7900	0.7858		
Dorough, Glass, Gresham, Malone, and Reid	[1941]	*166.1*	760	**−114.0**		**0.8177**		**1.4199**
Selected value	[1967]	^{e} 166.1±0.5	760	^{a} −114.0±	^{c} 0.8217	^{a} 0.8177		
		^{e} 55.1±0.5	10	0.5	±0.0010	±0.0010		
Antoine constants: *A* 7,2335, *B* 1601.4, *C* 208.1.								*dt/dp* at 760 mmHg, ^{e} 0.0483 °C/mmHg
4-Methyl-2-heptanol, $C_8H_{18}O$, mol wt. 130.232, state at 25 °C liq.								
Clarke	[1907]	168	760					
Bingham and Darrall	[1930]				**0.8026**			
Dorough, Glass, Gresham, Malone, and Reid	[1941]	**171.7**	760	**−102.0**		**0.7990**		**1.4225**
Selected value	[1967]	^{e} 171.6±0.5	760					
		^{e} 66.4±0.5	10					
Antoine constants: *A* 6.7364, *B* 1237.5, *C* 149.3								*dt/dp* at 760 mmHg, ^{e} 0.0476 °C/mmHg

Isomeric Octanols—Continued

5-Methyl-2-heptanol, $C_8H_{18}O$, mol wt. 130.323, state at 25 °C liq.

See also table 162

Investigators		Vapor Pressures and Boiling Points		Freezing Point	Density, *d* g cm^{-3}		Refractive Index, n_D	
		°C	mmHg	t_m, °C	20 °C	25 °C	20 °C	25 °C
Bingham and Darrall	[1930]				0.8133			
Dorough, Glass, Gresham, Malone, and Reid	[1941]	171.9	760	−120.0		0.8100		1.4218
Selected value	[1967]	[e] 171.9±0.5 [e] 63.5±0.5	760 10	[a] −120.0±0.5	[b] .8137 ±.0010	[d] .8098 ±.0010	[c] 1.424 ±0.002	[a] 1.4218 ±0.0010

Antoine constants: *A* 6.8882, *B* 1359.8, *C* 167.5. *dt/dp* at 760 mmHg, [e] 0.0484 °C/mmHg

6-Methyl-2-heptanol, $C_8H_{18}O$, mol wt. 130.232, state at 25 °C liq.

See also table 163

Investigators		Vapor Pressures and Boiling Points		Freezing Point	Density, *d* g cm^{-3}		Refractive Index, n_D	
		°C	mmHg	t_m, °C	20 °C	25 °C	20 °C	25 °C
Henry	[1906b]	171–172	760					
Buelens	[1908b]	171–172	760		0.8128		1.42381	
Guerbet	[1912b]	172–173	760					
Wallach	[1914]	171–172	760		.8155			
		173.5	760					
Escourrou	[1928]	165–166	743		.8069		1.4159	
Bingham and Darrall	[1930]				.8070			
Dorough, Glass, Gresham, Malone, and Reid	[1941]	171.8	760	−105.0		0.8034		1.4209
Herout, Zaoral, and Sorm	[1953]	80	25			0.8148	1.4250	
Zeiss and Tsutsui	[1953]	90–91	27					1.4222
Canonica, Bonati, Clerici, Gaudenzi, and Motta	[1959]	122	100					
Miropol'skaya, Fedstova, Veinberg, Yanotovskii, and Samokhvalov	[1962]	52	2.5		.8237		1.4290	
Selected value	[1967]	[e] 171.9±0.5 [e] 68.9±0.5	760 10	[a] −105.0±0.5	[d] .8071 ±.001	[d] 0.8033 ±0.001	[c] 1.423 ±0.002	[a] 1.4209 ±0.0010

Antoine constants: *A* 7.2176, *B* 1476.0, *C* 168.5. *dt/dp* at 760 mmHg, [e] 0.0449 °C/mmHg

Isomeric Octanols—Continued

Investigators	Vapor Pressures and Boiling Points		Freezing Point	Density, d g cm^{-3}		Refractive Index, n_D	
	°C	mmHg	t_m, °C	20 °C	25 °C	20 °C	25 °C
2-Methyl-3-heptanol, $C_8H_{18}O$, mol wt. 130.232, state at 25 °C liq.							
See also table 163							
Muset [1906]	153–154	760		0.825		1.42041	
Henry [1906b]	153–154	760					
Pickard and Kenyon [1912]	162	760		.8235	0.8203	1.4265	
Thole [1913]					.8211		
Wallach [1914]	167–168	760		.821		1.4249	
Bingham and Darrall [1930]				.8247			
Whitmore and Kreuger [1933]	159–164	740					
Tuot [1936]	73	19		.8123		1.4220	
Dorough, Glass, Gresham, Malone, and Reid [1941]	167.2	760	−85.0		.8210		1.4246
George [1943]	167.5	732		.8251		1.4265	
Malinovskii and Konvichev [1948]	153–155	760		.8280		1.4289	
Huston and Brault [1950]	165–167	740				1.4259	
Protiva, Exner, Borovicka, and Pliml [1952]	52–56	2					
Greenwood and Cohen [1963]	83	29					1.4240
Selected value [1967]	^{e} 167.6±0.5 ^{e} 64.2±0.5	760 10	^{a} −85.0± 0.5	^{d} .8245 ±.0005	^{d} .8205 ±.0005	^{b,c} 1.4266 ±0.0010	^{a} 1.4246 ±0.0010

Antoine constants: *A* 6.6097, *B* 1150.1, *C* 140.8 *dt*/*dp* at 760 mmHg, ^{e} 0.0473 °C/mmHg

Investigators	°C	mmHg	t_m, °C	20 °C	25 °C	20 °C	25 °C
3-Methyl-3-heptanol, $C_8H_{18}O$, mol wt. 130.232, state at 25 °C liq.							
See also table 163							
Konovalov, M. [1902]	158–160	745		0.8264		1.4270	
van Risseghem [1930]	163.5	760		.8285			
Bingham and Darrall [1930]				.8292			
Whitmore and Church [1933]	158–159	731				1.4238	
Whitmore and Badertscher [1933]	64–65	16				1.4283	
Whitmore and Woodburn [1933]	160	732		.8282	0.8249	1.4279	
Church, Whitmore, and McGrew [1934]	158–159	731				1.4238	
Dorough, Glass, Gresham, Malone, and Reid [1941]	159.4	760	−83.0		.8271		1.4263
Quayle and Smart [1944]					.8252	1.4284	1.4263
Wilberg and Foster [1961]					.823		1.4264
Selected value [1967]	^{e} 161.±0.5 ^{e} 59.2±0.5	760 10	^{a} −83.0± 0.5	^{d} .8293 ±.0005	^{d} .8251 ±.0005	^{b,c} 1.4283 ±0.0010	^{b} 1.4263 ±0.0010

Antoine constants: *A* 6.5807, *B* 1116.2, *C* 140.9. *dt*/*dp* at 760 mmHg, ^{e} 0.0467 °C/mmHg

Isomeric Octanols—Continued

Investigators		Vapor Pressures and Boiling Points		Freezing Point	Density, d g cm^{-3}		Refractive Index, n_D	
		°C	mmHg	t_m, °C	20 °C	25 °C	20 °C	25 °C
4-Methyl-3-heptanol, $C_8H_{18}O$, mol wt. 130.232, state at 25 °C liq.								
See also table 164								
Bjelous	[1912]	98.9	75			0.8268		1.42606
Bingham and Darrall	[1930]				**0.7980**			
Dorough, Glass, Gresham, Malone, and Reid	[1941]	**155.4**	760	**−123.0**		**.7946**		**1.4179**
Kallina and Kuffner	[1960]	155	760					
Selected value	[1967]	^{e}155.4±0.5 ^{e}44.9±0.5	760 10	^{a} −123.0± 0.5	^{d} .7981 ±.0005	^{d} .7940 ±.0005	^{c}1.420 ±0.002	^{a}1.4179 ±0.0010
Antoine constants: *A* 8.2151, *B* 2282.9, *C* 272.5.						*dt*/*dp* at 760 mmHg, ^{e} 0.0458 °C/mmHg		
5-Methyl-3-heptanol. $C_8H_{18}O$, mol wt. 130.232, state at 25 °C liq.								
See also table 164								
Guerbet	[1912d]	167–168	760					
Bingham and Darrall	[1930]				**0.8179**			
Powell and Secoy	[1931]	155	760			0.8417		1.433
Levene and Marker	[1931d]					0.814		
Dorough, Glass, Gresham, Malone, and Reid	[1941]	**153.4**	760	**−91.2**		**0.8162**		**1.4156**
Machinskaya and Barkhash	[1959]	70–72	28		0.8290			1.4233
Selected value	[1967]	^{e}153.6±0.5 ^{e}44.6±0.5	760 10	^{a} −91.2± 0.5	^{d}0.8185 ±0.0007	^{d}0.8143 ±0.001	^{c}1.418 ±0.002	^{a}1.4156 ±0.0010
Antoine constants: *A* 6,7551, *B* 1292.6, *C* 180.1.						*dt*/*dp* at 760 mmHg, ^{e} 0.0492 °C/mmHg		
6-Methyl-3-heptanol,* $C_8H_{18}O$, mol wt. 130.232, state at 25 °C liq								
Henry	[1906b]	165–166	760					
Buelens	[1908b]	165–166	760	−61.	0.8084		1.42011	
Bingham and Darrall	[1930]				**.7814**			
Kondo and Suzuki	[1936]	165–166	760					
Dorough, Glass, Gresham, Malone, and Reid	[1941]	**158.5**	760	**−58.5**		**0.7766**		1.4113
Henne and Matuszak	[1944]	169.7	760		.8220		1.4254	

* No selection was made for this compound. See discussion of Isomeric Octanols.

Isomeric Octanols—Continued

Investigators		Vapor Pressures and Boiling Points		Freezing Point	Density, *d* g cm^{-3}		Refractive Index, n_D	
		°C	mmHg	t_m, °C	20 °C	25 °C	20 °C	25 °C
2-Methyl-4-heptanol, $C_8H_{18}O$, mol wt. 130.232, state at 25 °C liq.								
See also table 164								
Henry	[1906b]	160–166	760					
Muset	[1906]	160	760		0.8207		1.42031	
Bingham and Darrall	[1930]				.8135			
Levene and Marker	[1931c]	80	25					1.4205
Tuot	[1936]	75	20		.8116		1.4219	
Bartlett, Kuno, and Levene	[1937]	72	15					
Dorough, Glass, Gresham, Malone, and Reid	[1941]	166.3	760	−81.0		0.8098		1.4196
Braude and Timmons	[1950]	113–114	130					1.4190
Shuikin and Bel'skii	[1957]	164–164.5	752		.8162		1.4220	
Selected value	[1967]	^{e} 166.1±0.5	760	^{a} −81.0±	^{d} .8136	^{d} 0.8098	^{b,c} 1.4216	^{a} 1.4196
		^{e} 65±1.	10	0.5	±.0010	±0.0007	±0.0010	±0.0010
Antoine constants: *A* 6.5565, *B* 1101.6, *C* 133.6								*dt*/*dp* at 760 mmHg, ^{e} 0.0466 °C/mmHg
3-Methyl-4-heptanol, $C_8H_{18}O$, mol wt. 130.232, state at 25 °C liq.								
See also table 165								
Bingham and Darrall	[1930]				0.8370			
Rhinesmith	[1936]	157–163	760					
Dorough, Glass, Gresham, Malone, and Reid	[1941]	164.7	760			0.8335		1.4211
Glacet	[1951]	68–69	12				1.4282	
Searles, Pollart, and Lutz	[1957]	82–84	38				1.4235	
Colonge, Descotes, and Bahurel	[1965]	170	760			.835		1.433
Selected value	[1967]	^{e} 164.7±0.5	760		^{d} .8371	^{d} .8329	^{a,c} 1.423	^{a} 1.4211
		^{e} 54.4±0.5	10		±.0005	±.0007	±0.002	±0.0010
Antoine constants: *A* 7.2456, *B* 1599.2, *C* 201.7.								*dt*/*dp* at 760 mmHg, ^{e} 0.0480 °C/mmHg
4-Methyl-4-heptanol, $C_8H_{18}O$, mol wt. 130.232, state at 25 °C liq.								
See also table 165								
Halse	[1914]	61–63	12					
Eykman	[1919]				0.8233			
Bingham and Darrall	[1930]				.8240			
Owen, Quayle, and Beavers	[1930]				.8225	0.8183		
Dorough, Glass, Gresham, Malone, and Reid	[1941]	160.8	760	−82.0		.8202		1.4240
Petrov and Kurbskii	[1944]	60–63	12					
Yur'ev and Belyakova	[1959]	58–59	10		.8227		1.4275	
Selected value	[1967]	^{e} 161.1±0.5	760	^{a} −82.0±	^{d} .8235	^{d} .8194	^{c} 1.426	^{a} 1.4240
		^{e} 59.0±0.5	10	0.5	±.0007	±.0010	±0.002	±0.0010
Antoine constants: *A* 6.9920, *B* 1337.0, *C* 164.1.								*dt*/*dp* at 760 mmHg, ^{e} 0.0452 °C/mmHg

Isomeric Octanols—Continued

2-Ethyl-1-hexanol, $C_8H_{18}O$, mol wt. 130.232, state at 25 °C liq.

See also table 165

Investigators		Vapor Pressures and Boiling Points		Freezing Point	Density, d g cm^{-3}		Refractive Index, n_D	
		°C	mmHg	t_m, °C	20 °C	25 °C	20 °C	25 °C
Guerbet	[1901a]	181	756					
Weizmann and Garrard	[1920]	180–185	760					
Levene and Taylor	[1922b]	181.3	743		0.8328		1.4328	
Bingham and Darrall	[1930]				.8316			
Morgan, Hardy and Procter	[1932]	180	760				1.431	
von Braun and Manz	[1934]	84.6	15		.8381			
Levene, Rothen and Meyer	[1936]	110	55			0.8293		1.4292
Shonle, Waldo, Keltch and Coles	[1936]	184.6	760					
Mastagli	[1937]	85	16		.8431		1.4374	
Mastagli	[1938]	85	15		.8431			1.4390
Magnani and McElvain	[1938]	179–182	760					
Goldwasser and Taylor	[1939]	184.6	760		.833			
Kenyon and Platt	[1939]	178–179	760		.8334		1.4313	
Whitmore, Whitaker, Mosher, Breivik, Wheeler, Miner, Sutherland, Wagner, Clapper, Lewis, Lux, and Popkin	[1941]	118	80				1.4302 to 1.4308	
		82	20				1.4305 to 1.4315	
Komarewsky and Smith	[1944]	183–184	760					
Häusermann	[1951]	82–83	11		.8340			
Bolle and Bourgeois	[1951]	181–183	760					
Sano	[1951]	181	760					
Suzuki et al.	[1951]	180–183	760					
Koga et al.	[1952]	180–183	760					
Union Carbide Corporation	[1953]	184.4	760					
Schmid and Bencge	[1953]	79	12					
Greiss	[1955]	80	11					
Union Carbide Corporation	[1956]	184.8	760	−70	.8324	.8287	1.4316	1.4290
Hornya and Cerny	[1956]	180–181	760					
Dvornikoff and Farmer	[1957]	180–182	760					
Union Carbide Corporation	[1958]	184.8	760					
Kutsenko and Lyubomilov	[1958]	180–183.5	760		0.8325		1.4325	
Lyubomilov and Belyanina	[1958]	183–184	760		.8325		1.4325	
Lyubomilov	[1958]	182–184	760		.8325		1.4325	
Hagemeyer, Wright, and Bobo	[1959]	91	20					
Fang, Huang, and Hou	[1959]	80–81	6					
Kallina and Kuffner	[1960]	183	760					
Tjebbes	[1960]				.8332	0.8291		
Miller and Bennett	[1961]	181–185	760					
Dykyj, Seprakova, and Paulech	[1961]	184.34	760		.8326		1.4320	
Lyubomilov and Merkula	[1963]	184	760		.8321		1.4310	
Union Carbide Corporation	[1965]	184.7	760	−70	.8325			
Selected value	[1967]	[e] 184.6±0.1	760	[a] −70.±1.	[d] .8327 ±.0007	[d] 0.8290 ±0.0007	[a] 1.4316 ±0.0010	[a] 1.4290 ±0.0010
		[e] 79.3±0.3	10					

Antoine constants: A 6.67138, B 1204.50, C 133.14

dt/dp at 760 mmHg, [e] 0.0479 °C/mmHg

Isomeric Octanols—Continued

Investigators		Vapor Pressures and Boiling Points		Freezing Point	Density, *d* g cm^{-3}		Refractive Index, n_D	
		°C	mmHg	t_m, °C	20 °C	25 °C	20 °C	25 °C
3-Ethyl-1-hexanol, $C_8H_{18}O$, mol wt. 130.232								
Levene and Marker	[1931e]					0.831		1.4323
4-Ethyl-1-hexanol, $C_8H_{18}O$, mol wt. 130.232								
Prout and Cason	[1949]	96	20					
Selected value	[1967]	[f] 85.±3.	10					
2,2-Dimethyl-1-hexanol, $C_8H_{18}O$, mol wt. 130.232, state at 25 °C liq								
Muset	[1906]	161–162	760					
Blondeau	[1928]	95	29					
Whitmore and Church	[1933]	80–82	14				1.4304 and 1.4296	
McElrath, Fritz, Brown, LeGall and Duke	[1960]	69–72	10					
Blood and Hagemeyer	[1964]	172.5	760	< −52	0.8265			1.4275
Selected value	[1967]	[e] 172.5±1. [e] 75.±2.	760 10				[b,c] 1.430 ±0.003	[a] 1.428 ±0.002
Antoine constants: *A* 9.6159, *B* 3001., *C* 273.					*dt*/*dp* at 760 mmHg, [e] 0.038 °C/mmHg			
2,4-Dimethyl-1-hexanol, $C_8H_{18}O$, mol wt. 130.232								
Graves	[1931]	173–175	760					
Shonle, Waldo, Keltch and Coles	[1936]	172–175	760					
Hagemeyer and Hudson	[1958]	177	760					
Selected value	[1967]	[b] 175.±5.	760					
2,5-Dimethyl-1-hexanol, $C_8H_{18}O$, mol wt. 130.232								
Carleton-Williams	[1879]	179–180	760		0.828	0.825		
3,3-Dimethyl-1-hexanol, $C_8H_{18}O$, mol wt. 130.232								
Stanley	[1964]	102	40		0.839		1.4328	
3,5-Dimethyl-1-hexanol, $C_8H_{18}O$, mol wt. 130.232								
Levene and Marker	[1932]					0.819		
Hoshiai and Nishio	[1959]	182.5	760		0.8282		1.4250	
4,4-Dimethyl-1-hexanol, $C_8H_{18}O$, mol wt. 130.232								
Gutman and Hickinbottom	[1951]	95–98	21				1.4351	

Isomeric Octanols—Continued

Investigators		Vapor Pressures and Boiling Points		Freezing Point	Density, *d* g cm^{-3}		Refractive Index, n_D	
		°C	mmHg	t_m, °C	20 °C	25 °C	20 °C	25 °C
3-Ethyl-2-hexanol, $C_8H_{18}O$, mol wt. 130.232								
Clark and Riegel	[1912]	167.5–168.5	760					
2,3-Dimethyl-2-hexanol, $C_8H_{18}O$, mol wt. 130.232								
Clarke	[1909]	150–161	756					
Huston, Guile, Sculati and Wasson	[1941]	159.6	748		0.8365		1.4335	
Stevens and Greenwood	[1943]	75	29			0.831		1.4280
							and	1.4290
Selected value	[1967]	^{e}160.1±1.	760		^{a}.836	^{c}.832	^{a}1.434	^{c}1.432
		^{e}62.±2.	10		±.001	±.001	±0.001	±0.002

Antoine constants: *A* 9.2833, *B* 2773., *C* 273. *dt/dp* at 760 mmHg, ^{e} 0.039 °C/mmHg

Investigators		°C	mmHg	t_m, °C	20 °C	25 °C	20 °C	25 °C
2,4-Dimethyl-2-hexanol, $C_8H_{18}O$, mol wt. 130.232								
Konovalov, M.	[1902]	158–160	745					
Clarke	[1908]	150.0 to 150.5	766					
Levene and Marker	[1931a]	64	20		0.827			
Huston, Guile, Sculati and Wasson	[1941]	150.2	748		.8099		1.4232	
Brokaw and Brode	[1948]	76.4 to 77.4	40				1.4253	
Thaker and Vasi	[1960]	56–70	20			0.804		1.422
Selected value	[1967]	^{e}150.7±1.	760		^{a}.810	^{c}.806	^{b}1.424	^{a}1.422
		^{e}51.±2.	10		±.001	±.002	±0.001	±0.002
2,5-Dimethyl-2-hexanol, $C_8H_{18}O$, mol wt. 130.232								
Konovalov, M.	[1902]				0.8227		1.42085	
Clarke	[1909]	152–154	760					
Meyer and Tout	[1933]	76	32		.8105		1.4214	
Huston, Guile, Sculati and Wasson	[1941]	151.6	748		.8158		1.4210	
George	[1943]	110	125					
Woods and Viola	[1956]	147–149	760			0.811		1.419
Barclay and Hilchie	[1957]	152–155	760					1.4216
Selected value	[1967]	^{e}152.5±0.5	760		^{a}.816	^{c}.812	^{b}1.4210	^{a,c}1.419
		^{e}58.±2.	10		±.001	±.002	±0.0010	±0.002

Antoine constants: *A* 6.5068, *B* 1006., *C* 125. *dt/dp* at 760 mmHg, ^{e} 0.044 °C/mmHg

Investigators		°C	mmHg	t_m, °C	20 °C	25 °C	20 °C	25 °C
3,3-Dimethyl-2-hexanol, $C_8H_{18}O$, mol wt. 130.232								
George	[1943]	110	125				1.4335	
Bol'shukhin and Egorov	[1957b]	85–86.5	28		0.8457		1.4353	
Egorov	[1958]	85–86.5	28		.8459		1.4353	
					^{a}.846	^{c}0.842	^{b}1.435	^{c}1.433
Selected value	[1967]	^{e}71.±2.	10		±.002	±0.003	±0.002	±0.003

Isomeric Octanols—Continued

Investigators		Vapor Pressures and Boiling Points		Freezing Point	Density, *d* g cm^{-3}		Refractive Index, n_D	
		°C	mmHg	t_m, °C	20 °C	25 °C	20 °C	25 °C
3,4-Dimethyl-2-hexanol, $C_8H_{18}O$, mol wt. 130.232								
Cook	[1952]	168.5	722				1.4362	
Selected value	[1967]	[f] 171.±2.	760					
3,5-Dimethyl-2-hexanol, $C_8H_{18}O$, mol wt. 130.232								
Bergmann and Herman	[1953]	160	760					
5,5-Dimethyl-2-hexanol, $C_8H_{18}O$, mol wt. 130.232								
Whitmore, Whitmore, and Cook	[1950]	166	760				1.4229	
3-Ethyl-3-hexanol, $C_8H_{18}O$, mol wt. 130.232, state at 25 °C								
See also table 166								
Masson	[1901]	159	760					
Clarke and Riegel	[1912]	160	760					
Halse	[1914]	158–159	760		0.8381		1.4294	
Eykman	[1919]	64	16		.8394			
Baerts	[1922]	160	760		.8373		1.42696	
Owen, Quayle and Beavers	[1930]				.8376	0.8333		
Church, Whitmore and McGrew	[1934]	158–160	733					
API Research Project 45	[1955]	58–59	9		.8398		1.4320	
Lanning and Moore	[1958]	160.1	760				1.4294	
Selected value	[1967]	[e] 159.±1.	760		[d] .8381	[d] 0.8337	[a] 1.427	[c] 1.425
		[e] 55.±2.	10		±.001	±0.001	±0.002	±0.003
Antoine constants: *A* 8.8289, *B* 2570., *C* 273.					*dt/dp* at 760 mmHg, [e] 0.042 °C/mmHg			
4-Ethyl-3-hexanol, $C_8H_{18}O$, mol wt. 130.232								
Winogradow	[1878]	164–166	760					
Fourneau and Tiffeneau	[1907]	162–164	760		0.819			
Warner	[1944]						1.4322	
Cook	[1952]	104	85				1.4321	
Selected value	[1967]	[e] 164.±3.	760		[a] .82		[b] 1.432	[c] 1.430
		[e] 59.±3.	10		±.01		±0.001	±0.002
Antoine constants: *A* 8.842, *B* 2605., *C* 273.					*dt/dp* at 760 mmHg, [e] 0.04 °C/mmHg			

Isomeric Octanols—Continued

2,2-Dimethyl-3-hexanol, $C_8H_{18}O$, mol wt. 130.232

Investigators		Vapor Pressures and Boiling Points		Freezing Point	Density, *d* g cm^{-3}		Refractive Index, n_D	
		°C	mmHg	t_m, °C	20 °C	25 °C	20 °C	25 °C
Haller and Bauer	[1913]	155–157	760					
Leroide	[1921]	156–157	760					
Conant, Webb and Mendum	[1929]	151–157	760					
Crooks	[1938]	148–153	741				1.4260 to 1.4276	
Whitmore	[1938]	152–163	744				1.4275	
Greenwood, Whitmore and Crooks	[1938]	152–153	744				1.4275	
Whitmore, Meyer, Pedlow and Popkin	[1938]						1.4245 to 1.4276	
Henne and Matuszak	[1944]	156.1	760		0.8342		1.4261	
Cadwallader, Fookson, Mears and Howard	[1948]	90–91	87–89					
		70–78	28–30				1.4262	
Powell and Wasserman	[1957]	153–155	760					1.4522
Selected value	[1967]	[e]156.1±0.5	760		[a].834	[c]0.830	[b]1.426	[c]1.424
		[e]42.±1.	10		±.002	±0.003	±0.002	±0.003

Antoine constants: *A* 8.0773, *B* 2229., *C* 273. *dt/dp* at 760 mmHg, [e]0.047 °C/mmHg

2,3-Dimethyl-3-hexanol, $C_8H_{18}O$, mol wt. 130.232

Investigators		Vapor Pressures and Boiling Points		Freezing Point	Density, *d* g cm^{-3}		Refractive Index, n_D	
		°C	mmHg	t_m, °C	20 °C	25 °C	20 °C	25 °C
Clarke	[1911]	158 to 158.2	758					
Stas	[1926]	61–62	18		0.8371		1.43087	
Whitmore and Evers	[1933]	42–43	16				1.4300	
Stevens and Greenwood	[1943]	72.5	29				1.4309	
Selected value	[1967]	[e]158.2±0.5	760				[b]1.4306	[c]1.428
		[e]52.±1.	10				±0.0010	±0.002

Antoine constants: *A* 8.5990, *B* 2466., *C* 273. *dt/dp* at 760 mmHg, [e]0.043 °C/mmHg

2,4-Dimethyl-3-hexanol, $C_8H_{18}O$, mol wt. 130.232

Investigators		Vapor Pressures and Boiling Points		Freezing Point	Density, *d* g cm^{-3}		Refractive Index, n_D	
		°C	mmHg	t_m, °C	20 °C	25 °C	20 °C	25 °C
Vaughan	[1944]	160.5	760					
Young and Roberts	[1945]	81.9	50				1.4325	
Whitmore, Whitmore and Cook	[1950]	160	760				1.4295 to 1.4300	
Botteron and Shulman	[1962a]	156–158	760					
Selected value	[1967]	[e]160.±1.	760				[a]1.431	[c]1.424
		[e]48.±1.	10				±0.002	±0.003

Antoine constants: *A* 8.2178, *B* 2314., *C* 273. *dt/dp* at 760 mmHg, [e]0.046 °C/mmHg

Isomeric Octanols—Continued

2,5-Dimethyl-3-hexanol, $C_8H_{18}O$, mol wt. 130.232, state at 25 °C

See also table 166

Investigators		Vapor Pressures and Boiling Points		Freezing Point	Density, d g cm^{-3}		Refractive Index, n_D	
		°C	mmHg	t_m, °C	20 °C	25 °C	20 °C	25 °C
Carleton-Williams	[1879]	106–163	755		0.817	0.814		
Michiels	[1912]	157–158	760		0.8212		1.42461	
Favorskii	[1913]	156	760		0.8221			
Tuot	[1936]	64	15		0.8145		1.4238	
George	[1943]	162	760		0.8195		1.4241	
		157.7	731					
		117.6	200					
Malinovskii and Konevichev	[1948]	160–162	760					
Sokolova	[1953]	154–157	760		0.8152		1.4221	
API Research Project 45	[1954]	158.9 to 159.2	760					
Botteron and Shulman	[1962a]	156–157	760					
Selected value	[1967]	^{e}159.±1.	760		^{d}0.8188	^{d}0.8146	^{b}1.424	^{c}1.422
		^{e}58.±2.	10		±0.001	±0.001	±0.002	±0.003

Antoine constants: *A* 6.2694, *B* 963., *C* 125. *dt/dp* at 760 mmHg, ^{e} 0.048 °C/mmHg

3,4-Dimethyl-3-hexanol, $C_8H_{18}O$, mol wt. 130.232, state at 25 °C

Investigators		Vapor Pressures and Boiling Points		Freezing Point	Density, d g cm^{-3}		Refractive Index, n_D	
		°C	mmHg	t_m, °C	20 °C	25 °C	20 °C	25 °C
Badertscher	[1934]	64	20				1.4380	
Huston, Goerner, Breining, Bostwick,		59–61	14					
Cline and Snyder	[1948]	150–152	740			0.8345	1.4350	
Selected value	[1967]	^{e}152.±2.	760		^{c}0.838	^{a}.834	^{a}1.436	^{c}1.433
		^{e}51.±2.	10		±.002	±.002	±0.002	±0.002

Antoine constants: *A* 8.9434, *B* 2576., *C* 273. *dt/dp* at 760 mmHg, ^{e} 0.04 °C/mmHg

3,5-Dimethyl-3-hexanol, $C_8H_{18}O$, mol wt. 130.232

Investigators		Vapor Pressures and Boiling Points		Freezing Point	Density, d g cm^{-3}		Refractive Index, n_D	
		°C	mmHg	t_m, °C	20 °C	25 °C	20 °C	25 °C
Clarke	[1908]	151	768					
Bodroux and Taboury	[1909]	151–153	750		0.826		1.4278	
Meyer and Tout	[1933]	59	15		.8228		1.4266	
Fischl	[1944]						1.4275	
Cymerman, Heilbron and Jones	[1945]	62–63	22				1.4272	
		60–60.5	20				1.4269	
Doering and Zeiss	[1948]	152	760		.826		1.425	
		152–153	760				1.427	
Doering and Zeiss	[1950]	152	760				1.427	1.4246
Cook	[1952]	93	100				1.4270	
Doering and Zeiss	[1953]	152–153	760					1.4241
Zeiss and Tsutsui	[1953]	152–153	760					1.4222
API Research Project 45	[1954]						1.4240 to 1.4244	
Woods and Viola	[1956]	152–153	760			0.827		1.433
Hickman and Kenyon	[1957]	150–151	760		.8329		1.426	
Pansevich-Kolyada and Osipenko	[1958]	44.5	10		.8288		1.4288	
Petrov, Zakharov and Krasnova	[1959]	54	14.5		.8261		1.4264	
Petrov and Zakharov	[1959]	54	14.5		.8261		1.4264	
Casey	[1959]	57–58	15				1.4266	
Sokolova, Shebanova and Shchepinov	[1961]	61	18		.8272		1.4288	
Selected value	[1967]	^{e}152.±1.	760		^{b}.827	^{c}.823	^{b}1.426	^{b,c}1.424
		^{e}43.±1.	10		±.002	±.004	±0.002	±0.002

Antoine constants: *A* 8.3311, *B* 2317., *C* 273. *dt/dp* at 760 mmHg, ^{e} 0.045 °C/mmHg

Isomeric Octanols—Continued

Investigators		Vapor Pressures and Boiling Points		Freezing Point	Density, *d* g cm^{-3}		Refractive Index, n_D	
		°C	mmHg	t_m, °C	20 °C	25 °C	20 °C	25 °C
4,4-Dimethyl-3-hexanol, $C_8H_{18}O$, mol wt. 130.232								
Rothrock	[1931]	159.2	760				1.4395	
Levina, Fainzil'berg, Tantsyreva, and Treshchova	[1951]	160 to 160.4	758		0.8341		1.4345	
Reeve and Karickhoff	[1956]	67	20					1.4315
Selected value	[1967]	[e] 159.±1.	760		[a] .834	[c] 0.830	[a] 1.434	[c] 1.432
		[e] 54.±1.	10		±.002	±0.003	±0.002	±0.003
Antoine constants: *A* 8.7031, *B* 2517., *C* 273.						*dt/dp* at 760 mmHg, [e] 0.042 °C/mmHg		
5.5-Dimethyl-3-hexanol, $C_8H_{18}O$, mol wt. 130.232								
Whitmore, Whitaker, Mattil and Popkin	[1938]	96	150				1.4248	
Whitmore, Popkin, Whitaker, Mattil, and Zech	[1938]	150–152	735					1.4250
Schmerling and Meisinger	[1953]	56–60	10				1.4262	
API Research Project 45	[1954]						1.4320 to 1.4324	
Benkeser, Hazdra and Burrous	[1959]	61	20				1.4258	
Selected value	[1967]	[e] 153.±2.	760				[a] 1.426	[c] 1.424
		[e] 50.±2.	10				±0.002	±0.003
Antoine constants: *A* 6.0660, *B* 886., *C* 125.						*dt/dp* at 760 mmHg, [e] 0.05 °C/mmHg		
2-*n*-Propyl-1-pentanol, $C_8H_{18}O$, mol wt. 130.232								
Koller and Kandler	[1931]	179	760					
Protiva, Exner, Brovicka and Pliml	[1952]	77–83	22					
Weiman and Thuan	[1958]	80–82	12		0.9		1.43	
Selected value	[1967]	[e] 179.±2.	760					
		[e] 79.±3.	10					
Antoine constants: *A* 9.4732, *B* 2980., *C* 273.						*dt/dp* at 760 mmHg, [e] 0.04 °C/mmHg		
2-Methyl-2-ethyl-1-pentanol, $C_8H_{18}O$, mol wt. 130.232								
Whitmore and Badertscher	[1933]	75.5–76	15				1.4353	
Badertscher	[1934]	75	15				1.4362	
Brannock	[1959]	174–175	760				1.4358	
Selected value	[1967]	174.±1	760				[b] 1.4358	[c] 1.434
							±0.0005	±0.001

Isomeric Octanols—Continued

4-Methyl-2-ethyl-1-pentanol, $C_8H_{18}O$, mol wt. 130.232

See also table 166

Investigators		Vapor Pressures and Boiling Points		Freezing Point	Density, d g cm^{-3}		Refractive Index, n_D	
		°C	mmHg	t_m, °C	20 °C	25 °C	20 °C	25 °C
Monsanto Chemical Company	[1958]	83	18		0.830			1.4271
Hagemeyer and Hudson	[1958]	176.5	760					
Hagemeyer, Wright, and Bobo	[1959]	176.5	760					
Dykyj, Seprakova, and Paulech	[1961]	177.05	760		.8273		1.4270	
		85.11	20					
Selected value	[1967]	177.1±0.2	760					
		73.2±0.5	10		^{a} .827± 0.001			

Antoine constants: A 6.9292, B 1326.1, C 150.5. dt/dp at 760 mmHg, ^{e} 0.0462 °C/mmHg

2,2,3-Trimethyl-1-pentanol, $C_8H_{18}O$, mol wt. 130.232, state at 25 °C

Investigators		Vapor Pressures and Boiling Points		Freezing Point	Density, d g cm^{-3}		Refractive Index, n_D	
		°C	mmHg	t_m, °C	20 °C	25 °C	20 °C	25 °C
Perry, Canter, DeBusk, and Robinson	[1958]	172–173	730				1.4388 and 1.4387	
McElrath, Fritz, Brown, LeGall, and Duke	[1960]	71	10					
		175	768					1.43828
Moffatt and Hutton	[1964]	72–74	16				1.4398	
Selected value	[1967]	^{e} 174.5±0.5	760				^{b} 1.439 ±0.001	^{c} 1.437 ±0.001
		^{e} 71.±0.5	10					

Antoine constants: A 9.121, B 2794., C 273. dt/dp at 760 mmHg, ^{e} 0.041 °C/mmHg

2,2,4-Trimethyl-1-pentanol, $C_8H_{18}O$, mol wt. 130.232, state at 25 °C liq.

See also table 167

Investigators		Vapor Pressures and Boiling Points		Freezing Point	Density, d g cm^{-3}		Refractive Index, n_D	
		°C	mmHg	t_m, °C	20 °C	25 °C	20 °C	25 °C
Terent'ev	[1925]	164–167	760		0.8232		1.4236	
James	[1943]						1.4299	
Davis and Hickinbottom	[1957]	79–80	23				1.4270 to 1.4285	
Union Carbide Corporation	[1958]	168.3	760	−70	.8384		1.4300	1.428
Hawthorne	[1958]	168–170	760					
Blake and Hammann	[1959]	82–83	30					1.4280
Brannock	[1959]	166–166.5	760				1.4300	
McElrath, Fritz, Brown, LeGall, and Duke	[1960]	72–73	15					
Hagemeyer, Hull, and Perry	[1960]	166	760					
Hasek, Clark, and Chaudet	[1961]	164–166.5	760				1.4292 to 1.4298	
Brannock	[1963]	164–166	760				1.4300	
Selected value	[1967]	^{e} 168.3±0.3	760	^{a} −70.±1.	^{a} .838 ±.001	^{c} 0.834 ±0.002	^{a} 1.4300 ±0.0010	^{c} 1.428 ±0.002
		^{e} 63.4±0.3	10					

Antoine constants: A 7.07819, B 1423.10, C 170.78. dt/dp at 760 mmHg, ^{e} 0.0462 °C/mmHg

Isomeric Octanols—Continued

Investigators	Vapor Pressures and Boiling Points		Freezing Point	Density, d g cm^{-3}		Refractive Index, n_D	
	°C	mmHg	t_m, °C	20 °C	25 °C	20 °C	25 °C
2,3,4-Trimethyl-1-pentanol, $C_8H_{18}O$, mol wt. 130.232							
Perry, Canter, DeBusk, and Robinson [1958]	182	730		0.8498		1.4392	
Perry and DeBusk [1959]	181–183	740					
Selected value [1967]	[c] 183.	760					
3,3,4-Trimethyl-1-pentanol, $C_8H_{18}O$, mol wt. 130.232							
Brändstrom [1959]	74–82	10					
2,4,4-Trimethyl-1-pentanol, $C_8H_{18}O$, mol wt. 130.232							
Sutherland [1940]				0.833			
Whitmore, Whitaker, Mosher, Brevik, Wheeler, Miner, Sutherland, Wagner, Clapper, Lewis, Lux, and Popkin [1941]	78–80	22				1.4278 to 1.4285	
Gasson, Millidge, Robson, and Wild [1953]	70–78	15					
	168–169	740					
Hadley, Hall, Heap, and Jacobs [1954]						1.4260	
Chambers and Foster [1959]	170–171	760					1.4259 to 1.4263
Selected value [1967]	[e] 171. ±1.	760		[a] .833	[c] 0.829	[c] 1.428	[a] 1.426
	[e] 63. ±2.	10		±.002	±0.003	±0.002	±0.001
Antoine constants: A 8.7978, B 2624., C 273.							
dt/dp at 760 mmHg, [e] 0.04 °C/mmHg							
2-Methyl-3-ethyl-2-pentanol, $C_8H_{18}O$, mol wt. 130.232							
Clarke [1908]	156	760					
Huston, Guile, Sculati, and Wasson [1941]	157.2	748		0.8382		1.4325	
American Petroleum Institute Research Project 45 [1954]	68	20					
Skinner and Florentine [1954]	38	2			0.8346		1.4303
Selected value [1967]	[e] 157.8±0.5	760		[a] .838	[a] 0.835		
	[e] 59. ±1.	10		±.001	±0.001		
Antoine constants: A 6.3920, B 993., C 125. dt/dp at 760 mmHg, [e] 0.046 °C/mmHg							
3-Methyl-3-ethyl-2-pentanol, $C_8H_{18}O$, mol wt. 130.232, state at 25 °C							
Reeve and Karickhoff [1956]	87	39					
Bol'shukhin and Egorov [1957a]	55–57	5		0.8576		1.4488	
Egorov [1958]	55–57	5		.8576		1.4488	
Selected value [1967]	[e] 67. ±3.	10		[b] .858	[c] 0.854	[b] 1.449	[c] 1.447
				±.002	±0.003	±0.002	±0.003
4-Methyl-3-ethyl-2-pentanol, $C_8H_{18}O$, mol wt. 130.232							
Clarke [1908]	172	760					
Whitmore, Whitmore, and Cook [1950]	164	760				1.4331	
Selected value [1967]	[a] 164. ±2.	760					

Isomeric Octanols—Continued

2,3,3-Trimethyl-2-pentanol, $C_8H_{18}O$, mol wt. 130.232, state at 25 °C liq

Investigators		Vapor Pressures and Boiling Points		Freezing Point	Density, *d* g cm^{-3}		Refractive Index, n_D	
		°C	mmHg	t_m, °C	20 °C	25 °C	20 °C	25 °C
Whitmore and Laughlin	[1932a]	82.5	58				1.4410 and 1.4280	
Whitmore and Laughlin	[1933]	86.5	60		0.861		1.4420	
Norton and Hass	[1936]	159.4	750			0.8151		1.4360
		78.5	50					
Huston, Guile, Sculati, and Wasson	[1941]	156.6	748		.8517		1.4393	
		45–47	6					
Brown and Kornblum	[1954]	77.8–78.0	40	−1.29			1.4420	
Selected value	[1967]	^{e} 160.0±0.5	760	* −0.5± 0.5	^{c} .819	^{a} .815	^{c} 1.438	^{a} 1.436
		^{e} 49.±1.	10		±.004	±.002	±0.004	±0.002

Antoine constants: *A* 5.8329, *B* 841., *C* 125. *dt/dp* at 760 mmHg, ^{e} 0.055 °C/mmHg

* Corrected for impurities.

2,3,4-Trimethyl-2-pentanol, $C_8H_{18}O$, mol wt. 130.232

Investigators		Vapor Pressures and Boiling Points		Freezing Point	Density, *d* g cm^{-3}		Refractive Index, n_D	
		°C	mmHg	t_m, °C	20 °C	25 °C	20 °C	25 °C
Huston and Guile	[1939]	155–157	752		0.8081		1.4372	
		43.8	5					
Huston, Guile, Sculati, and Wasson	[1941]	157.2	748		.8080		1.4365	
Selected value	[1967]	^{a,f} 158.±1.	760		^{a} .808 ±.001	^{c} 0.804 ±0.002	^{a} 1.437 ±0.001	^{c} 1.435 ±0.002

2,4,4-Trimethyl-2-pentanol, $C_8H_{18}O$, mol wt. 130.232

Investigators		Vapor Pressures and Boiling Points		Freezing Point	Density, *d* g cm^{-3}		Refractive Index, n_D	
		°C	mmHg	t_m, °C	20 °C	25 °C	20 °C	25 °C
Whitmore, Wilson, Capinjola, Tongberg, Fleming, McGrew, and Cosby	[1941]	143–145	760		0.8250		1.4270 to 1.4272	
		38	8					
Huston, Guile, Sculati, and Wasson	[1941]	145.8	748		.8225		1.4284	
Whitmore, Rowland, Wrenn, and Kilmer	[1942]	70.5	43				1.4286	
Ritter	[1948]	145–147	760			0.8297		1.4293
Brown and Berneis	[1953]	146–146.5	750					1.4256
Graham, Millidge, and Young	[1954]	143–145	760				1.4238	
Brown and Nakagawa	[1955]	60.5	28.4				1.4280	
Selected value	[1967]	^{e} 146.4±0.5	760		^{a} .823	^{c} .819	^{b} 1.428	^{a,c} 1.426
		^{e} 44.±1.	10		±.001	±0.002	±0.001	±0.002

Antoine constants: *A* 5.9629, *B* 837., *C* 125. *dt/dp* at 760 mmHg, ^{e} 0.050 °C/mmHg

3,3,4-Trimethyl-2-pentanol, $C_8H_{18}O$, mol wt. 130.232, state at 25 °C

Investigators		Vapor Pressures and Boiling Points		Freezing Point	Density, *d* g cm^{-3}		Refractive Index, n_D	
		°C	mmHg	t_m, °C	20 °C	25 °C	20 °C	25 °C
Meshcheryakov and Petrova	[1955]	164–165.5	760		0.8557		1.4381	

Isomeric Octanols—Continued

3,4,4-Trimethyl-2-pentanol, $C_8H_{18}O$, mol wt. 130.232, state at 25 °C crystal

Investigators		Vapor Pressures and Boiling Points		Freezing Point	Density, d g cm^{-3}		Refractive Index, n_D	
		°C	mmHg	t_m, °C	20 °C	25 °C	20 °C	25 °C
Sutherland	[1940]	157	760					
Wheeler	[1941]			27.3	0.8408			
Ansell, Hancock, and Hickinbottom	[1956]	159–160	760				1.4355	
Saunders and Carges	[1960]	93–95	67					1.4332
Selected value	[1967]	^{e}158.±2. ^{e}57.±3.	760 10	^{a}27.±0.5				

Antoine constants: A 9.041, B 2655., C 273. dt/dp at 760 mmHg, ^{e}0.040 °C/mmHg

2-Methyl-3-ethyl-3-pentanol, $C_8H_{18}O$, mol wt. 130.232

Investigators		Vapor Pressures and Boiling Points		Freezing Point	Density, d g cm^{-3}		Refractive Index, n_D	
		°C	mmHg	t_m, °C	20 °C	25 °C	20 °C	25 °C
Grigorovitsch and Povlov	[1891]	159.5–161	750		0.8295			
Papa, Villani, and Ginsberg	[1954]	158–160	760					
Selected value	[1967]	^{b}160.±2.	760					

2,2,3-Trimethyl-3-pentanol, $C_8H_{18}O$, mol wt. 130.232, state at 25 °C liq

See also table 167

Investigators		Vapor Pressures and Boiling Points		Freezing Point	Density, d g cm^{-3}		Refractive Index, n_D	
		°C	mmHg	t_m, °C	20 °C	25 °C	20 °C	25 °C
Clarke and Jones	[1912]	149–152	760					
Whitmore and Laughlin	[1932a]	75.8–76.2	39–41				1.4353	
Whitmore and Laughlin	[1033]	76.1–76.6	50		0.849		1.4354	
Norton and Hass	[1936]	151.8–152.4	743			0.8423		1.4330
Brooks, Howard, and Crafton	[1939]	74–76	40					
Ginnings and Coltrane	[1939]	153–154	760			.8420		
Schmerling, Friedman, and Ipatieff	[1940]	68–70	35				1.4352	
Cook	[1952]	98	124				1.4358	
Huston and Van Dyke	[1953]	148–150	750					
Brown and Kornblum	[1954]	44.5–45.0	11	−6.05			1.4357	
Brown and Okamoto	[1955]	44.5–45.0	11	−6.05			1.4357	
Petrov, Sushchinskii, Zakharov, and Rogozhnikova	[1957]	67.8–68.9	33.5		.8310		1.4352	
Saunders and Carges	[1960]	66–69	34					1.4319
Geiseler, Fruwert, and Stöckel	[1962]	95	100		.8473		1.4355	
Evans, Landor, and Taylor-Smith	[1903]	68–69	32					
Selected value	[1967]	^{e}152.5±1 ^{e}45.4±1.	760 10	−6.0±1.0	^{c}.846 ±.003	^{b}.842 ±.001	^{b}1.4355 ±0.0010	^{a,c}1.433 ±0.002

Antoine constants: A 7.3891, B 1642.0, C 211.6. dt/dp at 760 mmHg, ^{e}0.0462 °C/mmHg

Isomeric Octanols—Continued

Investigators		Vapor Pressures and Boiling Points		Freezing Point	Density, d g cm^{-3}		Refractive Index, n_D	
		°C	mmHg	t_m, °C	20 °C	25 °C	20 °C	25 °C
2,2,4-Trimethyl-3-pentanol, $C_8H_{18}O$, mol wt. 130.232, state at 25 °C liq								
See also table 167								
Favorskiĭ	[1913]	150–151	760	−13.				
Haller and Bauer	[1913]	145–148	760					
Conant and Blatt	[1929]	148–152	760					
Conant, Webb, and Mendum	[1929]	140–150	760					
Whitmore and Houk	[1932]	148–150	740				1.4288	
Whitmore and Laughlin	[1933]						1.428	
Whitmore, Meyer, Pedlow, and Popkin	[1938]	100	150				1.4290 to 1.4295	
Wibaut and Pelt	[1938]	54–54.5	18				1.4284	
Whitmore	[1938]	145	760				1.4281	
Greenwood, Whitmore, and Crooks	[1938]	145	738				1.4281	
Crooks	[1938]	145	760				1.4282	
Whitmore and Forster	[1942]	75.5	53				1.4268 to 1.4292	
Dixon, Cook, and Whitmore	[1948]	112.5	218				1.4290	
Cadwallader, Fookson, Mears, and Howard	[1948]	155 83	760 82				1.4280	
Huston and Brault	[1950]	55	15				1.4038	
Bridson-Jones, Buckley, Cross, and Driver	[1951]	148–150	760				1.4288	
Smith and Creitz	[1951]	151.3	760	−11.3	0.8322		1.4287	
Cook	[1952]	147	760				1.4289	
Zeiss and Tsutsui	[1953]	74	45					1.4262
Foley, Welch, La Combe, and Mosher	[1959]	150.9–151.1	760					
Kallina and Kuffner	[1960]	152–154	760					
Geiseler, Fruwert, and Stöckel	[1962]	96	100		.8326		1.4291	
Selected value	[1967]	^{e}151.0±0.5 ^{e}50.2±1.	760 10	−11.3±1.	^{b}.8324 ±.0010	^{c}0.828 ±0.002	^{b}1.4286 ±0.0010	^{c}1.427 ±0.002

Antoine constants: A 5.1306, B 498.1, C 70.4. dt/dp at 760 mmHg, ^{e}0.0562 °C/mmHg

Investigators		°C	mmHg	t_m, °C	20 °C	25 °C	20 °C	25 °C
2,3,4-Trimethyl-3-pentanol, $C_8H_{18}O$, mol wt. 130.232								
Stas	[1926]	156.5	760		0.8492		1.4353	
Whitmore and Laughlin		75–77	40				1.4341 to 1.4343	
Schmerling, Friedman, and Ipatieff	[1940]	73	30				1.4350 to 1.4356	
Whitmore and George	[1942]	101	125				1.4350	
Huston and Auvapara	[1944]	156–157	750					
Brown and Fletcher	[1951]	76–78	46					1.4326
Saunders and Carges	[1960]	50–53	16					1.4310
Kallina and Kuffner	[1960]	156–157	760					
Selected value	[1967]	^{e}157.±2. ^{e}43.±3.	760 10		^{a}.849 ±.002	^{c}.845 ±.003	^{b}1.435 ±0.001	^{c}1.433 ±0.002

Antoine constants: A 8.1164, B 2251., C 273. dt/dp at 760 mmHg, ^{e}0.047 °C/mmHg

Investigators		°C	mmHg	t_m, °C	20 °C	25 °C	20 °C	25 °C
3-Methyl-2-isopropyl-1-butanol, $C_8H_{18}O$, mol wt. 130.232								
Sarel and Newman	[1956]	171–172	741			0.8425		1.4324
Selected value	[1967]	^{a}173.±3.	760					

Isomeric Octanols—Continued

Investigators	Vapor Pressures and Boiling Points		Freezing Point	Density, d g cm^{-3}		Refractive Index, n_D	
	°C	mmHg	t_m, °C	20 °C	25 °C	20 °C	25 °C
2,2-Diethyl-1-butanol, $C_8H_{18}O$, mol wt. 130.232							
Whitmore and Badertscher [1933]	75–78	12				1.443	
Rice, Jenkins and Harden [1938]	76–77	11				1.4400	
Whitmore, Whitaker, Mosher, Breivik, Wheeler, Miner, Sutherland, Wagner, Clapper, Lewis, Lux, and Popkin [1941]	75	13				1.4430	
Whitmore and Lewis [1942]	96–100	40				1.4293 to 1.4412	
Sarel and Newman [1956]	92	25					1.4411
Selected value [1967]	^{c}69. ±2.	10				^{a,c}1.443 ±0.003	^{a}1.441 ±0.002
3,3-Dimethyl-2-ethyl-1-butanol, $C_8H_{18}O$, mol wt. 130.232							
Sarel and Newman [1956]	88–89	38			0.8425		1.4348
2,2,3,3-Tetramethyl-1-butanol, $C_8H_{18}O$, mol wt. 130.232 crystal							
Whitmore, Marker, and Plambeck [1941]			149–150				
McElrath, Fritz, Brown, LeGall, and Duke [1960]			149–151				
Selected value [1967]			^{b}150. ±3.				

Index to the Bibliography

Numbers refer to the Bibliography, page 1–389.

References to data used in the selection of refractive index, density, boiling point, vapor pressure, and melting point are in boldface type.

Numbers in parentheses refer to sources of reviews or theoretical calculations only.

Reference numbers under each property are listed in the order of date of publication.

References to the Properties of 2-Octanol

Refractive Index
378, 608, 235, 1381, 1378, 123, 509, 486, 1889, **1916**, **1926**, 1262, **2021**, 341, 444, 1222, 6, 706, **947**, **577**, **948**, 13, **1246**, **338**, 2016, 35, 377, 207, 343, 1824, 131, **944**, 610, **946**, **1487**, 1013, **586**, 1193, 1750

Density at 20–30 °C Only
235, 1349, 1381, 123, 1262, 1337, **2021**, 341, 1222, 173, 6, 1753, 205, 947, 1246, **338**, 35, 131, **944**, 610, **586**

Density at all Temperatures
608, 1559, **1378**, 1380, **1633**, 509, **149**, **486**, 1340, 92, **444**

Normal Boiling Point
378, 1576, 235, 1559, 1349, 868, 1395, 538, 1380, **1773**, 1009, 1121, 1597, **870**, 1847, 1889, **1916**, 1926, 2021, 1396, 6, 706, 1007, 1282, **338**, 49, 377, 2016, 207, 1643, 131

Vapor Pressure and Boiling Points at Other Pressures
1381, 1633, 695, 509, 888, 875, **486**, **982**, 341, 92, **444**, 173, **445**, **947**, **1246**, 377, 1824, **343**, **610**, 364, 944, 946, 1802, 232, 1193

Critical Temperature
218

Normal Melting Point
1773, **444**, **338**, 377

Calorimetric Heat of Vaporization at the Normal Boiling Point
219

Heat of Combustion
1085, 1086

Equilibrium Constants of Reactions in the Gas Phase
371

Molecular Vibration Frequencies and Spectra
1190

Association in the Liquid Phase
489

1-Nonanol

Properties of the Liquid Phase at Various Temperatures

Refractive Index

The range of conditions for available refractive index data are limited. Table 174 shows values for the Na$_D$ line at 20 and 25 °C. The only data outside this range are given by Stephan [1900] for the Na$_D$ line at 15 °C, and Vogel [1948] for three other wavelengths at 20 °C. The values at various wavelengths shown in table 173 were obtained by plotting the data of Vogel and adjusting it to agree with the value selected for n_D.

Density

Densities have been measured only from −5 to about 35 °C, and of these only 5 are at temperatures other than 20 °C. There are not enough data to permit a meaningful determination of the constant E in the Francis equation, and so the values in table 171 were calculated from a linear equation in temperature obtained by a least squares fit to the experimental points. Most of the experimental values are within about 0.001 g cm^{-3} of these calculated ones. At 20 °C the best values are those of Olivier [1937], Vogel [1948], Cook [1952], and von Erichsen [1952].

Vapor Pressure and Boiling Point

There are no accurate measurements of boiling points. Table 174 lists those values which deserve consideration in the selection. The boiling point calculated from the Antoine constants is within the experimental uncertainty implied by these data. No systematic measurements of vapor pressure at pressures other than 1 atm have been made. The selected Antoine constants are based on scattered measurements of boiling points at 1 atm and at pressures from about 7 to 20 mm Hg. The boiling point data of Krafft [1886], Verkade and Coops [1927], Ellis and Reid [1932], Haynes, Heilbron, Jones, and Sondheimer [1947], and Ställberg-Stenhagen [1948], besides those in table 174, were used to establish the Antoine constants. These were too inconsistent and too unevenly distributed to establish the constant C with any certainty. Although the final set of constants will reproduce these data as well as possible, it cannot be considered to have much physical significance. Royals and Corington [1955] report a boiling point of 72–76 °C at 3 mm Hg, although this was not used in fitting the constants. The selected Antoine constants predict a vapor pressure of 1.6 mm at 74 °C.

Critical Properties

Critical Temperature and Density

The only experimental data are from Efremov [1966]. He reported a temperature of 410 °C for the disappearance of the meniscus. However, extrapolation of his surface tension data to zero predicts a critical temperature of 404 °C, which was selected. The critical density was calculated from his values of saturated liquid and vapor densities for t_c of 404 °C.

Solid-Liquid Phase Equilibria

There is a definite scarcity of information on the melting point of 1-nonanol and a complete absence of any precise measurements. Krafft [1886], Sackmann and Sauerwald [1950], and Cook [1952] all report a melting point of approximately −5 °C. Guerbet [1902] found a melting point of −10 °C and a freezing point of −20 °C. A value of −5 °C was selected, with an uncertainty of at least 2 degrees. There are no data for heat of fusion or for any other condensed phase transitions.

Properties of the Liquid at 25 °C

The only liquid phase property which has been reported is the heat of combustion. When converted to modern units and standard state conventions, Verkade and Coops [1927] found $\Delta H_c^0(l) = -1420.5$ kcal mol^{-1}. Chao and Rossini [1965] obtained −1419.89 kcal mol^{-1} using modern techniques. The former value was selected. The entropy was calculated from the value selected for the ideal gas and the auxiliary data described below.

Vapor-Liquid Equilibrium at 25 °C

The vapor pressure data used to evaluate the Antoine constants did not extend below 95 °C. The constants predict a vapor pressure of 0.024 mm-Hg at 25 °C, but this is only a very rough indication of the true value. The Antoine equation does not produce a meaningful heat of vaporization this far below the experimental range, especially when the vapor pressure is so uncertain and so poorly distributed. Green [1960] calculated $\Delta H_v = 18.6$ kcal mol from another type of vapor pressure equation fitted to essentially the same set of data. Although this result cannot be considered as a direct experimental determination, it was selected as an estimate in calculating the heat of formation of 1-nonanol in the gas phase.

TABLE 171. 1-Nonanol. Selected values. Physical and thermodynamic properties

Temp. °C	Refractive Index, n_D	Density g cm^{-3}	Vapor Pressure, mmHg
0		0.8410	
10		.8345	
15	1.4358		
20	1.4338	.8280	
25	1.4319	.8247	
30		.8215	
40		.815	
104.			10
105			10.4
110			16.6
115			17.7
120			22.7
125			28.9
130			37.
135			46.
140			57.
145			71.
150			87.
153.			100
155			107.
160			130.
165			157.
170			187.
172.			200
175			226.
180			269.
185			318.
190			375.
192.			400
195			440
200			515.
205			600.
210			696.
213.1			760

Data For Phase Transitions

Initial	Final	Temp. °C	dt/dP deg mm^{-1}	Pressure mmHg	ΔH kcal mol^{-1}	$d\Delta H/dt$	ΔS	ΔC_p
						cal deg^{-1} mol^{-1}		
c	liq	−5.0±2						
liq	g	25		0.03±0.02	18.6±0.7		62.4±2	
liq	g	213.1±0.5	0.0456	760	13.0±1		26.7±2	

Condensed Phase Heat Capacity

State	Temp. °C	C_p
		cal deg^{-1} mol^{-1}

Properties of the Saturated Real Gas

Temp. °C	H^r-H^0	S^r-S^0	$C_p{}^r-C_p{}^0$
	kcal mol^{-1}	cal deg^{-1} mol^{-1}	

Data for the Standard States at 25 °C

State	Heat of Combustion $\Delta H_c{}^0$ kcal mol^{-1}	Heat of Formation $\Delta H_f{}^0$ kcal mol^{-1}	Entropy S^0 cal deg^{-1} mol^{-1}	Gibbs Energy of Formation $\Delta G_f{}^0$ kcal mol^{-1}	Heat Capacity, C_p cal deg^{-1} mol^{-1}
liq	−1420.4±0.4	−109.2±0.4	91.3±3	−32.4±1	
g	−1459.0±0.8	−90.6±0.8	133.5±0.7	−26.4±0.8	53.6±0.5

Critical Constants

Temp. 404 °C, 677. K	Pressure atm	Density 0.264 g cm^{-3}

Constants in Vapor Pressure and Density Equation

Antoine Equation				Francis Equation				
Temp. Range	A	B	C	Temp. Range	A	$B\times10^{-3}$	C	E
95 to 214 °C	7.8278	1953.8	181.9	−5 to 35 °C	0.84096	0.6495		

TABLE 172. 1-Nonanol. Selected values. Thermodynamic functions of the ideal gas at one atmosphere

Temperature K	Entropy S^0 cal deg^{-1} mol^{-1}	Heat Capacity C_p^0 cal deg^{-1} mol^{-1}	Enthalpy Function $(H^0-H^0_0)/T$ cal deg^{-1} mol^{-1}	Gibbs Energy Function $(G^0-H^0_0)/T$ cal deg^{-1} mol^{-1}	Heat of Formation ΔHf^0 kcal mol^{-1}	Gibbs Energy of Formation ΔGf^0 kcal mol^{-1}
0	0	0	0	0	−77.3	−77.3
273.15	128.96	50.33	32.85	−96.11	−89.7	−31.7
298.15	133.45	53.64	34.46	−98.99	−90.6	−26.4
300	133.75	53.91	34.56	−99.19	−90.7	−25.9
400	151.03	67.50	41.10	−109.93	−94.1	−3.8
500	167.46	80.01	47.66	−119.80	−97.0	19.1
600	182.90	90.60	53.93	−128.97	−99.2	42.6
700	197.53	99.71	59.79	−137.74	−100.9	66.4
800	211.39	107.46	65.30	−146.09	−102.1	90.4
900	224.40	114.15	70.40	−154.00	−102.9	114.5
1000	236.75	119.91	75.04	−161.71	−103.4	138.7

TABLE 173. 1-Nonanol. Selected values. Refractive index at various wavelengths at 20 °C

Symbol	Wavelength, Å	Refractive Index, n 20 °C
He_{red}	6678.2	1.4314
H_c	6562.8	1.4317
Na_D	5892.6	1.4338
Hg_e	5460.7	1.4356
He_{blue}	5015.7	1.4380
H_F	4861.3	1.4390
Hg_g	4358.3	1.4430
$H_{G'}$	4340.5	1.4432

Vapor-Liquid Equilibrium at the Normal Boiling Point

Using an estimated second virial coefficient of −1.5 liters mol^{-1}, a ΔH_v of 13.0 kcal mol^{-1} is calculated from the selected Antoine constants. Here also, in view of the uncertainty in the vapor pressure data, the result can be considered only as a rough indication of the correct value.

Properties of the Ideal Gas

Thermodynamic functions based on the incremental procedure have been published by Chermin [1961] and Green [1961]. To be consistent with the data selected for the other alcohols, the values of Green were selected. The heat capacity and entropy from these two sets of tables are within about 0.1 cal deg^{-1} mol^{-1} of each other at 298 K, and the difference increases to about 1 cal deg^{-1} mol^{-1} at 1000 K.

Table 174. 1-Nonanol. Reported values. Simple physical properties

Investigators		Vapor Pressures and Boiling Points		Freezing Point	Density, d g cm^{-3}		Refractive Index, n_D	
		°C	mmHg	t_m, °C	20 °C	25 °C	20 °C	25 °C
1-Nonanol, $C_9H_{20}O$, mol wt. 144.259, state at 25 °C liq								
Krafft	[1886a]			−5	0.8279			
Guerbet	[1902]	212–214	760	−10−−20				
Behal	[1919]	211–215	760		.8279		1.43105	
Wood and Comley	[1924]	213.2–213.5	760					
Verkade and Coops	[1927]					0.8239		
Malone and Reid	[1929]	213.6	760					
Ellis and Reid	[1932]	213.5				.82303		1.4320
Strating and Backer	[1936]	212.5–214	760					
Olivier	[1937]	213–213.5	760		.8271			
Muller	[1942]				.8304		1.4360	
Haynes, Heilbron, Jones, and Sondheimer	[1947]							1.4347
Vogel	[1948]	212	760		.8273		1.43325	
Sackmann and Sauerwald	[1950]			−5				
Cook	[1952]	213.3	760	−5	.8292		1.4327	
Stahl and Pessen	[1952]						1.4340	
von Erichsen	[1952]	214.6–214.7	760		.8284		1.4334	
McKenna, Tartar, and Lingafelter	[1953]	213.1						1.4318
Urry, Stacey, Huyser, and Juveland	[1954]						1.4342	
Royals and Covington	[1955]							1.4309
Goldfarb and Konstantinov	[1956]				.8305		1.4335	
Selected value	[1967]	213.1±0.5	760	−5±2.	.8280	0.8247	1.4338	1.4319
		104.±2.	10		±0.0005	±0.001	±0.001	±0.001

Antoine constants: A 7.8278, B 1953.8, C 181.9

dt/dp at 760 mmHg, ^{e} 0.0456 °C/mmHg

Index to the Bibliography

Numbers refer to the Bibliography on page 1–389.

References to data used in the selection of refractive index, density, boiling point, vapor pressure, and melting point are in boldface type.

Numbers in parentheses refer to sources of reviews or theoretical calculations only.

Reference numbers under each property are listed in the order of date of publication.

Refractive Index
123, **1113**, **486**, **1222**, 737, **1856**, **1865**, **338**, **1671**, **1152**, **1824**, **1515**, **612**

Density at 20–30 °C Only
123, **1113**, **486**, **1288**, **1222**, **1856**, **1865**, **338**, **612**

Density at all Temperatures
950, 1686, **1848**, 1527, 481

Normal Boiling Point
659, 123, **1981**, 1121, 1703, 1288, **1856**, **338**, 1152

Vapor Pressure and Boiling Points at Other Pressures
950, **1686**, **66**, **1848**, **486**, **727**, **1673**, **1824**, **1515**, **612**

Critical Volume and Density
481

Normal Melting Point
871, 950, 659, **1527**, **338**

Heat of Combustion
1848, (1507), (626), 287, 288

Molecular Vibration Frequencies and Spectra
1012, 456, 797

Thermodynamic Functions of the Ideal Gas
623, 291

Isomeric Nonanols

The observed data on simple physical properties have been summarized in the following unnumbered tables. There have been no systematic studies of this class of compounds by a single investigator and only a few studies of any property as a function of temperature. Thus most of the selections have been based on widely scattered data of questionable accuracy. Eykman [1919] has published refractive index values of 5-nonanol at various wavelengths in the visible region and at temperatures of 16 and 79.4 °C.

In a series of papers Pickard and Kenyon [1911], [1912], and [1913] have reported values of density of 2-nonanol, 3-nonanol, and 2-methyl-3-octanol over a wide range of temperatures. Ellis and Reid [1932] determined the density of 2-nonanol at 0 and 25 °C. Quayle and Smart [1944] measured the densities of 3-methyl-3-octanol and 4-methyl-4-octanol at temperatures from 25 to 55 °C and the refractive index at temperatures from 20 to 35 °C. Owen, Quayle, and Beavers [1930] reported surface tension and density data for 2-methyl-2-octanol from 0 to 65 °C. Stross, Gable, and Rounds [1947] accurately measured several properties, including density from 20 to 60 °C, viscosity from 0 to 40 °C, and refractive index at three wavelengths at 20 °C, of 2,6-dimethyl-4-heptanol. Their vapor pressure measurements over the range of 90 to 180 °C represent the only accurate vapor pressure data available for any of the isomeric nonanols. Values of density outside the range of 20 to 25 °C, which are listed in tables 175–178, have been calculated from the Francis equation constants based on these various sources of experimental density, along with values reported in the unnumbered tables. Since the available data were not adequate to determine the value of the constant, E, in the Francis equation, a value of 700 was assumed and the remaining constants were obtained by a least squares fit, as described in appendix B.

The Antoine constants and the corresponding vapor pressures listed for 2,6-dimethyl-4-heptanol in table 177 were taken from Stross, Gable, and Rounds [1947]. They also calculated a heat of vaporization of 10.50 kcal mol^{-1} at the normal boiling point for this compound. An estimate of the effect of gas imperfection was included in the calculation. Antoine constants for 2,2-dimethyl-4-heptanol, 2,2,3-trimethyl-3-hexanol, 2,4-dimethyl-3-ethyl-3-pentanol and 2,2,3,4-tetramethyl-3-pentanol which are given in tables 177 and 178 were calculated by a least squares fit to the experimental boiling point and vapor pressure data. George [1943] has reported vapor pressures at three points each for 2,2,3-trimethyl-3-hexanol and 2,4-dimethyl-3-ethyl-3-pentanol. The calculations for the other two compounds were based entirely on scattered boiling point values which are listed in the unnumbered tables.

The boiling point of 4-methyl-4-octanol at 50 mm Hg reported by Pomerantz, Fookson, Mears, Rothberg, and Howard [1954] appears to be the best value. However, it is about 20 °C higher than the boiling point obtained by interpolating the other values at this pressure. Because of this large discrepancy, no selection was made for boiling points below 760 mm Hg.

The Antoine constants reported for the other compounds in tables 175 and 176 and in the unnumbered tables have been obtained by a graphical procedure in which C was assumed to be either 125 or 273. These constants should be used only for rough interpolations between the experimental points.

Zubov [1903], as reported by Swietoslawski [1920], obtained a heat of combustion, ΔH_c^0, of 4-ethyl-4-heptanol of -1387.9 kcal mol^{-1}. This corresponds to $\Delta H_f^0(1) = -141.7$ kcal mol^{-1}. A more recent determination of the heat of combustion of 3,5,5-trimethyl-1-hexanol was made by Nicholson [1960]. His final corrected value was $\Delta H_c^0 = -1420.5$ kcal mol^{-1}, which gives $\Delta H_f^0(1) = -109.1$ kcal mol^{-1}.

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References to the Properties of 2-Nonanol

Numbers refer to the Bibliography, page 1–389.

References to data used in the selection of refractive index, density, boiling point, vapor pressure, and melting point are underlined.

Numbers in parentheses refer to sources of reviews or theoretical calculations only.

Reference numbers under each property are listed in the order of date of publication.

Refractive Index
1827, 693, 1378, 486, 844

Density at 20–30 °C Only
1827, 693, 1378

Density at all Temperatures
1418, 1136, 1380, 486

Normal Boiling Point
1418, 1827, 742, 1136, 693, 1380, 1121, 844

Vapor Pressure and Boiling Points at Other Pressures
1122, 779, 1761, 1827, 1378, 486, 1403

Normal Melting Point
1827

TABLE 175. Isomeric Nonanols. Selected values of physical properties of the liquid

2-Nonanol				3-Nonanol				2-Methyl-2-octanol			
Temp. °C	Refractive Index, n_D	Density g cm^{-3}	Vapor Pressure, mmHg	Temp. °C	Refractive Index, n_D	Density g cm^{-3}	Vapor Pressure, mmHg	Temp. °C	Refractive Index, n_D	Density g cm^{-3}	Vapor Pressure, mmHg
0		0.8372		10		0.832		0		0.8348	
10		.8302		20	1.431	.8250		10		.8274	
20	1.4310	.8231		25	1.419	.8214		20	1.428	.8198	
25	1.4290	.8195		30		.8178		25	1.426	.8158	
30		.8159		40		.8106		30		.8118	
40		.8084		50		.8033		40		.8035	
50		.8008		60		.7960		50		.7948	
60		.7929		70		.7886		60		.7858	
70		.7849		80		.7811		70		.7764	6.4
80		.7766		83.			10	77.			10
88.			10	90		.7736	15.	80			12.3
90		.7680	11.	100		.7659	26.	90			22.
100		.7591	18.	110		.7582	42.	100			38.
110		.7499	29.	120		.7504	66.	110			63.
120		.7404	45.	130.		.743	100	120			98.
130		.7304	69.	140			145.	130			150.
139.			100	149.			200	137.			200
140			102.	150			207.	140			220.
150			150.	160			286.	150			315.
158.			200	170			389.	157.			400
160			216.	171.			400	160			441.
170			305.	180			517.	170			601.
178.			400	190			674.	178.			760
180			426.	194.7			760				
190			585.								
198.5			760								

Constants	Temp. Range	A	B	C	E	Constants	Temp. Range	A	B	C	E	Constants	Temp. Range	A	B	C	E
Antoine eq	91 to 198 °C	9.0283	2900.	273.		Antoine eq	93 to 195 °C	6.3623	1113.	125.		Antoine eq	65 to 178 °C	6.630	1136.	125.	
Francis eq	0 to 130 °C	0.9472	4.141×10^{-4}	44.01	400	Francis eq	17 to 124 °C	0.9625	5.269×10^{-4}	86.3	700	Francis eq	0 to 65 °C	1.5574	-3.12×10^{-4}	505.9	700

TABLE 176. Isomeric Nonanols. Selected values. Physical properties of the liquid

2-Methyl-3-octanol			
Temp. °C	Refractive Index, n_D	Density g cm^{-3}	Vapor Pressure, mmHg
0		0.8448	
10		.8370	
20	1.431	.8289	
25	1.429	.8249	
30		.8275	
40		.8124	
50		.8039	
60		.7953	
70		.7864	
80		.7774	
90		.7682	
100		.7587	
110		.7490	67.
120		.7390	102.
130		.7289	149.
140		.7184	211.
150		.7077	293.
160		.697	397.
170			527.
180			687.
184.			760

Constants	Temp. Range	A	B	C	E
Antoine eq	115 to 180 °C	6.227	1034.	125.	
Francis eq	4 to 150 °C	1.1906	2.849×10^{-4}	242.1	700

3-Methyl-3-octanol			
Temp. °C	Refractive Index, n_D	Density g cm^{-3}	Vapor Pressure, mmHg
20	1.4324	0.8321	
25	1.4301	.8279	
30		.8237	
35	1.4256		
40		.8152	
50		.8068	
60		.798	5.
70			9.
80			16.
90			27.
100			43.
110			66.
120.			100

Constants	Temp. Range	A	B	C	E
Antoine eq	80 to 115 °C	6.0398	991.	125.	
Francis eq	20 to 55 °C	0.8490	8.43×10^{-4}		

4-Methyl-4-octanol			
Temp. °C	Refractive Index, n_D	Density g cm^{-3}	Vapor Pressure, mmHg
20	1.4320	0.8263	
25	1.4301	.8237	
30		.8206	
35	1.4256		
40		.8134	
50		.8045	
60		.794	

Constants	Temp. Range	A	B	C	E
Antoine eq					
Francis eq	20 to 55 °C	4.2194	-46.38×10^{-4}	2370.	700

TABLE 177. Isomeric Nonanols. Selected values. Physical properties of the liquid

2,2-Dimethyl-4-heptanol

Temp. °C	Refractive Index, n_D	Density g cm^{-3}	Vapor Pressure, mmHg
20	1.427		
25	1.425		
50			5.4
55			7.2
60			9.5
61.			10
65			12.
70			16.
75			21.
80			26.
85			33.
90			42.
95			52.
100			64.
105			78.
110			95.
111.			100
115			115.
120			139.
125			166.
130			199.
130.			200
135			236.
140			278.
145			327.
150			382.
151.			400
155			445.
160			516.
165			596.
170			686.
173.7			760
175			787.

Constants	Temp. Range	A	B	C	E
Antoine eq	47 to 172 °C	7.4780	1786.9	214.8	
Francis eq					

2,6-Dimethyl-4-heptanol

Temp. °C	Refractive Index, n_D	Density g cm^{-3}	Vapor Pressure, mmHg
10		0.8166	
20	1.4231	.8097	
25	1.4211	.8061	
30		.8025	
40		.7952	
50		.7876	
60		.7799	
70		.7719	
90			28.2
95			36.4
100			46.4
105			58.6
110			73.3
115			91.0
117.3			100
120			112.
125			136.
130			165.
135			199.
135.2			200
140			237.
145			281.
150			332.
155			389.
155.9			400
160			454.
165			527.
170			609.
175			700.
178.0			760
180			801.

Constants	Temp. Range	A	B	C	E
Antoine eq	90 to 180 °C	6.53806	1144.81	135.0	
Francis eq	20 to 60 °C	1.2595	0.434×10^{-4}	305.3	700

2,2,3-Trimethyl-3-hexanol

Temp. °C	Refractive Index, n_D	Density g cm^{-3}	Vapor Pressure, mmHg
20	1.4388	0.8464	
25	1.437	.842	
63.5			10
65			11.0
70			15.1
75			20.3
80			26.9
85			35.1
90			45.2
95			57.3
100			71.9
105			89.
107.8			100
110			109.
115			133.
120			160.
125			192.
126.2			200
130			227.
135			268.
140			312.
145			363.
148.3			400
150			419.
155			482.
160			550.
165			624.
170			707.
173.1			760
175			795.

Constants	Temp. Range	A	B	C	E
Antoine eq	70 to 171 °C	5.66401	755.9	98.6	
Francis eq					

TABLE 178. Isomeric Nonanols. Selected values. Physical properties of the liquid

2,4-Dimethyl-3-ethyl-3-pentanol

Temp. °C	Refractive Index, n_D	Density g cm^{-3}	Vapor Pressure, mmHg
20	1.4439	0.8588	
25	1.4416	.8543	
90			37.1
95			47.4
100			59.8
105			74.7
110			92.2
112.0			100
115			113.
120			136.
125			164.
130			195.
130.7			200
135			231.
140			271.
145			317.
150			367.
153.			400
155			423.
160			485.
165			553.
170			628.
175			710.
177.9			760
180			798.

Constants	Temp. Range	*A*	*B*	*C*	*E*
Antoine eq Francis eq	96 to 178 °C	5.7123	786.2	99.8	

2,2,3,4-Tetramethyl-3-pentanol

Temp. °C	Refractive Index, n_D	Density g cm^{-3}	Vapor Pressure, mmHg
15		0.861	
20	1.4428	.8565	
25	1.4405	.8523	
55			5.7
60			8.2
62.8			10
65			11.6
70			16.0
75			21.7
80			29.
85			28.
90			48.
95			61.
100			77.
150			95.
106.3			100
110			116.
115			140.
120			168.
125			199.
125.1			200
130			235.
135			275.
140			319.
145			368.
148.0			400
150			422.
155			482.
160			546.
165			616.
170			692.
174.2			760
175			774.

Constants	Temp. Range	*A*	*B*	*C*	*E*.
Antoine eq Francis eq	56 to 175 °C	5.32404	625.7	81.9	

Isomeric Nonanols

2-Nonanol, $C_9H_{20}O$, mol wt. 144.26, state at 25 °C liq

See also table 175

Investigators		Vapor Pressures and Boiling Points		Freezing Point	Density, *d* g cm^{-3}		Refractive Index, n_D	
		°C	mmHg	t_m, °C	20 °C	25 °C	20 °C	25 °C
Mannich	[1902]	193–194	760					
Houben	[1902]	193–194	760					
Power and Lees	[1902]	198–200	765					
Thomas and Mannich	[1903]	193–194	760					
van Gysegem	[1906]	197–198	747	−35 to − 36	0.84708		1.43533	
Henry	[1906b]	197.198	760					
Masson	[1909]	195–196	760					
Haller and Lassieur	[1910]	190–195	760			0.823		1.4233
Pickard and Kenyon	[1911]	105	19		.8230	.8202	1.4299	1.4279
Pickard and Kenyon	[1912]	193	760					
Malone and Reid	[1929]	198.2	760					
Ellis and Reid	[1932]	198.3	760			.81910		1.4290
Polgar and Robinson	[1945]	91	13					
Jasperson and Jones	[1947]	200	760				1.4333	
Selected value	[1967]	[e] 198.5±1. [e] 88.±2	760 10	[a] −35.±2.	[d] .8231 ±.0005	[d] .8195 ±.0005	[c] 1.4310 ±0.0010	[a] 1.4290 ±0.0010

Antoine constants: *A* 9.0283, *B* 2900., *C* 273. *dt/dp* at 760 mmHg, [e] 0.044 °C/mmHg

3-Nonanol, $C_9H_{20}O$, mol wt. 144.259, state at 25 °C liq

See also table 175

Investigators		Vapor Pressures and Boiling Points		Freezing Point	Density, *d* g cm^{-3}		Refractive Index, n_D	
		°C	mmHg	t_m, °C	20 °C	25 °C	20 °C	25 °C
Wagner	[1891]	194.5–195	760					
Gerard	[1907]			22–23				
Pickard and Kenyon	[1911]	118–121	65		0.8260		1.4308	
Pickard and Kenyon	[1913]	97	17		.8265		1.4308	
Tuot	[1936]	93	18		.8196		1.4289	
Zeiss and Tsutsui	[1953]	91–91.5	29					1.4286
Sparks and Knobloch	[1954]	94	13				1.4308	
Selected value	[1967]	[e] 194.7±0.5 [e] 83.±1.	760 10	[a] 22.±2.	[d] .8250 ±.001	[d] 0.8214 ±.001	[b] 1.431 ±0.002	[a,c] 1.429 ±0.002

Antoine constants: *A* 6.3623, *B* 1113, *C* 125. *dt/dp* at 760 mmHg, [e] 0.052 °C/mmHg

4-Nonanol, $C_9H_{20}O$, mol wt. 144.259, state at 25 °C liq

Investigators		Vapor Pressures and Boiling Points		Freezing Point	Density, *d* g cm^{-3}		Refractive Index, n_D	
		°C	mmHg	t_m, °C	20 °C	25 °C	20 °C	25 °C
Pexsters	[1906]	192–193	760				1.41971	
Zeiss and Tsutsui	[1953]	101–101.5	30					1.4275
Shuikin and Belskii	[1957]	191–192.5	750		0.8263		1.4292	
Selected value	[1967]	[e] 193.±1. [e] 81.±2.	760 10		[a] 0.826 ±0.002	[c] 0.822	[c] 1.4295 ±0.0020	[a] 1.4275 ±0.0010

Antoine constants: *A* 6.361, *B* 1105, *C* 125. *dt/dp* at 760 mmHg, [e] 0.05 °C/mmHg

Isomeric Nonanols—Continued

Investigators	Vapor Pressures and Boiling Points		Freezing Point	Density, *d* g cm^{-3}		Refractive Index, n_D	
	°C	mmHg	t_m, °C	20 °C	25 °C	20 °C	25 °C
5-Nonanol, $C_9H_{20}O$, mol wt. 144.259, state at 25 °C liq							
Henry [1906b]	193	760					
Malengreau [1906b]	193	766		0.823			
Eykman [1919]	92	14		.8212			
Vavon and Ivanoff [1923]	194	760		.821		1.4281	
Dillion and Lucas [1928]	77–79.5	10					
Vavon and Barbier [1931]	84	10					
Böeseken and Hanegraaff [1942]	190–194	760		.8360		1.4282	
Tuot and Guyard [1947]	103	27		.8257		1.4289	
Mears, Fookson, Pomerantz, Rich,	195.09	760					
Dussinger and Howard [1950]	145	150	+5.6	.8220	0.8183	1.4295	1.4267
Cook [1952]	133	100				1.4293 to 1.4297	
Protiva, Exner, Borovicka and Plimal [1952]	97–98	20					
Zeiss and Tsutsui [1953]	106–107	30					1.4295
Stapp and Rabjohn [1959]	90–92	20					1.4360
Landa and Markovec [1964]	116–117	15	24.0 to 24.2				
Selected value [1967]	^{e}195.1±0.2	760	^{a}+5.6 ±0.3	^{a}.8220	^{a}.8183	^{a}1.4295	^{a}1.4267
	^{e}89.1±1.	10		±0.0010	±.0010	±0.0010	±0.0010

Antoine constants: *A* 6.6791, *B* 1216, *C* 125. *dt/dp* at 760 mmHg, ^{e}0.048 °C/mmHg

Investigators	Vapor Pressures and Boiling Points		Freezing Point	Density, *d* g cm^{-3}		Refractive Index, n_D	
	°C	mmHg	t_m, °C	20 °C	25 °C	20 °C	25 °C
2-Methyl-1-octanol, $C_9H_{20}O$, mol wt. 144.259, state at 25 °C liq							
Bouveault and Blanc [1904b]	98–99	16		0.8289			
3-Methyl-1-octanol, $C_9H_{20}O$, mol wt. 144.259, state at 25 °C							
Levene and Marker [1931b]	110	25			0.826		1.4328
Polgar and Robinson [1945]	108	22				1.4346	
Selected value [1967]	^{f}95.±3.	10					
4-Methyl-1-octanol, $C_9H_{20}O$, mol wt. 144.259, state at 25 °C							
Levene and Marker [1931b]	106	17			0.822		1.4335
Cason, Brewer and Pippen [1948]	104–105	19					1.4328
Selected value [1967]						^{c}1.435 ±0.002	^{b}1.4331 ±0.0020
5-Methyl-1-octanol, $C_9H_{20}O$, mol wt. 144.259							
Levene and Marker [1933]	110	25			0.827		

Isomeric Nonanols—Continued

6-Methyl-1-octanol, $C_9H_{20}O$, mol wt. 144.259

Investigators		Vapor Pressures and Boiling Points		Freezing Point	Density, *d* g cm^{-3}		Refractive Index, n_D	
		°C	mmHg	t_m, °C	20 °C	25 °C	20 °C	25 °C
Levene and Marker	[1933]	100	20			0.829		
Milburn and Truter	[1954]	204–208	760					
Crombie, Manzoor-i-Khuda and Smith	[1957]	55	0.1				1.4360	
Selected value	[1967]	[e] 206. ±2.	760					
		[e] 85. ±2.	10					

Antoine constants: *A* 8.4407, *B* 2664, *C* 273. *dt/dp* at 760 mmHg, [e]0.049 °C/mmHg

7-Methyl-1-octanol, $C_9H_{20}O$, mol wt. 144.259

Investigators		Vapor Pressures and Boiling Points		Freezing Point	Density, *d* g cm^{-3}		Refractive Index, n_D	
		°C	mmHg	t_m, °C	20 °C	25 °C	20 °C	25 °C
Levene and Allen	[1916]	206.0	761			0.8260		
Mathers and Pro	[1954]							1.43160
Selected value	[1967]	[a] 206. ±1.	760					

2-Methyl-2-octanol, $C_9H_{20}O$, mol wt. 144.259

See also table 175

Investigators		Vapor Pressures and Boiling Points		Freezing Point	Density, *d* g cm^{-3}		Refractive Index, n_D	
		°C	mmHg	t_m, °C	20 °C	25 °C	20 °C	25 °C
Masson	[1901]	178	760					
Owen, Quayle, and Beavers	[1930]				0.8174	0.8134		
Southgate	[1934]	84	16					
Gredy	[1935]	80	12.5					
Whitmore and Orem	[1938]				.8210			1.4280
Whitmore and Southgate	[1938]	82–5	20				1.427	
Prevost and Singer	[1950]	82	15					
Urry, Stacey, Huyster, and Juveland	[1954]	66	8				1.4282	
Kornblum, Smiley, Ungnade, White, Taub, and Herbert	[1955]	65	2					
Tarasova, Taits, and Plate	[1956]	91–91.5	24		.8239		1.4281	
Herbertz	[1959]	80	12		.8935		1.43680	
Rabilloud	[1964]	85	13				1.4287	
Selected value	[1967]	[e] 178. ±1.	760		[d] .8198	[d] 0.8158	[b] 1.428	[c] 1.426
		[e] 77. ±2.	10		±.001	±0.001	±0.002	±0.002

Antoine constants: *A* 6.630, *B* 1136., *C* 125. *dt/dp* at 760 mmHg, [e]0.046 °C/mmHg

3-Methyl-2-octanol, $C_9H_{20}O$, mol wt. 144.259

Investigators		Vapor Pressures and Boiling Points		Freezing Point	Density, *d* g cm^{-3}		Refractive Index, n_D	
		°C	mmHg	t_m, °C	20 °C	25 °C	20 °C	25 °C
Powell, Murray and Baldwin	[1933]	75	15			0.833		1.438
Adams, Harfenist and Loewe	[1949]	85–87	7				1.4330	
Selected value	[1967]	[f] 80. ±3.	10				[a] 1.433	[c] 1.431
							±0.002	±0.003

5-Methyl-2-octanol, $C_9H_{20}O$, mol wt. 144.259

Investigators		Vapor Pressures and Boiling Points		Freezing Point	Density, *d* g cm^{-3}		Refractive Index, n_D	
		°C	mmHg	t_m, °C	20 °C	25 °C	20 °C	25 °C
Levene and Marker	[1931d]					0.821		

Isomeric Nonanols—Continued

Investigators		Vapor Pressures and Boiling Points		Freezing Point	Density, *d* g cm^{-3}		Refractive Index, n_D	
		°C	mmHg	t_m, °C	20 °C	25 °C	20 °C	25 °C
7-Methyl-2-octanol, $C_9H_{20}O$, mol wt. 144.259								
Heilborn, Jones and Weedon	[1944]	57	3				1.4309	
2-Methyl-3-octanol, $C_9H_{20}O$, mol wt. 144.259								
See also Table 176								
Pickard and Kenyon	[1912]	184	760		0.8270		1.4314	
George	[1943]	143.7	200		.8331		1.4286	
Ruof	[1948]	115	83				1.4320	
Nielsen and Ovist	[1954]	180–183	690					
Herbertz	[1959]	110	(?)					
Selected value	[1967]	[e] 184. ±2.	760		[d] 0.8289	[d] 0.8249	[b] 1.431	[c] 1.429
		[c] 73. ±3.	10		±.001	±.001	±0.002	±0.002
Antoine constants: *A* 6.227, *B* 1034., *C* 125.					*dt/dp* at 760 mmHg, [e]0.05 °C/mmHg			
3-Methyl-3-octanol, $C_9H_{20}O$, mol wt. 144.259								
See also table 176								
Davies, Dixon and Jones	[1930]	97.5	50			0.8108		1.4257
Whitmore and Williams	[1933]	80–81	15			.8258	1.4315	
Green	[1934]	36–37	3		0.8216			
Church, Whitmore and McGrew	[1934]	78–79	15				1.4323	
Quayle and Smart	[1944]					.8275	1.4324	1.4301
Cook	[1952]	115	83				1.4324	
Pomerantz, Fookson, Mears, Rothberg and Howard	[1954]				.8331		1.4298	
Rabjohn and Latina	[1954]	100–102	30				1.4321	
Sokolova, Shebanova and Shchepinov	[1961]	96	30		.8322		1.4340	
Selected value	[1967]	[e] 189. ±3.	760		[d] .8321	[d] 0.8279	[a] 1.4324	[a] 1.4301
		[e] 72. ±2.	10		±.001	±0.001	±0.001	±0.001
Antoine constants: *A* 6.0398, *B* 991., *C* 125.					*dt/dp* at 760 mmHg, 0.057[e] °C/mmHg			
4-Methyl-3-octanol, $C_9H_{20}O$, mol wt. 144.259								
Green	[1934]	132–133	20			0.8437		
Selected value	[1967]	[f] 122. ±3	10					
6-Methyl-3-octanol, $C_9H_{20}O$, mol wt. 144.259								
Powell and Baldwin	[1936]	81–83	15			0.8320		1.4372
Selected value	[1967]	[f] 76. ±3.	10					
7-Methyl-3-octanol, $C_9H_{20}O$, mol wt. 144.259								
Thoms and Kahre	[1925]	74–79	18		0.8338			

Isomeric Nonanols—Continued

Investigators	Vapor Pressures and Boiling Points		Freezing Point	Density, *d* g cm^{-3}		Refractive Index, n_D	
	°C	mmHg	t_m, °C	20 °C	25 °C	20 °C	25 °C
2-Methyl-4-Octanol, $C_9H_{20}O$, mol wt. 144.259							
Malengreau [1906b]	184	766		0.815			
Levene and Marker [1931f]	87	20					1.4258
Tuot [1936]	91	23		0.8130		1.4262	
Protiva, Exner, Borovicka and Pliml [1952]	60–67	4					
Dubois and Luft [1954b]	76–78	10			0.815		1.4263
				and		and	
					0.816		1.4257
Selected value [1967]	[e] 184.±1.	760		[c] 0.819	[a] 0.815	[c] 1.428	[b] 1.426
	[c] 77.±1.	10		±0.003	±0.002	±0.002	±0.002
Antoine constants: A 6.4225, *B* 1095., *C* 125.					***dt/dp* at 760 mmHg, [e]0.050 °C/mmHg**		
3-Methyl-4-octanol, $C_9H_{20}O$, mol wt. 144.259							
Vavon and Ivanoff [1923]	180	760		0.832		1.4317	
Vavon and Barbier [1931]	82	12					
Selected value [1967]	[c] 80.±2.	10					
4-Methyl-4-octanol, $C_9H_{20}O$, mol wt. 144.259							
See also table 176							
Woodburn [1931]	180	760					
Whitmore and Woodburn [1938]	178–179	732		0.8267	0.8237	1.4327	
Quayle and Smart [1944]					0.8252	1.4325	1.4301
Protiva, Exner, Borovicka, and Pliml [1952]	73–75	7					
Pomerantz, Fookson, Mears, Rothberg and Howard [1954]	113	50		.8284		1.4316	
Wynberg and Logothetis [1956]	178–180	740					1.4317
Yur'ev, Belyakova, and Volkov [1959]	70–72	10		.8227		1.4275	
Selected value [1967]	[c] 181.±2.	760		[d] .8263	[d] 0.8237	[b] 1.4320	[a] 1.4301
		10		±.002	±0.002	±0.001	±0.001
					***dt/dp* at 760 mmHg, [e]0.052 °C/mmHg**		
5-Methyl-4-octanol, $C_9H_{20}O$, mol wt. 144.259							
Bjelous [1912]	74–76	9			0.8156		1.42616
Selected value [1967]				[c] 0.820	[a] .816	[c] 1.428	[a] 1.4262
	[f] 76.±3.	10		±.003	±.002	±0.002	±0.0010
6-Methyl-4-octanol, $C_9H_{20}O$, mol wt. 114.259							
Levene and Marker [1931d]					.820		

Isomeric Nonanols—Continued

Investigators		Vapor Pressures and Boiling Points		Freezing Point	Density, *d* g cm^{-3}		Refractive Index, n_D	
		°C	mmHg	t_m, °C	20 °C	25 °C	20 °C	25 °C
7-Methyl-4-octanol, $C_9H_{20}O$, mol wt. 144.259								
Thoms and Kahre	[1925]	79–84	14					
Tuot	[1936]	89	18		0.8136		1.4260	
Selected value	[1967]	^{f}80.±3.	10					
2-Ethyl-1-heptanol, $C_9H_{20}O$, mol wt. 144.259								
Royals and Corington	[1955]	65–73	3				1.4320	
Selected value	[1967]	^{f}75.±5.	10					
3-Ethyl-1-heptanol, $C_9H_{20}O$, mol wt. 144.259								
Levene and Marker	[1931e]					0.832		
Paul and Tchelitcheff	[1956]	206–207	760					
Taylor, A. W. C.	[1958]	110–112	20					
Watanabe and Saga	[1963]	79–80	6					
Selected value	[1967]	^{e}207.±2. ^{e}89.±3.	760 10		^{c}0.836 ±0.003	^{a}0.832 ±0.002		
Antoine constants: *A* 8.6484, *B* 2769., *C* 273.						dt/dp at 760 mmHg, ^{e}0.048 °C/mmHg		
5-Ethyl-1-heptanol, $C_9H_{20}O$, mol wt. 144.259								
Colonge, Descotes and Soula	[1962]	109	30			0.848		1.4350
2,2-Dimethyl-1-heptanol, $C_9H_{20}O$, mol wt. 144.259								
Whitmore and Badertscher	[1933]	88–89	15				1.4339	
Brannock	[1959]	191.5 to 192	760				1.4336	
Selected value	[1967]	192.±2. ^{c}80.±3.	760 10				^{b}1.4338 ±0.0010	^{c}1.432 ±0.002
4,6-Dimethyl-1-heptanol, $C_9H_{20}O$, mol wt. 144.259								
Julia, Julia, Tchen and Graffin	[1961]	62	1				1.4323	
Julia, Julia, Tchen and Graffin	[1964]	63–64	1				1.4315	
Selected value	[1967]	^{f}72.±2.	10				^{b}1.432 ±0.001	^{c}1.430 ±0.002
6,6-Dimethyl-1-heptanol, $C_9H_{20}O$, mol wt. 144.259								
Gol'dfarb and Konstantinov	[1956]	86–88	12		0.8439		1.4430	
Selected value	[1967]	^{f}85.±3.	10					
2-Ethyl-2-heptanol, $C_9H_{20}O$, mol wt. 144.259								
Sparks and Kobloch	[1955]						1.4377	

Isomeric Nonanols—Continued

Investigators		Vapor Pressures and Boiling Points		Freezing Point	Density, d g cm^{-3}		Refractive Index, n_D	
		°C	mmHg	t_m, °C	20 °C	25 °C	20 °C	25 °C
3-Ethyl-2-heptanol, $C_9H_{20}O$, mol wt. 144.259								
Arcus and Smyth	[1955]	91–92	22				1.4308	
Selected value	[1967]	[f] 80.±3.	10					
2,3-Dimethyl-2-heptanol, $C_9H_{20}O$, mol wt. 144.259								
Nazarov and Torguv	[1948]	80–81	19				1.4404	
Selected value	[1967]	[f] 70.±2.	10					
2,4-Dimethyl-2-heptanol, $C_9H_{20}O$, mol wt. 144.259								
Levene and Marker	[1931]	134–136	?					
Colonge and Gaumont	[1959]	81	40			0.828		1.4290
2,5-Dimethyl-2-heptanol, $C_9H_{20}O$, mol wt. 144.259								
Levene and Marker	[1931a]	75	15		0.832			
2,6-Dimethyl-2-heptanol, $C_9H_{20}O$, mol wt. 144.259								
Pastureau and Zamenhot	[1926]	48	7		0.8186		1.4242	
Escourrou	[1928]	170–172	760		.8162 (10.5°)		1.42831 (10.5°)	
Selected value	[1967]	[c] 54±3.	10		[a] .819 ±0.003	[c] 0.815 ±0.003	[a] 1.424 ±0.002	[c] 1.422 ±0.002
4,6-Dimethyl-2-heptanol, $C_9H_{20}O$, mol wt. 144.259								
Guerbet	[1909]	194–195	760		0.8787 (0°C)			
Guerbet	[1912d]	194–195	760		0.8801 (0°C)			
Selected value	[1967]				[c] 0.863 ±0.010	[c] 0.859 ±0.010		
5,6-Dimethyl-2-heptanol, $C_9H_{20}O$, mol wt. 144.259								
Wallach	[1911]	191.5–192.5	760		0.833		1.4348	
Zeiss and Tsutsui	[1953]							1.4480
Selected value	[1967]						[c] 1.4501 ±0.010	[a] 1.4480 ±0.0010

Isomeric Nonanols—Continued

Investigators		Vapor Pressures and Boiling Points		Freezing Point	Density, d g cm^{-3}		Refractive Index, n_D	
		°C	mmHg	t_m, °C	20 °C	25 °C	20 °C	25 °C
3-Ethyl-3-heptanol, $C_9H_{20}O$, mol wt. 144.259								
Conant and Blatt	[1929]	116–118	105		0.8409		1.4360	
Whitmore and Woodburn	[1933]	180–180.5	733		0.8399	.8365	1.4362	
Church, Whitmore, and McGrew	[1934]	78–80	18				1.4362	
Whitmore and Southgate	[1938]	95.7	36					
Whitmore and Orem	[1938]				0.8429			1.4360
Selected value	[1967]	^{e}182.2±1.	760		^{b}0.841	^{a,c}0.837	^{b}1.436	1.434
		^{e}72.±2.	10		±0.002	±0.002	±0.002	±0.002
Antoine constants: *A* 6.2617, *B* 1039., *C* 125.					*dt/dp* at 760 mmHg, ^{e}0.052 °C/mmHg			
2,2-Dimethyl-3-heptanol, $C_9H_{20}O$, mol wt. 144.259								
Leroide	[1921]	76–79	16					
Whitmore, Popkin, Whitaker, Mattil,		71	15					
and Zech	[1938]	65.6–67	11				1.4329	
Whitmore	[1938]	71	15				1.4321	
		67	11					
Pedlow	[1940]	122	50					
Foley, Welch, LaCombe, and Mosher	[1959]	76	23			0.824	1.4320 (dl)	
Colonge and Lagier	[1949]	80–81	18		0.828		1.429	
Selected value	[1967]				^{a}0.828	^{a}0.824	^{b}1.433	^{c}1.431
		^{c}63.±2.	10		±0.003	±0.002	±0.002	±0.003
2,3-Dimethyl-3-heptanol, $C_9H_{20}O$, mol wt. 144.259								
Whitmore and Evers	[1933]	56–57	5		0.8395		1.4365	
Whitmore and Southgate	[1938]	75–78	16				1.4355	
Ruof	[1948]	106	60				1.4360	
Nazarov and Bakhmutskaya	[1950]	172–174	760		0.8349		1.4365	
Cook	[1952]	105	64				1.4362	
Selected value	[1967]	^{e}174.±2.	760		^{b}0.837	^{c}0.833	^{b}1.4361	^{c}1.434
		^{e}74.±2.	10		±0.003	±0.003	±0.0010	±0.002
Antoine constants: *A* 6.6261, *B* 1120., *C* 125.					*dt/dp* at 760 mmHg, ^{e}0.046 °C/mmHg			
2,6-Dimethyl-3-heptanol, $C_9H_{20}O$, mol wt. 144.259								
Michiels	[1912]	175	760		0.8212		1.42461	
Thoms and Kahre	[1925]	173–178	760					
Tuot	[1936]	88	25		0.8148		1.4275	
Selected value	[1967]	^{e}175.±2.	760		^{a}0.821	^{c}0.817	^{a}1.425	^{c}1.423
		^{e}73.±2.	10		±0.002	±0.003	±0.002	±0.002
Antoine constants: *A* 6.5122, *B* 1090., *C* 125.					*dt/dp* at 760 mmHg, ^{e}0.047 °C/mmHg			

Isomeric Nonanols—Continued

Investigators		Vapor Pressures and Boiling Points		Freezing Point	Density, d g cm^{-3}		Refractive Index, n_D	
		°C	mmHg	t_m, °C	20 °C	25 °C	20 °C	25 °C
3,5-Dimethyl-3-heptanol, $C_9H_{20}O$, mol wt. 144.259								
Davies, Dixon, and Jones	[1930]	95–97	50			0.8177		1.4251
Brokaw and Brode	[1948]	88.4–88.6	35					
Machinskaya and Barkhash	[1959]	49–51	15		0.824			1.4325
Thaker and Vasi	[1960]	70–82	20			.8237		1.428
Selected value	[1967]	[c] 40.±2.	10		[c] .824 ±.004	[b] .820 ±.004	[c] 1.431 ±0.003	[b] 1.429 ±0.003
3,6-Dimethyl-3-heptanol, $C_9H_{20}O$, mol wt. 144.259								
Konovalov, M.	[1904]				0.8253		1.4309	
Meyer and Tout	[1933]						1.4308	
Ruof	[1948]						1.4308	
Cook	[1952]						1.4308	
Selected value	[1967]						[b] 1.4308 ±0.0010	[c] 1.429 ±0.002
3-Ethyl-4-heptanol, $C_9H_{20}O$, mol wt. 144.259								
Zerner	[1911]	80–81	10					
4-Ethyl-4-heptanol, $C_9H_{20}O$, mol wt. 144.259								
Eykman	[1919]	78 61	14 2.5		0.8352			
Stas	[1926]				0.8337		1.4332	
Owen, Quayle, and Beavers	[1930]				0.8245			
Church, Whitmore, and McGrew	[1934]	76–78	17					
Cook	[1952]	178	734				1.4340	
Nazarov and Kakhniashvili	[1954a]	179–180	760		0.8364		1.433	
Selected value	[1967]	[e] 179.±1. [e] 73.±1.	760 10		[b] .835 ±0.002	[c] 0.831 ±0.003	[b] 1.4336 ±0.0010	[c] 1.432 ±0.002
Antoine constants: A 6.3684, B 1061., C 125.					dt/dp at 760 mmHg, [e] 0.050 °C/mmHg			
2,2-Dimethyl-4-heptanol, $C_9H_{20}O$, mol wt. 144.259, state at 25 °C								
Whitmore, Popkin, Whitaker, Matill, and Zech	[1938]	172 58–60 85	733 10 29				1.4220–1.4290 1.4300–1.4315 1.4260	
Whitmore, Whitaker, Mattil, and Popkin	[1938]	120–121	150				1.4270	
Whitmore and Forster	[1942]	47.5	5				1.4261–1.4278	
Ansell, Davis, Hancock, and Hickinbottom	[1955]	72	16				1.4281	
Selected value	[1967]	[e] 173.7±1. [e] 61.±2.	760 10				[b] 1.427 ±0.002	[c] 1.425 ±0.003
Antoine constants: A 7.47800, B 1786.9, C 214.8.					dt/dp at 760 mmHg, [e] 0.053 °C/mmHg			

Isomeric Nonanols—Continued

Investigators		Vapor Pressures and Boiling Points		Freezing Point	Density, d g cm^{-3}		Refractive Index, n_D	
		°C	mmHg	t_m, °C	20 °C	25 °C	20 °C	25 °C
2,4-Dimethyl-4-heptanol, $C_9H_{20}O$, mol wt. 144.259, state at 25 °C								
See also table 177								
Bodroux and Taboury	[1909a]	170–171	750		0.826		1.4310	
Meyer and Tuot	[1933]	75	19		.8215		1.4292	
Henze, Allen, and Leslie	[1942]	171.3–171.8	758		.8254		1.4298	
Ruof	[1948]						1.4300	
Cook	[1952]	101	60				1.4320	
Nazarov and Kakhniashvili	[1954a]	170–171	760		.8242		1.432	
Petrov and Zakharov	[1959]	67	6		.8242		1.4297	
Petrov, Zakharov, and Krasnova	[1959]	67	6		.8242		1.4297	
Selected value	[1967]	[e] 171.4±0.5 [e] 64.±1.	760 10		[b] 0.825 ±.003	[c] 0.821 ±0.003	[b] 1.430 ±.002	[c] 1.428 ±0.002

Antoine constants: A 6.2054, B 985., C 125. *dt/dp* at 760 mmHg, [e] 0.051 °C/mmHg

Investigators		°C	mmHg	t_m, °C	20 °C	25 °C	20 °C	25 °C
2,6-Dimethyl-4-heptanol, $C_9H_{20}O$, mol wt. 144.259, state at 25 °C liq.								
See also table 177								
Vavon	[1914]	174–175	760		0.809		1.423	
Wilcox and Brunel	[1916]	171.4–173.4	760					
Tuot	[1936]	79	15		.8114		1.4242	
Ipatieff and Haensel	[1942]	179	760				1.4238	
Stross, Gable, and Rounds	[1947]	178.02	760		.80969		1.42314	
Union Carbide Corporation	[1953]			−65	.8106			
Zeiss and Tsutsui	[1953]	91–91.5	25					1.4220
Union Carbide Corporation	[1955]	178.1	760					
Jadot and Braine	[1956]	173	760					
Union Carbide Corporation	[1958]			−65				
Selected value	[1967]	[e] 178.0±0.1 [e] 71.7±0.3	760 10	−65±1.	[d] 0.8097 ±0.0005	[d] 0.8061 ±0.0010	[a] 1.4231 ±0.0005	[c] 1.4211 ±0.0010

Antoine constants: A 6.53806, B 1144.81, C 135.0 *dt/dp* at 760 mmHg, [e] 0.0488 °C/mmHg

Investigators		°C	mmHg	t_m, °C	20 °C	25 °C	20 °C	25 °C
3,3-Dimethyl-4-heptanol, $C_9H_{20}O$, mol wt. 144.259								
Conant, Webb, and Mendum	[1929]	175–178	760					
3,5-Dimethyl-4-heptanol, $C_9H_{20}O$, mol wt. 144.259								
Vavon and Ivanoff	[1923]	171	760		0.834		1.4322	
Kopp	[1944]	100	48				1.4379	
Cook	[1952]	189–192	726				1.4270	
Levina, Shusherina, and Treschova	[1952]	185–187	755		0.8592		1.4283	
Selected value	[1967]	[e] 187.±2 [e] 70.±3.	760 10		[a] 0.859 ±0.005	[c] .855 ±0.005	[b] 1.428 ±0.002	[c] 1.426 ±0.003

Antoine constants: A 6.001, B 973., C 125. *dt/dp* at 760 mmHg, [e] 0.057 °C/mmHg

Isomeric Nonanols—Continued

Investigators		Vapor Pressures and Boiling Points		Freezing Point	Density, *d* g cm^{-3}		Refractive Index, n_D	
		°C	mmHg	t_m, °C	20 °C	25 °C	20 °C	25 °C
2-*n*-Propyl-1-hexanol, $C_9H_{20}O$, mol wt. 144.259								
Meakin, Mumford, and Ward	[1959]	103–104	22					1.4925
3-*n*-Propyl-1-hexanol, $C_9H_{20}O$, mol wt. 144.259								
Keil and Schiller	[1947]	106	18					
		92–94	8					
Fieser, Berliner, Bondhus, Chang, Dauben, Ettlinger, Fawaz, Fields, Heidelberger, Heymann, Vaughan, Wilson, Wilson, Wu, Leffler, Hamlin, Matson, Moore, Moore, and Zaugg	[1948]	84–85	9				1.4358	
2-Methyl-2-ethyl-1-hexanol, mol wt. 144.259								
Whitmore and Badertscher	[1933]	85.5–86	11				1.4401	
2-Methyl-3-ethyl-1-hexanol, $C_9H_{20}O$, mol wt. 144.259								
Nazarov and Kakhniashivili	[1954c]	192–194	760		0.8496		1.4455	
		56–57	3					
		191–192	760		.8512		1.4454	
		55–57	3					
Selected value	[1967]	[e] 192. ±2.	760		[b] .850	[c] 0.846	[a] 1.4454	[c] 1.443
		[e] 78. ±2.	10		±0.002	±0.002	±0.0020	±0.003

Antoine constants: *A* 8.6953, *B* 2704., *C* 273. *dt/dp* at 760 mmHg, [e] 0.046 °C/mmHg

Investigators		°C	mmHg	t_m, °C	20 °C	25 °C	20 °C	25 °C
3-Methyl-2-ethyl-1-hexanol, $C_9H_{20}O$, mol wt. 144.259								
Connor and Adkins	[1932]	83–86	10			0.8358		1.4356
4-Methyl-2-ethyl-1-hexanol, $C_9H_{20}O$, mol wt. 144.259								
Hagemeyer and Hudson	[1958]	195	760		0.8288		1.43313	
5-Methyl-2-ethyl-1-hexanol, $C_9H_{20}O$, mol wt. 144.259								
Connor and Adkins	[1932]	84–86	10			0.8208		1.4304
3,3,5-Trimethyl-1-hexanol, $C_9H_{20}O$, mol wt. 144.259								
Finch, Furman, and Ballard	[1951]	94.0–95.4	18				1.4345	
DuPont de Nemours, E. I., and Co.	[1951]	81	10					

Isomeric Nonanols—Continued

Investigators		Vapor Pressures and Boiling Points		Freezing Point	Density, *d* g cm^{-3}		Refractive Index, n_D	
		°C	mmHg	t_m, °C	20 °C	25 °C	20 °C	25 °C
3,4,4-Trimethyl-1-hexanol, $C_9H_{20}O$, mol wt. 144.259								
Freedman and Becker	[1951]	191	760					1.4308
3,5,5-Trimethyl-1-hexanol, $C_9H_{20}O$, mol wt. 144.259, state at 25 °C liq.								
Keulemans, Kwantes, and Van Bavel	[1948]	192.9	760					
Bruner	[1949]	193–194	760	< −70		0.8236		1.4300
Gutman and Hickinbottom	[1951]	85					1.4330	
Freedman and Becker	[1951]	191	760					1.4308
Turner and Turner	[1951]	192.7	759					1.4305
Gresham, Brooks, and Bruner	[1952]	190	760					1.4300
Selected value	[1967]	[e] 193.0±0.5	760		[c] 0.828	[a] 0.824	[c] 1.4320	[b] 1.4300
		[e] 83.±1.	10		±0.003	±0.003	±0.0020	±0.0010
Antoine constants: *A* 6.4606, *B* 1138., *C* 125.					*dt/dp* at 760 mmHg, [e] 0.05 °C/mmHg			
4,5,5-Trimethyl-1-hexanol, $C_9H_{20}O$, mol wt. 144.259								
Dean	[1954]	202–204	760				1.4406	
2-Methyl-3-ethyl-2-hexanol, $C_9H_{20}O$, mol wt. 144.259								
Nazarov and Kakhniashvili	[1954c]	177–178	760		0.8468		1.4401	
Skinner and Florentine	[1954]	71–75	14			0.8334		1.4331
Selected value	[1967]	[e] 65.±1.	10		[c] 0.837 ±0.002	[a] 0.8334 ±0.0010	[c] 1.435 ±0.002	[a] 1.4331 ±0.0010
Antoine constants: *A* 8.5183, *B* 2540., *C* 273.					*dt/dp* at 760 mmHg, [e] 0.046 °C/mmHg			
2,3,4-Trimethyl-2-hexanol, $C_9H_{20}O$, mol wt. 144.259								
Colonge	[1935a]	57–58	5		0.8313		1.4395	
2,4,4-Trimethyl-2-hexanol, $C_9H_{20}O$, mol wt. 144.259								
Mosher	[1940]	70	30		0.8475		1.4425	
2,4,5-Trimethyl-2-hexanol, $C_9H_{20}O$, mol wt. 144.259								
Lux	[1933]				0.8320			
Ruof	[1948]	102	83				1.4322	
2,5,5-Trimethyl-2-hexanol, $C_9H_{20}O$, mol wt. 144.259								
Botteron and Shulman	[1962b]	72–74	25				1.4260	

Isomeric Nonanols—Continued

Investigators		Vapor Pressures and Boiling Points		Freezing Point	Density, *d* g cm^{-3}		Refractive Index, n_D	
		°C	mmHg	t_m, °C	20 °C	25 °C	20 °C	25 °C
2-Methyl-3-ethyl-3-hexanol, $C_9H_{20}O$, mol wt. 144.259								
Stas	[1926]	176.5 to 177.5	755		0.8596		1.4398	
George	[1943]	182.3	734				1.4274 to 1.4282	
Skinner and Florentine	[1954]	66.5	13			0.8445		1.4369
Selected value	[1967]	[e] 184.1±0.5	760		[c] 0.849	[a] 0.8445	[c] 1.439	[a] 1.4369
		[e] 62.0±0.5	10		±0.002	±0.0010	±0.002	±0.0010
Antoine constants: *A* 5.7588, *B* 890., *C* 125.								*dt/dp* at 760 mmHg, [e] 0.061 °C/mmHg
2-Methyl-4-ethyl-3-hexanol, $C_9H_{20}O$, mol wt. 144.259								
George	[1943]				0.8275			
Warner	[1944]	87	30				1.4373	
3-Methyl-4-ethyl-3-hexanol, $C_9H_{20}O$, mol wt. 144.259								
Skinner and Florentine	[1954]	41	6			0.8994		1.4405
Selected value	[1967]	[f] 45.±2.	10					
4-Methyl-3-ethyl-3-hexanol, $C_9H_{20}O$, mol wt. 144.259								
Prelog and Zalan	[1944]	63–65	11		0.857			
Papa, Villani, and Ginsberg	[1954]	69–70	10					
Selected value	[1967]	[a] 69.±3.	10					
5-Methyl-3-ethyl-3-hexanol, $C_9H_{20}O$, mol wt. 144.259								
Masson	[1901]	172	760					
Halse	[1914]	171–172	760		0.8412		1.4318	
Selected value	[1967]	[b] 172.±2.	760					
2,2,3-Trimethyl-3-hexanol, $C_9H_{20}O$, mol wt. 144.259								
See also table 177								
Leroide	[1921]	170	760					
George	[1943]	171.1	728		0.8464		1.4390	
Ruof	[1948]	96	58		0.8485		1.4384	
Cook	[1952]	107	107				1.4394	
Petrov, Sushchinskii and Konoval'chikov	[1955]	87	55		0.8463		1.4370	
Maretina and Petrov	[1961]	68–73	16		0.8460		1.4382	
Selected value	[1967]	[e] 173.1±0.5	760		[b] 0.8464	[c] 0.842	[b] 1.4388	[c] 1.437
		[e] 63.5±0.5	10		±0.0020	±0.003	±0.0020	±0.003
Antoine constants: *A* 5.66401, *B* 755.9, *C* 98.6.								*dt/dp* at 760 mmHg, [e] 0.053 °C/mmHg

Isomeric Nonanols—Continued

Investigators		Vapor Pressures and Boiling Points		Freezing Point	Density, *d* g cm^{-3}		Refractive Index, n_D	
		°C	mmHg	t_m, °C	20 °C	25 °C	20 °C	25 °C
2,2,4-Trimethyl-3-hexanol, $C_9H_{20}O$, mol wt. 144.259								
Haller and Bauer	[1913]	169	760					
2,2,5-Trimethyl-3-hexanol, $C_9H_{20}O$, mol wt. 144.259, state at 25 °C liq. (*dl*)								
Whitmore, Meyer, Pedlow, and Popkin	[1938]	111–112	150				1.4299 to 1.4302	
Pedlow	[1940]						1.4301	
Whitmore and Forster	[1942]	74	23					
Foley, Welch, LaCombe and Mosher	[1959]	115–116	150	17(*dl*) 40 to 41(*d*)	0.789		1.4309	
Selected value	[1907]	[e] 160. ±3.	760	17. ± 1. (*dl*)			[b] 1.430	[c] 1.428
		[e] 58. ±2.	10	40. ± 1. (*d*)			±0.001	±0.002
Antoine constants: *A* 9.0040, *B* 2653., *C* 273.								*dt/dp* at 760 mmHg, [e] 0.040 °C/mmHg
2,3,4-Trimethyl-3-hexanol, $C_9H_{20}O$, mol wt. 144.259, state at 25°C								
Vaughan	[1944]	93	85				1.4410	
Cook	[1952]	113	104				1.4410	
Selected value	[1967]						[b] 1.4410	[c] 1.439
		[e] 49. ±2.	10				±0.0010	±0.0020
Antoine constants: *A* 8.651, *B* 2460., *C* 273.								
2,3,5-Trimethyl-3-hexanol, $C_9H_{20}O$, mol wt. 144.259								
Meyer and Tout	[1933]	72	21		0.8256		1.4321	
Shine and Turner	[1950]	45.3	3				1.4321	
Petrov, Zakharov and Krasnova	[1959]	52–54	7		.8312		1.4292	
Selected value	[1967]	[f] 61. ±2.	10		[b] .828 ±.003	[c] 0.824 ±0.004	[a] 1.432 ±0.002	[c] 1.430 ±0.002
2,4,4-Trimethyl-3-hexanol, $C_9H_{20}O$, mol wt. 144.259								
Haller and Bauer	[1913]	170–171	760					
Conant, Webb, and Mendum	[1929]	167–177	760					
Whitmore and Forster	[1942]	52–53	6.5				1.4395 to 1.4400	
Ruof	[1948]	112	100		0.8488			
Cook	[1952]	112	100				1.4387	
Selected value	[1967]	[e] 171. ±2.	760				[a] 1.4387	[c] 1.437
		[e] 62. ±2.	10				±0.0010	±0.0020
Antoine constants: *A* 8.6683, *B* 2568., *C* 273.								*dt/dp* at 760 mmHg, [e] 0.044 °C/mmHg

Isomeric Nonanols—Continued

Investigators		Vapor Pressures and Boiling Points		Freezing Point	Density, *d* g cm^{-3}		Refractive Index, n_D	
		°C	mmHg	t_m, °C	20 °C	25 °C	20 °C	25 °C
2,5,5-Trimethyl-3-hexanol, $C_9H_{20}O$, mol wt. 144.259								
Whitmore and Forster	[1942]	74.8	25		0.825		1.4286 to 1.4295	
		76.7	32				1.4283 to 1.4302	
Selected value	[1967]						^{b}1.429 ±0.002	^{c}1.427 ±0.003
3,4,4-Trimethyl-3-hexanol, $C_9H_{20}O$, mol wt. state at 25 °C liq.								
Konovalov, Miller, and Timchenho	[1906]	165–166	760		0.833		1.43367	
Mosher	[1940]	75	30	23.5			1.4466	
Cook	[1952]	75	30				1.4470	
Selected value	[1967]	^{e}166.±2.	760				^{a}1.4470 ±0.0010	^{c}1.445 ±0.002
		^{e}52.±2.	10					
Antoine constants: *A* 8.2778, *B* 2367., *C* 273.								*dt/dp* at 760 mmHg, ^{e}0.046 °C/mmHg
3,5,5-Trimethyl-3-hexanol, $C_9H_{20}O$, mol wt. 144.259								
Whitmore and Laughlin	[1933]	62–62.5	14				1.4340	
Whitmore, Popkin, Whitaker, Mattil, and Zech	[1938]	44	4				1.4335 to 1.4375	
Howard, Mears, Fookson, Pomerantz and Brooks	[1947]	71	25		0.8350		1.4352	
Selected value	[1967]				^{a}0.8350 ±0.0010	^{c}0.831 ±0.002	^{a}1.4352 ±0.0010	^{c}1.433 ±0.002
		^{c}57.±1.	10					
4-Methyl-2-*n*-propyl-1-pentanol, $C_9H_{20}O$, mol wt. 144.259								
Hagemeyer and Hudson	[1958]	192–192.5	760		0.82556		1.83120	
4-Methyl-2-isopropyl-1-pentanol, $C_9H_{20}O$, mol wt. 144.259								
Hagemeyer and Hudson	[1958]	187	760					
2,2-Dimethyl-3-ethyl-1-pentanol, $C_9H_{20}O$, mol wt. 144.259								
Gleim	[1941]	86	50				1.4325	
3,3-Diethyl-2-pentanol, $C_9H_{20}O$, mol wt. 144.259, state at 25 °C								
Zeiss and Tsutsui	[1953]	91.5	20					1.4480

Isomeric Nonanols—Continued

Investigators	Vapor Pressures and Boiling Points		Freezing Point	Density, d g cm^{-3}		Refractive Index, n_D	
	°C	mmHg	t_m, °C	20 °C	25 °C	20 °C	25 °C
2,4-Dimethyl-2-ethyl-1-pentanol, $C_9H_{20}O$, mol wt. 144.259							
Doering, Farber, Sprecher and Wiberg [1952]	187–189	760			0.837		1.4380
Brannock [1959]	186–188	760				1.4396	
Selected value [1967]	^{b}188.±2.	760				^{a}1.440 ±0.002	^{a}1.438 ±0.002
2,3-Dimethyl-3-ethyl-2-pentanol, $C_9H_{20}O$, mol wt. 144.259							
Laughlin [1933]	76	18				1.4472	
Selected value [1967]	^{f}69.±3.	10					
4,4-Dimethyl-3-ethyl-2-pentanol, $C_9H_{20}O$, mol wt. 144.259							
Mosher and Cox [1950]	90–92	10					1.4320
Ansell, Hancock, and Hickinbottom [1956]	66	12				1.4436	
2,3,3,4-Tetramethyl-2-pentanol, $C_9H_{20}O$, mol wt. 144.259							
Cook [1952]	93	47				1.4482	
2,3,4,4-Tetramethyl-2-pentanol, $C_9H_{20}O$, mol wt. 144.259							
Cook [1952]	110	90				1.4461	
3,3,4,4-Tetramethyl-2-pentanol, $C_9H_{20}O$, mol wt. 144.259, state at 25 °C crystal							
Locquin and Sung [1924]	179–180	746	50				
Selected value [1967]	^{c}180.±2.	760					
2,2-Dimethyl-3-ethyl-3-pentanol, $C_9H_{20}O$, mol wt. 144.259, state at 25 °C liq.							
Whitmore, Meyer, Pedlow, and Popkin [1938]	114.5	150		0.8524		1.4424	
Whitmore and Forster [1942]	84	40				1.4230	
Howard, Mears, Fookson, Pomerantz, and Brooks [1947]	174 94	760 50	−19.0	.8572	0.8526	1.4429	1.4405
Selected value [1967]	^{e}174.0±0.5 ^{e}58.1±0.5	760 10		^{a}.8572 ±.0010	^{a}0.8526 0.0010	^{a}1.4429 ±0.0010	^{a}1.4405 ±0.0010

Antoine constants: A 5.8503, B 888.0, C 125.

dt/dp at 760 mmHg, ^{e}0.058 °C/mmHg

Isomeric Nonanols—Continued

2,4-Dimethyl-3-ethyl-3-pentanol, $C_9H_{20}O$, mol wt. 144.259, state at 25 °C liq.

See also table 178

Investigators		Vapor Pressures and Boiling Points °C	mmHg	Freezing Point t_m, °C	Density, d g cm^{-3} 20 °C	25 °C	Refractive Index, n_D 20 °C	25 °C
Stas	[1926]	176–177	755		0.8610		1.4434	
Whitmore and George	[1942]	117.	125				1.4440	
George	[1943]	176.4	727		.8600		1.4441	
		109.6	90					
		103.5	70					
Huston and Auvapara	[1944]	176–177	750		.8485		1.4388	
Howard, Mears, Fookson, Pomerantz,		177.9	760					
and Brooks	[1947]	96	50	−16.0	.8588	0.8543	1.4439	1.4416
Smith and Creitz	[1951]	177.9	760	−16.0	0.8588		1.4439	
Selected value	[1967]	[e] 177.9±0.5	760	[a] −16.0±	[a] 0.8588	[a] 0.8543	[a] 1.4439	[a] 1.4416
		[e] 67.±1.	10	0.5	±0.0010	±0.0010	±0.0010	±0.0010

Antoine constants: *A* 5.7123, *B* 786.2, *C* 99.8

dt/dp at 760 mmHg, 0.0561 °C/mmHg

2,2,3,4-Tetramethyl-3-pentanol, $C_9H_{20}O$, mol wt. 144.259, state at 25 °C liq.

See also table 178

Investigators		Vapor Pressures and Boiling Points °C	mmHg	Freezing Point t_m, °C	Density, d g cm^{-3} 20 °C	25 °C	Refractive Index, n_D 20 °C	25 °C
Conant and Blatt	[1929]	56–57	6		0.8564		1.4430	
Whitmore and Laughlin	[1933]	62	12		.856		1.4440	
Nazarov	[1936]			+15	.8582		1.4483	
Whitmore, Whitaker, Mosher, Breivik,		185–191	736				1.4476	
Wheeler, Miner, Sutherland,								
Wagner, Clapper, Lewis, Lux, and								
and Popkin	[1941]							
Howard, Mears, Fookson, Pomerantz,		173.4	760	+12.8	0.8565	0.8523	1.4428	1.4405
and Brooks	[1947]	94	50					
Cadwallader, Fookson, Mears, and		175	760		0.8550		1.4397	
Howard	[1948]	111–112	128					
Cook	[1952]	90	50				1.4431	
Selected value	[1967]	[e] 174.2±0.5	760	[a] 12.8±0.5	[a] 0.8565	[a] 0.8523	[a] 1.4428	[a] 1.4405
		[e] 62.8±1.	10		±0.0020	±0.0020	±0.0020	±0.0020

Antoine constants: *A* 5.32404, *B* 625.7, *C* 81.9.

dt/dp at 760 mmHg, [e] 0.052 °C/mmHg

Isomeric Nonanols—Continued

Investigators		Vapor Pressures and Boiling Points		Freezing Point	Density, d g cm^{-3}		Refractive Index, n_D	
		°C	mmHg	t_m, °C	20 °C	25 °C	20 °C	25 °C
2,2,4,4-Tetramethyl-3-pentanol, $C_9H_{20}O$, mol wt. 144.259, state at 25 °C crystal								
Haller and Bauer	[1913]	165–166	760	50				
Willcox and Brunel	[1916]	171.4–173.4	760					
Vavon and Barbier	[1931]	165.5	760	51				
Whitmore and Stahly	[1933]	117–118	166	50–51				
Crooks	[1938]	165–167	760					
Whitmore	[1938]	163–166	760					
Greenwood, Whitmore, and Crooks	[1938]	163–166	737					
Enyeart	[1942]	89.5–90	50				1.4433	
Bartlett and Schneider	[1945]			50				
Zeiss and Tsutsui	[1953]			46–48				
Bartlett and Stiles	[1955]			46–48				
Hansley	[1956]	169.5	760	52.2				
Petrov, Sokolova, and Chin-Lan	[1957]	116	164	51				
Petrov, Kao, and Semenkin	[1960]	165–167	?	51–52				
Petrov, Sokolova, and Kao	[1960]	116	164	51–52				
Selected value	[1967]	[e] 167.±2. [e] 62.±2.	760 10	[b] 50.±2.			[a] 1.4433 ±0.002	[c] 1.441 ±0.003

Antoine constants: A 6.2314, B 980., C 125.

dt/dp at 760 mmHg, [e] 0.050 °C/mmHg

1-Decanol

Properties of the Liquid Phase at Various Temperatures

Refractive Index

Most of the refractive index data have been reported at the Na_D line and 20 °C. Even here, as can be seen in table 182, the values scatter over a range of about 0.004. The principal difficulty is in obtaining pure samples. The value selected at 20 °C was close to these measurements where some care was taken to insure purity. The two values at 25 °C differ considerably, and the selected value was obtained by applying the temperature coefficient obtained from data at other temperatures to the selected value at 20 °C. Rathmann, Curtis, McGeer, and Smyth [1956] reported values at 31 and 80 °C, and Weissler [1948] at 30 °C. The value of Rathmann et al. at 20 °C was a little lower than the selected value, and the values at other temperatures were taken from a straight line parallel to their data passing through the selected value. Refractive indices at other wavelengths have been reported by Talvitie [1927], Komppa and Talvitie [1932], and Vogel [1948]. The selected values in table 181 were taken from a plot of these data versus $1/(\lambda - 1000)^{1.6}$. They are very close to the values of Talvitie.

Density

The earliest significant measurement of density was by Krafft [1883], who reported values at 7, 20, and 98.7 °C. The apparent best values at 20 and 25 °C are by Béhal [1919], Talvitie [1927], Jones, Bowden, Yarnold, and Jones [1948], Cook [1952], and Blood and Hagemeyer [1964]. These are within 0.0005 g. cm^{-3} of the calculated ones. Most of the data at other temperatures are from Kuss [1955], who covered the range 20 to 85 °C, and Costello and Bowden [1958], from 20 to 280 °C. In the region of overlap the data of Kuss were about 0.003 to 0.004 g cm^{-1} higher than those of Costello and Bowden. The data of Kuss matched those of other investigators at low temperatures better than did those of Costello and Bowden. Kuss also determined the density as a function of pressure, with an upper limit ranging from 800 kg cm^{-2} at 25 °C to 1400 kg cm^{-2} at 80 °C. Rathmann, Curtis, McGeer and Smyth [1956] reported densities at 31 and 80 °C. Efremov [1966] has determined the saturated liquid and vapor densities from 20 °C to near the critical temperature. Because of the method used for measuring these densities, the values for the liquid are not as accurate as the other data in the low temperature range.

TABLE 179. 1-Decanol. Selected values. Physical and thermodynamic properties

Temp. °C	Refractive Index, n_D	Density g cm^{-3}	Vapor Pressure, mmHg
0		0.8431	
10		.8365	
20	1.4371	.8297	
25	1.4353	.8263	0.009
30	1.4335	.8229	0.015
40	1.4299	.8159	0.041
50	1.4263	.8089	0.10
60	1.4227	.8017	
70	1.4190	.7943	
80	1.4155	.7868	
90		.7792	
100		.7714	
110		.7635	7.7
114.6			10
115			10.2
120		.7553	13.4
125			17.3
130		.7470	22.2
135			28.2
140		.7385	35.5
145			44.3
150			54.8
155			67.4
160			82.3
165			99.8
165.1			100
170			120.2
175			144.
180			171.
184.5			200
185			203.
190			239.
195			280.
200			327.
205			380.
206.7			400
210			439.
215			506.
220			581.
225			664.
230			755.
230.2			760

Data For Phase Transitions

Initial	Final	Temp. °C	dt/dP deg mm^{-1}	Pressure mmHg	ΔH kcal mol^{-1}	$d\Delta H/dt$	ΔS	ΔC_p
						cal deg^{-1} mol^{-1}		
c	liq	6.9		760	9.0±2		32±6	
c	liq	6.9		0.0011				
liq	g	25	1050.	0.0091	18.6±0.5		62.4±1.5	
liq	g	230.2±0.5	0.0515	760	11.9±2		24±4	

Condensed Phase Heat Capacity

State	Temp. °C	C_p
		cal deg^{-1} mol^{-1}

Properties of the Saturated Real Gas

Temp. °C	H^r-H^0	S^r-S^0	$C_p{}^r-C_p{}^0$
	kcal mol^{-1}	cal deg^{-1} mol^{-1}	

Data for the Standard States at 25 °C

State	Heat of Combustion $\Delta H_c{}^0$ kcal mol^{-1}	Heat of Formation $\Delta H_f{}^0$ kcal mol^{-1}	Entropy S^0 cal deg^{-1} mol^{-1}	Gibbs Energy of Formation $\Delta G_f{}^0$ kcal mol^{-1}	Heat Capacity, C_p cal deg^{-1} mol^{-1}
liq	−1577.4±0.3	−114.6±0.3	102.9±1.6	−31.6±0.5	
g	−1596.0±0.5	−96.0±0.5	142.8±0.7	−24.9±0.6	59.1±0.5

Critical Constants

Temp. 427 °C, 700. K	Pressure atm	Density 0.264 g cm^{-3}

Constants in Vapor Pressure and Density Equation

Antoine Equation

Temp. Range	A	B	C
103 to 230 °C	6.92244	1472.01	133.98
25 to 52 °C	11.560	4055	273.2

Francis Equation

Temp. Range	A	$B\times10^3$	C	E
5 to 140 °C	1.01817	0.3668	105.03	600

TABLE 180. 1-Decanol. Selected values. Thermodynamic functions of the ideal gas at one atmosphere

Temperature K	Entropy S^0 cal deg^{-1} mol^{-1}	Heat Capacity C_p^0 cal deg^{-1} mol^{-1}	Enthalpy Function $(H^0-H^0_0)/T$ cal deg^{-1} mol^{-1}	Gibbs Energy Function $(G^0-H^0_0)/T$ cal deg^{-1} mol^{-1}	Heat of Formation ΔHf^0 kcal mol^{-1}	Gibbs Energy of Formation ΔGf^0 kcal mol^{-1}
0	0	0	0	0	−81.5	−81.5
273.15	137.81	55.44	36.00	−101.81	−95.0	−30.7
298.15	142.76	59.11	37.79	−104.97	−96.0	−24.9
300	143.09	59.41	37.90	−105.19	−96.1	−24.4
400	162.15	74.44	45.16	−116.99	−99.9	0.2
500	180.28	88.26	52.43	−127.85	−102.9	25.5
600	197.31	99.94	59.37	−137.94	−105.4	51.5
700	213.45	109.99	65.85	−147.60	−107.3	77.8
800	228.74	118.53	71.94	−156.80	−108.6	104.4
900	243.09	125.90	77.58	−165.51	−109.4	131.1
1000	256.71	132.24	82.70	−174.01	−109.9	157.8

Vapor Pressures and Boiling Points

Normal boiling points reported by various investigators scatter over about a three degree range. A selection of the better ones is given in table 182. The selected value, as calculated from the Antoine constants, is very close to the measured value of Stavely and Spice [1952] who applied considerable care in purifying their sample. In the range above one mm, there has been only one systematic study of the vapor pressure as a function of temperature. This was done by Rose, Papahronis, and Williams [1958] who determined the boiling points by an ebulliometric method from 104 to 188 °C. In addition Verkade and Coops [1927] reported the boiling point at 8 mm, Talvite [1927] reported the boiling point at 15.5 mm and Braun and Manz [1934] at 13 mm. These data, along with the normal boiling points underlined in the Index, determined the selected Antoine constants listed in tables 179 and 182.

TABLE 181. 1-Decanol. Selected values. Refractive index at various wavelengths at 20 °C

Symbol	Wavelength, Å	Refractive Index, n 20 °C
He_{red}	6678.2	1.4347
H_c	6562.8	1.4350
Na_D	5892.6	1.4371
Hg_e	5460.7	1.4389
He_{blue}	5015.7	1.4413
H_F	4861.3	1.4423
Hg_g	4358.3	1.4465
$H_{G'}$	4340.5	1.4466

Two sets of measurements of the vapor pressure in the low pressure range have been published. Spizzichino [1956] measured the vapor pressure from 7 to 42 °C by a static method, and Davies and Kybett [1965] measured the vapor pressure of the solid from −9 to 0 °C and of the liquid from 25 to 52 °C by the Knudsen effusion method. Davies and Kybett did not report the experimental measurements directly but gave the equations log P(mm Hg) = 18.490 − 6028/T for the solid and log P(mm Hg) = 11.560 − 4055/T for the liquid. The data of Spizzichino can be represented by the Antoine equation, log P(mm Hg) = 4.71835 − 776.34/(93.49 + t) to within about 2 percent for most of the pressures. The liquid vapor pressures calculated from the two equations agree fairly well at 10 °C, but diverge at increasing temperatures, so that at 50 °C the vapor pressure calculated from Spizzichino's data is about twice as large as that from Davies and Kybett. There is no obvious reason for this discrepancy, but similar results are found for several other alcohols. Although the effusion method is subject to large errors, the data of Davies and Kybett are considered more reliable because they used carefully purified samples and calibrated their apparatus with benzoic acid and benzophenone. Their equation gives a more reasonable heat of vaporization than does the one for Spizzichino's data. Therefore, the Antoine constants are taken from Davies and Kybett's equation. This cannot be considered to give reliable values outside their experimental range of temperature however.

Critical Properties

The only observed critical properties are the critical temperature and density of Efremov (1966). His observed critical temperature is 435 °C. Extrapolation of his surface tension measurements to zero predicts a critical temperature of 427°. Since his observed critical temperatures agree fairly well with such extrapolations for all the other alcohols except 1-nonanol, the lower temperature was selected. His value for the critical density was selected.

TABLE 182. 1-Decanol. Reported values. Simple physical properties

Investigators		Vapor Pressures and Boiling Points		Freezing Point	Density, *d* g cm^{-3}		Refractive Index, n_D	
		°C	mmHg	t_m, °C	20 °C	25 °C	20 °C	25 °C
1-Decanol, $C_{10}H_{22}O$, mol wt. 158.286, state at 25 °C liq.								
Krafft	[1883a]			7	0.8297			
Schultz	[1909]	231	760	6.5	.8300			
Behal	[1919]				.8297		1.43605	
Lecat	[1927]	232.9	760					
Talvite	[1927]	228	760				1.43719	
Verkade and Coops	[1927]			6.4				
Komppa and Talvite	[1932]	230–233	760				1.43719	
Meyer and Reid	[1933]			5.99				
Drake and Marvel	[1937]						1.4355	
Komarewsky and Coley	[1941a]	230.0–230.1	760				1.4379	
Muller	[1942]				.8305		1.4393	
Hoerr, Harwood, and Ralson	[1944]			6.88				
Vogel	[1948]	229	760		.8283			
Jones, Bowden, Yarnold, and Jones	[1948]					0.8263		
Newman, Underwood, and Renoll	[1949]						1.4373	
Pratt and Draper	[1949]						1.4352	
Baldacci	[1950]						1.4343	
Sackmann and Sauerwald	[1950]			4.7				
con Erichsen	[1952]	235.8–235.9	760		.8310		1.4375	
Cook	[1952]			6	.8297		1.4371	
Anderson and Smith	[1952]			5				
Stavely and Spice	[1952]	229.84	760		.8298			
McKenna, Tartar, and Lingafelter	[1953]	231.4	760					1.4360
Petrov, Sushchinshii, and Konovalchikov	[1955]				.8252		1.4322	
Kuss	[1955]				.8301	.8269		
Spizzichino	[1956]			6.5			1.4370	
Rathmann, Curtis, McGreer, and Smyth	[1956]						1.43670	
Costello and Bowden	[1958]	231	760	6.9	.8260			
Lin and Tuan	[1958]					.82882		1.4344
Blood and Hagemeyer	[1964]				.8300			
Davies and Kybett	[1965a]			6.2–6.7				
Rose, Papahronis, and Williams	[1958]	114.7	10.1					1.43529
Selected value	[1967]	230.2±0.5	760	6.9	.8297	.8263	1.4371	1.4353
		114.6±0.7	10	±0.5	±.0005	±.001	±0.001	±0.001

Antoine constants: *A* 6.92244, *B* 1472.01, *C* 133.98.

Solid-Liquid Phase Equilibria

Normal Melting Point and Triple Point

Table 182 shows the more reliable values for the melting point of 1-decanol. The "solidification point" of Spizzichino [1956] is found by direct observation, while the "triple point" is obtained from her vapor pressure curve. According to the data on this table, the true melting point is probably somewhere in the range from 6.5 to 6.9 °C, with something near the upper end more likely. The temperature at which the vapor pressure curves for the solid and liquid phases obtained by Davies and Kybett [1965] cross is 11.5 °C. However, this cannot be considered a reasonable estimate of the triple point.

Heat of Fusion

The only value available for the heat of fusion is calculated from the difference in heats of sublimation of the solid and heat of vaporization of the liquid, based on the vapor pressure curves of Davies and Kybett [1965]. Since the opportunities for introduction of errors into this calculation are many, the uncertainty in the result is large. The equilibrium vapor pressure at the triple point is 0.0012 mm Hg, as calculated from the equation of Davies and Kybett [1965] for the liquid, and 0.00093 mm Hg as calculated from their equation for the solid.

Properties of the Liquid at 25 °C

Absolute Entropy

There are no data for the heat capacity of the liquid. The entropy was derived from the selected entropy of the ideal gas, the heat of vaporization, and the vapor pressure at 25 °C.

Heat of Combustion

Two experimental determinations have been reported. When converted to modern units and standard state, the enthalpy of combustion obtained by Verkade and Coops [1927] is -1577.10 kcal mol^{-1}. The more recent value of Chao and Rossini [1965] is -1577.35 kcal mol^{-1}. This represents very good agreement, considering the estimated uncertainties in the data. The value of Chao and Rossini was adopted.

Vapor-Liquid Equilibrium at 25 °C

Vapor Pressure

Spizzichino's measurements predict 0.015 mm Hg, while Davies and Kybett [1965] give 0.0091 mm Hg. The latter figure was selected, for the reasons given in the section on Vapor Pressure and Boiling Point.

Heat of Vaporization

The only available values are those calculated from vapor pressure measurements. Results obtained in this way are shown in table 183. Two values have been obtained from the data of Spizzichino [1956]. One was given in the original article, and the other calculated from the Antoine constants fitted to these data as given in the section on Vapor Pressure and Boiling Point. The result calculated from the vapor pressure of Davies and Kybett [1965a] has been selected.

TABLE 183. 1-Decanol. Reported values. Heat of vaporization at 25 °C

Investigator	ΔH_v at 25 °C kcal mol^{-1}
Spizzichino [1956], as reported	20.3
Spizzichino [1956] from Antoine constants	22.5
Green [1960], from previous vapor pressure data	19.82
Davies and Kybett [1965]	18.6

Vapor-Liquid Equilibrium at the Normal Melting Point

The Heat of vaporization reported in table 179 was calculated from the Antoine constants given there, with the assumption that the second virial coefficient is -2.1 liters mol^{-1}. As a result of the uncertainty in the vapor pressure curve and in the behavior of the real gas, this result has only a very approximate significance.

Properties of the Ideal Gas State

The thermodynamic functions of the ideal gas shown on table 180 have been taken from Green [1961]. As described in the corresponding section for 1-pentanol, these were obtained by applying the methylene increment to data for the first three normal alkanols. This long extrapolation introduces considerable uncertainty into the final result. An error in the entropy at 800 K in the original paper has been corrected in the table. Chermin [1961] has also published tables of the ideal gas thermodynamic functions obtained in a similar manner. In the temperature range of 298 to 1000 K, the heat capacities and entropies in these two sets of tables agree to within about 0.5 cal deg^{-1} mol^{-1}.

Index to the Bibliography

Numbers refer to the Bibliography, page 1–389.

References to data used in the selection of refractive index, density, boiling point, vapor pressure, and melting point are in boldface type.

Numbers in parentheses refer to sources of reviews or theoretical calculations only.

Reference numbers under each property are listed in the order of date of publication.

Refractive Index
123, **1726**, 1113, 931, **449**, **926**, **1222**, **1856**, 1893, **1264**, **1420**, 75, **1865**, **338**, **1152**, 1364, **1460**, **1669**, **1067**, **1498**

Density at 20–30 °C Only
123, **1726**, 1113, **1222**, **1856**, **853**, 1810, 1682, **1865**, **338**, 1364, **1067**, **165**

Density at all Temperatures
953, **1581**, **1848**, **1893**, **1527**, **978**, 1460, **347**

Normal Boiling Point
950, 1008, 1580, 931, 1842, **926**, **1856**, **1007**, **1682**, 1152, **347**, **165**

Vapor Pressure and Boiling Points at Other Pressures
953, 1581, 123, **1848**, **1726**, 312, **1863**, 449, 1264, 1865, **978**, 1364, 1460, **1669**, 1067, 232, **1498**, **398**

Normal Melting Point
953, 1581, **1848**, **1169**, 64, 766, 2027, 1527, 338, 29, **1669**, 1736, 347, **389**

Heat of Combustion
1848, (1507), (626), 287, 288

Isomeric Decanols

As for the nonanols, no systematic study of the physical properties of the isomeric decanols, as a class, has been made. In fact, there have been few systematic studies even of a particular property of individual compounds. Data of any kind have been found for only about 22 percent of the 507 theoretically possible isomers of decanol. Reported values of the simple physical properties are given in the following unnumbered tables.

The only systematic measurement of vapor pressure as a function of temperature for this class of compounds has been reported by Union Carbide Corporation for 2-*n*-propyl-1-heptanol. Although they also reported the Antoine constants for this compound, they do not correspond to the values of vapor pressure listed. The Antoine constants given in table 186 have been adjusted to fit the data. Antoine constants for other isomeric decanols are based on scattered boiling point measurements collected from various sources. In a few cases all three constants could be evaluated by a least square calculation. The values of these constants, along with tables of vapor pressures calculated from them, are given in tables 184 through 187.Because of the large uncertainties in the experimental data, these Antoine constants are not reliable and have only limited value in interpolating vapor pressure values between the observed points. In some other cases the data were insufficient to determine the constant C and a value of 125 or 273 was assumed.

Refractive indices at 20 and 25 °C have been summarized in the unnumbered tables, and values at a few other temperatures are given in the numbered tables. Arndt, Barbour, Engels, Horn, and Sutton [1959] reported the refractive indices of 5-methyl-1-nonanol, 5-methyl-2-nonanol, 5-methyl-3-nonanol, 5-methyl-4-nonanol, and 2-*n*-butyl-1-hexanol at 30 °C. Baykut and Ozeris [1957] measured refractive indices of 2-, 3-, 4-, and 5-decanol at 70 °C. Quayle and Smart [1944] determined the refractive indices of carefully purified samples of 4-methyl-4-nonanol and 5-methyl-5-nonanol at 20, 25, and 30 °C. Thaker and Vasi [1960] reported a value for 4, 6-dimethyl-4-octanol at 30 °C, and Carson, Brewer, and Pippen [1948] reported a value for 4-methyl-1-nonanol at 30 °C. The only measurements at wavelengths other than the sodium D-line have been made by Eykman [1919], who listed values throughout the visible range for 4-*n*-propyl-4-heptanol at 17.2 °C.

Reported and selected values of density at 20 and 25 °C are given in the unnumbered tables. In addition there have been a few measurements of densities at other temperatures. Pickard and Kenyon [1912] and [1913] measured the densities of 3-decanol and 2-methyl-3-nonanol from about 10 to 150 °C. Owen, Quayle, and Beavers [1930] reported the density of 3-methyl-3-nonanol from 0 to 65 °C, and Quayle and Smart [1944] reported densities of 4-methyl-4-nonanol and 5-methyl-5-nonanol from 25 to 55 °C. Kuss [1955] measured the density of 8-methyl-2-nonanol over the temperature range of 20 to 85 °C and also at pressures up to 2000 kg cm^{-2}. Stas [1926] measured the density of 2,4-dimethyl-3-*n*-propyl-3-pentanol from 0 to 30 °C. A few additional measurements at temperatures below 20 °C have been reported by Guerbet [1912a], Grignard, V. [1904b], and Freylon [1910].

No other physical or thermodynamic properties have been located for the isomeric decanols.

Index to the Bibliography

References to the Properties of 2-Decanol

Numbers refer to the Bibliography, page 1–389.

References to data used in the selection of refractive index, density, boiling point, vapor pressure, and melting point are in bold face type.

Numbers in parentheses refer to sources of reviews or theoretical calculations only.

Reference numbers under each property are listed in the order of date of publication.

Refractive Index
1378, 732, 1431, 1264, 1824, 1825, 2016, 111, 52, 942

Density at 20–30 °C Only
942, 52

Density at all Temperatures
1378, 1380

Normal Boiling Point
1378, 1380, 732, 1431

Vapor Pressure and Boiling Points at Other Pressures
1431, 1264, 2016, 1825, 1824, 52

Normal Melting Point
1431, 111, 52

TABLE 184. Isomeric Decanols. Selected values. Physical properties of the liquid

2-Decanol				3-Decanol				8-Methyl-2-nonanol			
Temp. °C	Refractive Index, n_D	Density g cm^{-3}	Vapor Pressure, mmHg	Temp. °C	Refractive Index, n_D	Density g cm^{-3}	Vapor Pressure, mmHg	Temp. °C	Refractive Index, n_D	Density g cm^{-3}	Vapor Pressure, mmHg
10		0.8328		10		0.8337		20		0.8252	
20	1.434	.8254		20	1.434	.8266		25		.8211	
25	1.432	.8216		25	1.432	.8230		30		.8170	
30		.8178		30		.8193		40		.8089	
40		.8102		40		.8119		50		.8007	
50		.8025		50		.8043		60		.7926	
60		.7947		60		.7965		70		.7844	
70	1.412	.7868		70	1.410	.7886		80		.7763	
80		.7787		80		.7804		90		.7681	
90		.7607		90		.7721					
100		.7624	8.3	100		.7635					
104.			10	105.			10				
110		.7541	13.9	110		.7547					
120		.7456	22.7	120		.7457					
130		.7370	36.	130		.7364					
140		.7283	57.	140		.7270					
150		.7194	86.								
154.			100								
160		.710	129.								
170			190.								
171.			200								
180			275.								
190			392.								
200			549.								
209.7			760								

Constants	Temp. Range	*A*	*B*	*C*	*E*	Constants	Temp. Range	*A*	*B*	*C*	*E*	Constants	Temp. Range	*A*	*B*	*C*	*E*
Antoine eq		9.5348	3214.	273.		Antoine eq						Antoine eq					
Francis eq		1.02397	4.712×10^{-4}	128.64	700	Francis eq		1.1791	2.083×10^{-4}	236.9	700	Francis eq		0.8415	8.152×10^{-4}		

Table 185. Isomeric Decanols. Selected values. Physical properties of the liquid

2-Methyl-3-nonanol				3-Methyl-3-nonanol				4-Methyl-4-nonanol			
Temp. °C	Refractive Index, n_D	Density g cm^{-3}	Vapor Pressure, mmHg	Temp. °C	Refractive Index, n_D	Density g cm^{-3}	Vapor Pressure, mmHg	Temp. °C	Refractive Index, n_D	Density g cm^{-3}	Vapor Pressure, mmHg
0		0.8435		0		0.8475		20	1.4350	0.8297	
10		.8362		10		.8392		25	1.4332	.8259	
20	1.4343	.8287		20	1.438	.8309		30	1.4310	.8220	
25	1.4320	.8249		25	1.436	.8267		40	1.427	.8143	
30		.8211		30		.8226		50		.8067	
40		.8133		40		.8142		60		.7990	
50		.8053		50		.8059		80.			10
60		.7971		60		.7976					
70		.7888		70		.7893					
80		.7802		86.			10				
90		.7715									
100		.7625									
110		.7533									
120		.7439									
130		.7341									
140		.7242									
143.			100								
150		.7139	129.								
160		.7033	184.								
162.			200								
170			256.								
180			349.								
185.			400								
190			466.								
200			611.								
208.6			760								
210			788.								

Constants	Temp. Range	*A*	*B*	*C*	*E*	Constants	Temp. Range	*A*	*B*	*C*	*E*	Constants	Temp. Range	*A*	*B*	*C*	*E*
Antoine eq		6.4934	1205.	125.		Antoine eq						Antoine eq					
Francis eq		1.2003	2.154×10^{-4}	249.7	700	Francis eq		0.8475	8.323×10^{-4}			Francis eq		0.8450	7.681×10^{-4}		

Table 186. Isomeric decanols. Selected values. Physical properties of the liquid

5-Methyl-5-nonanol			
Temp. °C	Refractive Index, n_D	Density g cm^{-3}	Vapor Pressure, mmHg
20	1.4350	0.8297	
25	1.4326	.8256	
30	1.4303	.8216	
40	1.426	.8135	
50		.8054	
60		.7973	
85.			10

Constants	Temp. Range	A	B	C	E
Antoine eq					
Francis eq		0.8459	8.103×10^{-4}		

2-*n*-Propyl-1-heptanol			
Temp. °C	Refractive Index, n_D	Density g cm^{-3}	Vapor Pressure, mmHg
20	1.4370	0.8322	
25	1.436		
103.			10
105			11.1
110			14.5
115			18.8
120			24.1
125			30.5
130			38.
135			48.
140			59.
145			73.
150			89.
153.			100
155			107.
160			129.
165			154.
170			184.
172.			200
175			217.
180			256.
185			300.
190			349.
195.			400
200			468.
205			538.
210			616.
215			704.
217.9			760
220			801.

Constants	Temp. Range	A	B	C	E
Antoine eq		6.8998	1448.6	142.5	
Francis eq					

4-*n*-Propyl-4-heptanol			
Temp. °C	Refractive Index, n_D	Density g cm^{-3}	Vapor Pressure, mmHg
0		0.8496	
10		.7638	
20	1.435	.8324	
25	1.433	.8281	
30		.8316	
40		.8153	
50		.8067	
60		.7981	
70		.7896	
81.			10
85			13.3
90			18.2
95			24.4
100			32.2
105			42.
110			53.
115			67.
120			83.
125.			100
130			124.
135			149.
140			177.
144.			200
145			209.
150			245.
155			285.
160			329.
165			378.
167.			400
170			431.
175			489.
180			552.
185			620.
190			693.
194.3			760
195			771.

Constants	Temp. Range	A	B	C	E
Antoine eq		5.2052	590.2	59.6	
Francis eq		0.8496	8.573×10^{-4}		

TABLE 187. Isomeric Decanols. Selected values. Physical properties of the liquid

2-*n*-Butyl-1-hexanol

Temp. °C	Refractive Index, n_D	Density g cm^{-3}	Vapor Pressure, mmHg
20	1.436		
25	1.434		
106.			10
110			15.7
115			24.3
120			36.
125			50.
130			67.
135			87.
138.			100
140			110.
145			136.
150			165.
156.			200
160			231.
170			300.
180			390.
181.			400
190			481.
200			577.
210			678.
218.			760

Constants	Temp. Range	*A*	*B*	*C*	*E*
Antoine eq		3.9268	183.0	−43.	
Francis eq					

2,4-Dimethyl-3-*n*-propyl-3-pentanol

Temp. °C	Refractive Index, n_D	Density g cm^{-3}	Vapor Pressure, mmHg
0		0.8689	
10		.8621	
20	1.444	.8552	
25	1.442	.8518	
30		.8484	
66.			10
80			18.
90			28.
100			41.
110			61.
120			89.
123.			100
130			127.
140			181.
143.			200
150			253.
160			351.
164.			400
170			482.
180			654
185.			760

Constants	Temp. Range	*A*	*B*	*C*	*E*
Antoine eq		10.9478	5058.	442.	
Francis eq		0.8689	6.81×10^{-4}		

2,4-Dimethyl-3-isopropyl-3-pentanol

Temp. °C	Refractive Index, n_D	Density g cm^{-3}	Vapor Pressure, mmHg
20	1.4480	0.8632	
25	1.4458	.8591	
74.			10
75			10.7
80			13.9
85			18.0
90			23.
95			29.
100			36.
105			45.
110			56.
115			68.
120			83.
125			100.
130			120.
135			142.
140			168.
145			197.
150			231.
155			268.
160			311.
165			358.
169.			400
170			411.
175			470.
180			534.
185			606.
190			684.
194.4			760
195			770.

Constants	Temp. Range	*A*	*B*	*C*	*E*
Antoine eq		6.3781	1206.	150.4	
Francis eq					

Table 188. Isomeric Decanols. Selected values. Physical properties of the liquid

2,2,3,4,4-Pentamethyl-3-pentanol

Temp. °C	Refractive Index, n_D	Density g cm^{-3}	Vapor Pressure, mmHg
70			10
80			17.
90			28.
100			44.
110			66.
120			96.
121.			100
130			135.
140			187.
142.			200
150			252.
160			332.
167.			400
170			431.
180			549.
190			688.
194.6			760

Constants	Temp. Range	*A*	*B*	*C*	*E*
Antoine eq		5.8559	956.5	126.9	
Francis eq					

Isomeric Decanols

Investigators	Vapor Pressures and Boiling Points		Freezing Point	Density, *d* g cm^{-3}		Refractive Index, n_D	
	°C	mmHg	t_m, °C	20 °C	25 °C	20 °C	25 °C
2-Decanol, $C_{10}H_{22}O$, mol wt. 158.29, State at 25 °C liq.							
See also table 184							
Pickard and Kenyon [1911]	210–211	760		0.8250	0.8214	1.4344	
Pickard and Kenyon [1912]	210	760					
Heilbron, Jones, and Raphael [1934]	209	760					1.4328
Prout, Cason, and Ingersoll [1948]	122	28	−2.4				1.4327
	124–126	31					
	127–129	35					
Newman, Underwood, and Renoll [1949]	104.5–106	13				1.4340	1.4320
Zeiss and Tsutsui [1953]	125–126	29					1.4334
Urry, Stacey, Juveland, and McDonnell [1953]	52–54	1				1.4357	
Urry, Stacey, Huyser and Juveland [1954]	30–33	.2–.3				1.4358	
Baykut and Ozeris [1957]			−2 to 0			1.4120	
Asinger, Geiseler, and Schmiedel [1959]	108	13	−1.7	0.8249		1.4346	
Kromer and Petrov [1960]	95–97	10		0.8256		1.4330	
Selected value [1967]	[e] 209.7±1.	760	[b] −2.±1.	[d] 0.8254 ±0.0005	[d] 0.8216 ±0.0005	[b] 1.434 ±0.002	[b] 1.432 ±0.002
	[e] 104.±2.	10					

Antoine constants: *A* 9.5348, *B* 3214., *C* 273.

dt/*dp* at 760 mmHg, [e] 0.041 °C/mmHg

Isomeric Decanols—Continued

Investigators		Vapor Pressures and Boiling Points		Freezing Point	Density, d g cm^{-3}		Refractive Index, n_D	
		°C	mmHg	t_m, °C	20 °C	25 °C	20 °C	25 °C
3-Decanol, $C_{10}H_{22}O$, mol wt. 158.286, state at 25 °C liq.								
See also table 184								
Pickard and Kenyon	[1913]	**108**	15		**0.8272**		**1.4336**	
Woods and Lederle	[1951]	**105–107**	13				1.4348	
Zeiss and Tsutsui	[1953]	105–105.5	45					**1.4325**
Baykut and Ozeris	[1957]			−4 to −2.5			1.4100	
Asinger, Geiseler, and Schmiedel	[1959]	**101**	12	−7.5	0.8266		1.4348	
Selected value	[1967]				[d] 0.8266	[d] 0.8230	[a] 1.434	[a] 1.432
		[c] 105.±3.	10	[f] −5.±3.	±0.0005	±0.0005	±0.002	±0.002
4-Decanol, $C_{10}H_{22}O$, mol wt. 158.286, state at 25 °C liq.								
Wagner, G.	[1891]	**210**	759					
Heilbron, Jones, and Raphael	[1943]	71	1				1.4316	
Zeiss and Tsutsui	[1953]	**116.5 to 117**	30					1.4340
Petrov, Nefedov, and Grigor'ev	[1957]	96	13		0.8262		1.4320	
Baykut and Ozeris	[1957]	67	1	−11.2 to −8.8				
Asinger, Geiseler, and Schmiedel	[1959]	**101**	12	**−11.6**	**0.8238**		1.4334	
Selected value	[1967]	[e] 210.±1.	760	−11.4	[a] 0.824	[c] 0.820	[a] 1.4334	[c] 1.431
		[e] 98.±1.	10	±0.5	±0.002	±0.003	±0.0010	±0.002
Antoine constants: *A* 6.6163, *B* 1252., *C* 125.								*dt/dp* at 760 mmHg, [e] 0.051 °C/mmHg
5-Decanol, $C_{10}H_{22}O$, mol wt. 158.286, state at 25 °C liq.								
Woods and Lederle	[1951]	**118–120**	30					1.4329
Protiva, Exner, Borovicka, and Pliml	[1952]	95–97	3					
Zeiss and Tsutsui	[1953]	117–118	31					**1.4310**
Franzen	[1954b]	**98**	8				1.4320	
Goldfarb and Konstantinov	[1956]	**111–113**	27		0.82766			1.4335
Baykut and Ozeris	[1957]			8 to 9				
Asinger, Geiseler, and Schmiedel	[1959]	99	11	8.7	**0.8238**		1.4333	
Selected value	[1967]	[e] 201.±3.	760	8.7±0.5	[a] 0.824	[c] 0.820	[a] 1.4333	[a] 1.431
		[e] 98.±2.	10		±0.002	±0.003	±0.0010	±0.002
Antoine constants: *A* 6.9317, *B* 1320., *C* 125.								*dt/dp* at 760 mmHg, [e] 0.046 °C/mmHg
2-Methyl-1-nonanol, $C_{10}H_{22}O$, mol wt. 158.286								
Guerbet	[1902]	**221–223**	760					
Levene and Mikeska	[1929]	80–82	0.4					
Selected value	[1967]	[a] 222.±2.	760					

Isomeric Decanols—Continued

Investigators		Vapor Pressures and Boiling Points		Freezing Point	Density, d g cm^{-3}		Refractive Index, n_D	
		°C	mmHg	t_m, °C	20 °C	25 °C	20 °C	25 °C
3-Methyl-1-nonanol, $C_{10}H_{22}O$, mol wt. 158.286								
Bouveault and Blanc	[1903]	114–116	14					
Levene and Taylor	[1922b]	103–103.5	9		0.8342		1.4361	
Levene and Marker	[1931b]	122	24			0.835		1.4348
Cymerman, Heilbron, and Jones	[1944]	121–121.5	24				1.4368	
Polgar and Robinson	[1945]	117–118	14					
Cason, Pippen, Taylor, and Winans	[1950]	108–109	11					
Legoff, Ulrich, and Denney	[1958]	88–89	2.5–3.0		0.829		1.4372	
Landa and Markovec	[1964]	115–117	19				1.4372	
Selected value	[1967]	[e] 105.±1.	10		[a] 0.834 ±0.002	[c] 0.830 ±0.003	[a] 1.437 ±0.002	[a,c] 1.435 ±0.002
4-Methyl-1-nonanol, $C_{10}H_{22}O$, mol wt. 158.286								
Levene and Marker	[1931b]	120	17			0.828		1.4364
Cason, Brewer, and Pippen	[1948]	111–112	14				1.4333 (30°C)	
		115–116	17					1.4358
Selected value	[1967]	[f] 110.±3.	10		[c] 0.832 ±.003	[a,c] .828 ±.002	[c] 1.438 ±0.003	[a] 1.436 ±0.002
5-Methyl-1-nonanol, $C_{10}H_{22}O$, mol wt. 158.286								
Levene and Marker	[1933]	125	25			0.830		
Arndt, Barbour, Engles, Horn, and Sutton	[1959]						1.4340 (30°C)	
Selected value	[1967]	[f] 110.±3.	10				[c] 1.438 ±0.003	[a,c] 1.436 ±0.002
7-Methyl-1-nonanol, $C_{10}H_{22}O$, mol wt. 158.286								
Kuss	[1956]					0.8211		
Lardicci, Salvadori, and Pino	[1962]	115–116	16			.8282		1.4361
Selected value	[1967]	[f] 110.±2.	10		[c] 0.824 ±0.003	[a] .828 ±.002		
8-Methyl-1-nonanol, $C_{10}H_{22}O$, mol wt. 158.286								
Milburn and Truter	[1954]	110–111	11.5				1.4352	
Selected value	[1967]	[f] 108.±2.	10					
2-Methyl-2-nonanol, $C_{10}H_{22}O$, mol wt. 158.286								
Houben	[1902]	96–98	13.5					
Prevost and Singer	[1950]	104	25					
Oliver	[1961]	101.0 to 101.8	21.6				1.4320	
Selected value	[1967]	[c] 91.±3.	10					

Isomeric Decanols—Continued

Investigators		Vapor Pressures and Boiling Points		Freezing Point	Density, *d* g cm^{-3}		Refractive Index, n_D	
		°C	mmHg	t_m, °C	20 °C	25 °C	20 °C	25 °C
3-Methyl-2-nonanol, $C_{10}H_{22}O$, mol wt. 158.286, state at 25 °C								
Gredy	[1935]	94.5–95	20		0.847			1.424
Petrov, Nefedov, and Grigor'ev	[1957]	86–88	8		0.8353		1.4386	
Selected value	[1967]	[c] 90.±2.	10		[a] 0.835 ±0.010	[c] 0.831 ±0.010	[a] 1.438 ±0.010	[c] 1.436 ±0.010
5-Methyl-2-nonanol, $C_{10}H_{22}O$, mol wt. 158.286								
Arndt, Barbour, Engels, Horn, and Sutton	[1959]	*202 to 202.1*	655					1.4320
6-Methyl-2-nonanol, $C_{10}H_{22}O$, mol wt. 158.286								
Shvarts and Petrov	[1961]	96–97.5	12		0.8332		1.4408	
Selected value	[1967]	[f] 95.±2.	10					
7-Methyl-2-nonanol, $C_{10}H_{22}O$, mol wt. 158.286								
Heilbron, Johnson, Jones, and Raphael	[1943]	93	4				1.4322	
8-Methyl-2-nonanol, $C_{10}H_{22}O$, mol wt. 158.286								
See also table 184								
Kuss	[1955]				0.8251	0.8211		
Selected value	[1967]				[d] .8252 ±.0005	[d] .8211 ±0.0005		
2-Methyl-3-nonanol, $C_{10}H_{22}O$, mol wt. 158.286								
See also table 185								
Pickard and Kenyon	[1912]	200	760		0.8290			1.4346
Petrov and Ol'dekop	[1948]	194–195	737		.8287		1.435	
Mears, Fookson, Pomerantz, Rich, Dussinger, and Howard	[1950]	**208.4** 154	760 150		**.8281**	0.8245	1.4343	1.4320
Selected value	[1967]	[e] 208.6±0.2 [c] 94.4±0.5	760 10		[d] .8287 ±.0005	[d] .8249 ±.0005	[a] 1.4343 ±0.0005	[a] 1.4320 ±0.0005

Antoine constants; *A* 6.4934, *B* 1205., *C* 125.

dt/dp at 760 mmHg, [e] 0.0527 °C/mmHg

Isomeric Decanols—Continued

Investigators	Vapor Pressures and Boiling Points		Freezing Point	Density, d g cm^{-3}		Refractive Index, n_D	
	°C	mmHg	t_m, °C	20 °C	25 °C	20 °C	25 °C
3-Methyl-3-nonanol, $C_{10}H_{22}O$, mol wt. 158.286							
See also table 185							
Owen, Quayle, and Beavers [1930]				0.8292	0.8251		
Gredy [1935]	91	13					
Whitmore and Orem [1938]				.8311			1.4358
Sokolova, Shebanova, and Shchepinov [1961]	112	40		.8350		1.4362	
Selected value [1967]	[c] 86.±2.	10		[d] .8309 ±.001	[d] .8267 ±.001	[c] 1.438 ±0.002	[a] 1.436 ±0.002
5-Methyl-3-nonanol, $C_{10}H_{22}O$, mol wt. 158.286							
Arndt, Barbour, Engels, Horn, and Sutton [1959]	197.5 to 197.6	655					1.4328 1.4312
Selected value [1967]						[c] 1.435 ±0.002	[a,b,c] 1.433 ±0.002
2-Methyl-4-nonanol, $C_{10}H_{22}O$, mol wt. 156.286							
Levene and Marker [1931c]	117	40					1.4302
Union Carbide Corporation [1936]	92–93	13					
Dubois and Luft [1954b]	93–94	14			0.820		1.4306
Selected value [1967]	[f] 90.±2.	10				[c] 1.432 ±0.002	[b] 1.430 ±0.002
4-Methyl-4-nonanol, $C_{10}H_{22}O$, mol wt. 158.286							
See also table 185							
Whitmore and Williams [1933]	92–93	15			0.8245	1.4338	
Church, Whitmore, and McGrew [1934]	84–86	15				1.4344	
Quayle and Smart [1944]					0.8271	1.4350	1.4332
Lukes and Kovar [1954]	78–82	10					
Selected value [1967]	[f] 80.±3.	10		[d] 0.8297 ±0.001	[d] 0.8259 ±0.001	[a] 1.4350 ±0.0007	[a] 1.4332 ±0.0007
5-Methyl-4-nonanol, $C_{10}H_{22}O$, mol. wt. 158.286							
Powell and Nielson [1948]	80–81	6			0.828		1.4338
Arndt, Barbour, Engels, Horn, and Sutton [1959]	197.8 to 198.0	654					1.4340
7-Methyl-4-nonanol, $C_{10}H_{22}O$, mol wt. 158.286							
Heilbron, Johnson, Jones, and Raphael [1943]	94	12				1.4325	
Selected value [1967]	[f] 92.±2.	10					

Isomeric Decanols—Continued

Investigators		Vapor Pressures and Boiling Points		Freezing Point	Density, *d* g cm^{-3}		Refractive Index, n_D	
		°C	mmHg	t_m, °C	20 °C	25 °C	20 °C	25 °C
2-Methyl-5-nonanol, $C_{10}H_{22}O$, mol wt. 158.286								
Powell and Hageman	[1944]	111.5–113	28.5		0.8215		1.4310	
3-Methyl-5-nonanol, $C_{10}H_{22}O$, mol wt. 158.286								
Letsinger and Traynham	[1950]	97–99	17			0.821		1.4307
Selected value	[1967]	[f] 90. ±4.	10					
5-Methyl-5-nonanol, $C_{10}H_{22}O$, mol wt. 158.286								
See also table 186								
Whitmore and Woodburn	[1938]	91.4 to 92.4	15		0.8290	0.8253	1.4341	
Whitmore, Popkin, Whitaker, Mattil, and Zech	[1938]	100	24				1.4348 to 1.4351	
Quayle and Smart	[1944]					.8258	1.4350	1.4326
Armstrong, Lutte, and Doak	[1944]	100	24				1.4349	
Petrov and Kurbskii	[1944]	88	100					
Jeremias and MacKenzie	[1948]	91–92	15					
Protiva, Exner, Borovicka, and Pliml	[1952]	78–80	3					
Yur'ev and Belyakova	[1959]	85–86	10		.8305		1.4352	
Selected value	[1967]	[e] 85. ±2.	10		[d] .8297 ±.001	[d] .8256 ±.001	[a,c] 1.4350 ±0.0010	[a] 1.4326 ±0.0010
2-Ethyl-1-octanol, $C_{10}H_{22}O$, mol wt. 158.286								
Hoaglin, Kubler, and Leech	[1958]	104	10				1.4380	
3-Ethyl-1-octanol, $C_{10}H_{22}O$, mol wt. 158.286								
Levene and Marker	[1931e]				0.835			
4-Ethyl-1-octanol, $C_{10}H_{22}O$, mol wt. 158.286								
Keil	[1942]	108–110	10					
6-Ethyl-1-octanol, $C_{10}H_{22}O$, mol. wt. 158.286								
Prout and Cason	[1949]	121–123.5	18					
Selected value	[1967]	[f] 115. ±5.	10					
2,2-Dimethyl-1-octanol, $C_{10}H_{22}O$, mol wt. 158.286								
Blood and Hagemeyer	[1964]	208	760	<-53	0.8300			1.4350

Isomeric Decanols—Continued

Investigators		Vapor Pressures and Boiling Points		Freezing Point	Density, *d* g cm^{-3}		Refractive Index, n_D	
		°C	mmHg	t_m, °C	20 °C	25 °C	20 °C	25 °C
2,6-Dimethyl-1-octanol, $C_{10}H_{22}O$, mol wt. 158.286								
Vavon	[1914]	107–108	12		0.828		1.437	
Selected value	[1967]	^{f}105.±5.	10					
3,3-Dimethyl-1-octanol, $C_{10}H_{22}O$, mol wt. 158.286								
Mousseron and Bolle	[1957]	110–112	15					
Selected value	[1967]	^{f}105.±3.	10					
3,7-Dimethyl-1-octanol, $C_{10}H_{22}O$, mol wt. 158.286								
Ipatieff	[1912]	104–105	12		0.8280			
Ishizake	[1914]	212–213	760					
von Braun and Kaiser	[1923]	104–105	12		.836			
Longinov and Margoliss	[1924]	118.5 to 119	18		.8310		1.4392	
Escourrou	[1928]	84–85	10			0.8374 (11°)		1.43773 (11°)
Palfray	[1940]	106	12		.8299		1.4367	
Müller, Arno	[1942]				.8285		1.4355	
Smith and Rouault	[1947]	98–99	9				1.4430	
Sorensen and Mehlum	[1948]	114–116	21				1.4351	
Sorm, Suchy, and Herout	[1951]	111	11		.8357		1.4430	
Inoue	[1952]	85–86	4		.835			1.4435
Parham and Holmquist	[1954]	85–95	7					
Riniker, Arigoni, and Jeger	[1954]	102–104	12			0.8265	1.435	
Sanin and Ul'yanova	[1956]	108.5 to 109	15					
Quilico, Grunanger, and Piozzi	[1957]	114–115	17				1.4407	
Sax and Stross	[1957]	107	10				1.4379 to 1.4381	
Lebedeva and Kukhareva	[1958]	95–96	9		0.8402		1.4391	
Inoue and Takano	[1958]	88–89.5	4					
Porsch and Farnow	[1960]				0.8271		1.4360	
Yey, P. H.	[1961]	108–109	10		0.841		1.4470	
Yeh, P. H.	[1963]	108–111	13		0.8409		1.4491	
Disselkoetter and Kurtz	[1964]	102	10					
Selected value	[1967]	^{e}212.±2. ^{e}101.±2.	760 10		^{b}0.836 ±0.004	^{c}0.832 ±0.004	^{b}1.440 ±0.004	^{c}1.438 ±0.004
Antoine constants: *A* 9.1778, *B* 3057., *C* 273.								*dt/dp* at 760 mmHg, ^{e}0.044 °C/mmHg
4,5-Dimethyl-1-octanol, $C_{10}H_{22}O$, mol wt. 158.286								
Crombie, Manzoor-i-Khuda, and Smith	[1957]	78–79	0.3					1.4416
4,6-Dimethyl-1-octanol, $C_{10}H_{22}O$, mol wt. 158.286								
Crombie, Manzoor-i-Khuda, and Smith	[1957]	68	0.2				1.4411	

Isomeric Decanols—Continued

Investigators		Vapor Pressures and Boiling Points		Freezing Point	Density, d g cm^{-3}		Refractive Index, n_D	
		°C	mmHg	t_m, °C	20 °C	25 °C	20 °C	25 °C
4,7-Dimethyl-1-octanol, $C_{10}H_{22}O$, mol wt. 158.286								
Crombie, Manzoor-i-Khuda, and Smith	[1957]	125	50					1.4380
7,7-Dimethyl-1-octanol, $C_{10}H_{22}O$, mol wt. 158.286								
Gutman and Hickinbottom	[1951]	103–104	15				1.4384	
Selected value	[1967]	[f] 98.±2.	10				[c] 1.440 ±0.002	[a] 1.438 ±0.002
2,4-Dimethyl-2-octanol, $C_{10}H_{22}O$, mol wt. 158.286								
Nazarov and Torgov	[1948]	75–76	8		0.8257		1.4330	
Selected value	[1967]	[f] 77.±2.	10					
2,6-Dimethyl-2-octanol, $C_{10}H_{22}O$, mol wt. 158.286								
Sutherland, M. D.	[1953]	80.5	10			0.8023		1.4220
Nazarov, Krasnaya and Makin	[1957]	82–83	10		0.8335		1.4352	
Houlihan, Levy, and Mayer	[1959]	83	12		0.8260		1.4332	
Ohloff, Siebel, and Kovats	[1964]	83–85	12		0.8273		1.4322	
Selected value	[1967]	[a] 81.±1.	10		[b] 0.828 ±0.004	[c] 0.824 ±0.005	[b] 1.430 ±0.005	[c] 1.428 ±0.006
2,7-Dimethyl-2-octanol, $C_{10}H_{22}O$, mol wt. 158.286								
Zal'kind and Chelpanova	[1951]	68–70	4					
Audier, L.	[1957]	86	11				1.431	
Selected value	[1967]	[f] 83.±2.	10					
3,7-Dimethyl-2-octanol, $C_{10}H_{22}O$, mol wt. 158.286								
Naves, Desalbres and Ardizio	[1956]	62–63	1.3		0.8291		1.4355	
Selected value	[1967]				[a] .829 ±.002	[c] 0.825 ±.002	[a] 1.436 ±0.002	[c] 1.434 ±0.003
3-Ethyl-3-octanol, $C_{10}H_{22}O$, mol wt. 158.286								
Masson	[1901]	199	760					
Whitmore and Williams	[1933]	89.5 to 91.5	15			0.8361	1.4390	
Church, Whitmore, and McGrew	[1934]	83–85	12				1.4391	
Selected value	[1967]	[e] 199.±2.	760				[a] 1.4390 ±0.0020	[c] 1.437 ±0.003
		[e] 82.±2.	10					

Antoine constants: *A* 8.5916, *B* 2696., *C* 273. *dt/dp* at 760 mmHg, [e] 0.047 °C/mmHg

Isomeric Decanols—Continued

Investigators		Vapor Pressures and Boiling Points °C	Vapor Pressures and Boiling Points mmHg	Freezing Point t_m, °C	Density, *d* g cm^{-3} 20 °C	Density, *d* g cm^{-3} 25 °C	Refractive Index, n_D 20 °C	Refractive Index, n_D 25 °C
6-Ethyl-3-octanol, $C_{10}H_{22}O$, mol wt. 158.286								
Powell and Baldwin	[1936]	90–92	20					1.4367
Selected value	[1967]	[f] 80.±3.	10					
2,2-Dimethyl-3-octanol, $C_{10}H_{22}O$, mol wt. 158.286								
Whitmore, Meyer, Pedlow, and Popkin	[1933]	86–88	18				1.4340 to 1.4342	
Selected value	[1967]	[f] 80.±3.	10				[a] 1.4341 ±0.0020	[c] 1.432 ±0.003
2,3-Dimethyl-3-octanol, $C_{10}H_{22}O$, mol wt. 158.286								
Whitmore and Evers	[1933]	69–70	5		0.8401		1.4380	
Mears, Fookson, Pomerantz, Rich, Dussinger, and Howard	[1950]	189.1	760		.8293	0.8249	1.4375	1.4351
		138	150					
Selected value	[1967]	[e] 189.1±0.2	760		.8293 ±.0010	.8249 ±.0010	1.4375 ±0.0010	1.4351 ±0.0010
		[e] 74.0±0.5	10					
Antoine constants: *A* 8.5498, *B* 2620., *C* 273.					*dt/dp* at 760 mmHg, [e] 0.047 °C/mmHg			
2,7-Dimethyl-3-octanol, $C_{10}H_{22}O$, mol wt. 158.286, state at 25 °C								
Michiels	[1912]	193–194	756		0.8152		1.43021	
Selected value	[1967]	[a] 194.±2.	760					
3,5-Dimethyl-3-octanol, $C_{10}H_{22}O$, mol wt. 158.286								
Colonge and Gaumont	[1959]	106	4			0.837		1.4361
3,6-Dimethyl-3-octanol, $C_{10}H_{22}O$, mol wt. 158.286								
Dupont	[1913]	192	760		0.8331		1.4387	
3,7-Dimethyl-3-octanol, $C_{10}H_{22}O$, mol wt. 158.286								
Wallach, O.	[1914]	195.5–197	760		0.8280			
Escourrou	[1928]	84–85	10		.8374 (11°C)		1.43773 (11°C)	
Stevens and McNiven	[1939]	89.0	15			0.8647		1.4320
Palfray	[1940a]	87	15		.8331		1.4350	
Nazarov, Gussev, and Gunar	[1958]	71–73	6					
Verkade, de Vries, and Wepster	[1964]	96–98	21					1.4331
Selected value	[1967]	[e] 196.±2.	760		[b] .830 ±.003	[c] .826 ±.003	[a,c] 1.435 ±0.002	[b] 1.433 ±0.002
		[e] 81.±3.	10					

Isomeric Decanols—Continued

Investigators		Vapor Pressures and Boiling Points		Freezing Point	Density, d g cm^{-3}		Refractive Index, n_D	
		°C	mmHg	t_m, °C	20 °C	25 °C	20 °C	25 °C
Antoine constants: A 8.6484, B 2705., C 273.								dt/dp at 760 mmHg, [e] 0.046 °C/mmHg
3-Ethyl-4-octanol, $C_{10}H_{22}O$, mol wt. 158.286								
Woods and Lederle	[1951]	92–95	10					1.4389
Mousseron and Bolle	[1956]	74–75	3					
4-Ethyl-4-octanol, $C_{10}H_{22}O$, mol wt. 158.286								
Whitmore and Woodburn	[1933]	88.8–89.6	15		0.8369	0.8337	1.4378	
Rabjohn and Latina	[1954]	101–103	20				1.4381	
Selected value	[1967]	[f] 80.±3.	10		[a] .837 ±.002	[a] 0.834 ±0.002	[b] 1.438 ±0.001	[c] 1.436 ±0.002
2,2-Dimethyl-4-octanol, $C_{10}H_{22}O$, mol wt. 158.286								
Whitmore, Whitaker, Mattil, and Popkin	[1938]	92	100				1.4295 to 1.4305	
Whitmore, Popkin, Whitaker, Mattil, and Zech	[1938]	190–200 186–190 95	733 735 24		0.8212		1.4260 to 1.4308	
Selected value	[1967]						[b] 1.430 ±0.005	
2,4-Dimethyl-4-octanol, $C_{10}H_{22}O$, mol wt. 158.286								
Meyer and Tout	[1933]	97	27		0.8238		1.4338	
Sokolova, Krasnova and Zhurleva	[1958]	82.5–85	3		0.8236		1.4340	
Nogaidel and Dzagnidze	[1959]	62–64	5–6		0.8328		1.4410	
Petrov and Zakharov	[1959]	73.5–75	5		0.8227		1.4325	
Petrov, Zakharov, and Krasnova	[1959]	73.5–75	5		0.8227		1.4325	
Selected value	[1967]	[e] 83.±3.	10		[b] 0.8232 ±0.0010	[c] 0.819 ±0.002	[b] 1.4332 ±0.0010	[c] 1.431 ±0.002
2,5-Dimethyl-4-octanol, $C_{10}H_{22}O$, mol wt. 158.286								
Bjelous	[1912]	102–104	34			0.8125		1.42596
2,6-Dimethyl-4-octanol, $C_{10}H_{22}O$, mol wt. 158.286								
Verkade, de Vries and Wepster	[1964]	87.5–89.0	12				1.4309	
Selected value	[1967]	[f] 85.±3.	10					
2,7-Dimethyl-4-octanol, $C_{10}H_{22}O$, mol wt. 158.286								
Tuot	[1936]	96	18		0.8140		1.4280	
Powell and Hagemann	[1944]	107–108	29.5		0.8183		1.4297	
Selected value	[1967]	[f] 92.±2.	10		[b] 0.816 ±0.002	[c] 0.812 ±0.003	[b] 1.429 ±0.002	[c] 1.427 ±0.003

Isomeric Decanols—Continued

Investigators	Vapor Pressures and Boiling Points		Freezing Point	Density, d g cm^{-3}		Refractive Index, n_D	
	°C	mmHg	t_m, °C	20 °C	25 °C	20 °C	25 °C
3,4-Dimethyl-4-octanol, $C_{10}H_{22}O$, mol wt. 158.286							
Shine and Turner [1949]	64–65	3				1.4418	
Selected value [1967]	^{f}72.±3.	10					
3,6-Dimethyl-4-octanol, $C_{10}H_{22}O$, mol wt. 158.286							
Thi, T. S. L. [1962]	106–107	12		0.837		1.449	
Selected value [1967]	^{f}103.±2.	10					
4,6-Dimethyl-4-octanol, $C_{10}H_{22}O$, mol wt. 158.286							
Thaker and Vasi [1960]	95–103	20			0.8282		1.433
4,7-Dimethyl-4-octanol, $C_{10}H_{22}O$, mol. wt. 158.286							
Guerbet [1912a]	192	760		0.8421 (0 °C)			
2-*n*-Propyl-1-heptanol, $C_{10}H_{22}O$, mol wt. 158.286, state at 25 °C liq.							
See also table 186							
Karrer, Canal, Zohner, and Widmer [1928]	95–103	10–11					
Weizmann, Bergmann, and Sulzbacher [1950]	112–115	14					
Pratt and Kubler [1954]							1.4356
Griess [1955]	114	15					
Union Carbide Corporation [1956]	217.9	760	< −75	0.8322		1.4370	
Selected value [1967]	^{e}217.9±0.2	760				^{a}1.4370 ±0.0010	^{a}1.436 ±0.002
	^{e}103.±0.5	10					
Antoine constants: A 6.8998, B 1448.6, C 142.5				dt/dp at 760 mmHg, ^{e}0.0529 °C/mmHg			
3-Isopropyl-1-heptanol, $C_{10}H_{22}O$, mol wt. 158.286, state at 25 °C							
Kitaoka [1957]	215.5	766			0.8381		1.4397
	115	20					
Selected value [1967]	^{e}215.2±0.5	760					
	^{e}100.±1.	10					
Antoine constants: A 8.9958, B 2986., C 273.				dt/dp at 760 mmHg, ^{e}0.046 °C/mmHg			
2,3,6-Trimethyl-2-heptanol, $C_{10}H_{22}O$, mol wt. 158.286							
Barbier and Locquin [1913]	92–95	18					
Selected value [1967]	^{f}86.±4.	10					

Isomeric Decanols—Continued

Investigators		Vapor Pressures and Boiling Points		Freezing Point	Density, *d* g cm^{-3}		Refractive Index, n_D	
		°C	mmHg	t_m, °C	20 °C	25 °C	20 °C	25 °C
2,4,6-Trimethyl-2-heptanol, $C_{10}H_{22}O$, mol wt. 158.286								
Braude and Coles	[1952]	85–88	25					1.4344
Selected value	[1967]	[f] 71. ±4.	10					
2,5,6-Trimethyl-2-heptanol, $C_{10}H_{22}O$, mol wt. 158.286								
Wallach	[1911]	192–194	760		0.831		1.4355	
4,6,6-Trimethyl-2-heptanol, $C_{10}H_{22}O$, mol wt. 158.286								
Doumani	[1946]	91.0–94.4	25					1.4313
Selected value	[1967]	[f] 77. ±4.	10					
2-Methyl-3-ethyl-3-heptanol, $C_{10}H_{22}O$, mol wt. 158.286								
Wallach and Gröppel	[1914]	191–195	760		0.8455		1.4378	
2-Methyl-5-ethyl-3-heptanol, $C_{10}H_{22}O$, mol wt. 158.286								
Fourneau and Matti	[1931]	92	28					
4-Methyl-3-ethyl-3-heptanol, $C_{10}H_{22}O$, mol wt. 158.286								
Bergmann and Bondi	[1936]	92–93	32					
4-Methyl-5-ethyl-3-heptanol, $C_{10}H_{22}O$, mol wt. 158.286								
Colonge and Joly	[1943]	86–88	14		0.863		1.4553	
Selected value	[1967]	[f] 83. ±3.	10					
6-Methyl-3-ethyl-3-heptanol, $C_{10}H_{22}O$, mol wt. 158.286								
Grignard, V.	[1904a]	83–86	15		0.836		1.4371	
Selected value	[1967]	[f] 80. ±4.	10					
2,2,3-Trimethyl-3-heptanol, $C_{10}H_{22}O$, mol wt. 158.286								
Conant and Blatt	[1929]	84–87	13		0.8487		1.4409	
Mosher	[1954]	186	757		.8454		1.4410	
Selected value	[1967]	[e] 186. ±1. [e] 77. ±2.	760 10		[a] .845 ±.002	[c] 0.841 ±.003	[b] 1.441 ±0.001	[c] 1.439 ±0.002

Antoine constants: *A* 8.9057, *B* 2766., *C* 273.

dt/dp at 760 mmHg, [e] 0.044 °C/mmHg

Isomeric Decanols—Continued

Investigators	Vapor Pressures and Boiling Points		Freezing Point	Density, d g cm^{-3}		Refractive Index, n_D	
	°C	mmHg	t_m, °C	20 °C	25 °C	20 °C	25 °C
2,2,6-Trimethyl-3-heptanol, $C_{10}H_{22}O$, mol wt. 158.286							
Whitmore, Meyer, Pedlow, and Popkin [1938]	133.2 to 133.5	150		0.8236		1.4320 to 1.4323	
2,3,6-Trimethyl-3-heptanol, $C_{10}H_{22}O$, mol wt. 158.286							
Thomas, Palluy, Willhalm, and Stoll [1963]	73	8		0.8398		1.4377	
Selected value [1967]	^{f} 75.±2.	10					
3,5,5-Trimethyl-3-heptanol, $C_{10}H_{22}O$, mol wt. 158.286							
Mosher [1940]	86	30		0.8513		1.4455	
Stehman [1947]	180	760				1.4450	
Stehman, Cook, Percival, and Whitmore [1950]	195.6	760		.8558		1.4453	
Selected value [1967]	^{e} 195.6±1. ^{e} 60.±1.	760 10		^{a} 0.856 ±0.003	^{c} 0.852 ±0.003	^{b} 1.445 ±0.001	^{c} 1.443 ±0.002
Antoine constants: A 7.4786, B 2155., C 273.					dt/dp at 760 mmHg, ^{e} 0.058 °C/mmHg		
4-n-Propyl-4-heptanol, $C_{10}H_{22}O$, mol wt. 158.286,							
See also table 186							
Konovalov, M. [1902]	193–195	737				1.4359	
Halse [1914]	84–85	12					
Eykman [1919]	77	8		0.8328			
Leroide [1921]	192–194	760					
Owen, Quayle, and Beavers [1930]				0.8311	0.8268		
Moyer and Marvel [1931]	89–92	20					
Church, Whitmore, and McGrew [1934]	89–90	15					
Challenger and Pantony [1954]	89–92	17					
Desgrandchamps, Peluzarche, and Maillard [1961]	75	8.5				1.4354	
Meshcheryakov, Erzyutova, and Kuo [1961]	193–195	760		0.8340		1.4340	
Selected value [1967]	^{e} 194.3±0.5 ^{e} 81.±1.	760 10		^{d} 0.8324 ±0.001	^{d} 0.8281 ±0.001	^{b} 1.435 ±0.001	^{c} 1.433 ±0.002
Antoine constants: A 5.2052, B 590.2, C 59.6					dt/dp at 760 mmHg, ^{e} 0.047 °C/mmHg		

Isomeric Decanols—Continued

Investigators		Vapor Pressures and Boiling Points		Freezing Point	Density, d g cm^{-3}		Refractive Index, n_D	
		°C	mmHg	t_m, °C	20 °C	25 °C	20 °C	25 °C
4-Isopropyl-4-heptanol, $C_{10}H_{22}O$, mol wt. 158.286								
Stas	[1926]	188–190	760		0.8449		1.4390	
		79–81	14					
Nazarov and Kakhniashvili	[1954a]	81	15		.8471		1.442	
Selected value	[1967]	[e] 190.±2.	760		[a] .845 ±0.001	[c] 0.841 ±.002	[a] 1.439 ±0.001	[c] 1.437 ±0.002
		[e] 73.±2.	10					
Antoine constants: A 8.4173, B 2563., C 273.								dt/dp at 760 mmHg, [e] 0.048 °C/mmHg
2,2,4-Trimethyl-4-heptanol, $C_{10}H_{22}O$, mol wt. 158.286								
Whitmore, Popkin, Whitaker, Mattil, and Zech	[1938]	74.5	14				1.4367 to 1.4371	
Moersch	[1942]	119.8	100		0.833		1.4371	
Moersch and Whitmore	[1949]	119.8	100		.833		1.4373	
		59.6	7					
Selected value	[1967]	[e] 181.±3.	760		[b] .833 ±.002	[c] 0.829 ±0.002	[b] 1.437 ±0.001	[c] 1.435 ±0.002
		[e] 68.±1.	10					
Antoine constants: A 8.552, B 2574., C 273.								dt/dp at 760 mmHg, [e] 0.046 °C/mmHg
2,2,5-Trimethyl-4-heptanol, $C_{10}H_{22}O$, mol wt. 158.286								
Petrov, Sumin, Meerovich, Kudrina, and Tikhonova	[1939]	95–97	25		0.8361			
Selected value	[1967]	[f] 80.±4.	10					
2,2,6-Trimethyl-4-heptanol, $C_{10}H_{22}O$, mol wt. 158.286								
Whitmore and Forster	[1942]	75	15				1.4237 to 1.4279	
		34.4	3				1.4232 to 1.4282	
Selected value	[1967]	[f] 60.±5.	10				[a] 1.424 ±0.004	[c] 1.422 ±0.005
2,4,5-Trimethyl-4-heptanol, $C_{10}H_{22}O$, mol wt. 158.286								
Shine and Turner	[1949]	54–55	3				1.4382	

Isomeric Decanols—Continued

Investigators	Vapor Pressures and Boiling Points		Freezing Point	Density, d g cm^{-3}		Refractive Index, n_D	
	°C	mmHg	t_m, °C	20 °C	25 °C	20 °C	25 °C
2,4,6-Trimethyl-4-heptanol, $C_{10}H_{22}O$, mol wt. 158.286							
Bodroux and Taboury [1909a]	180–182	753		0.824		1.4326	
Halse [1914]	78–80	12					
Meyer and Tout [1933]	81	19		.8186		1.4312	
Takemoto and Nakajima [1957]	65–66	5					
Petrov, Zakharov, and Krasnova [1959]	94–96	25		.8241		1.4319	
Selected value [1967]	^{e}182.±2.	760		^{a}.819 ±0.001	^{c}0.815 ±0.002	^{a}1.431 ±0.001	^{c}1.429 ±0.002
	^{e}68.±2.	10					
Antoine constants: A 8.4783, B 2549., C 273.	dt/dp at 760 mmHg, ^{e}0.046 °C/mmHg						
3,3,6-Trimethyl-4-heptanol, $C_{10}H_{22}O$, mol. wt. 158.286							
Takemoto and Nakajima [1957]					0.838		1.4376
2-n-Butyl-1-hexanol, $C_{10}H_{22}O$, mol wt. 158.286							
See also table 187							
Levene and Allen [1916]	218–219	760					
Levene and Cretcher [1918]	218–219	760					
Levene and Taylor [1922b]	210–212	731					
Protiva, Exner, Borovicka, and Pliml [1952]	95–97	3					
Franzen, V. [1954a]	107	12				1.4360	
Arndt, Barbour, Engels, Horn, and Sutton [1959]	209.4	655					1.4348
Landa and Markovec [1964]	112.5 *to* 113.9	20				1.4354	
Selected value [1967]	^{e}218.±2	760				^{b}1.436 ±0.001	^{a}1.434 ±0.002
	^{e}106.±2	10					
Antoine constants: A 3.9268, B 183.0, C −43.	dt/dp at 760 mmHg, ^{e}0.046 °C/mmHg						
4-Methyl-2-n-propyl-1-hexanol, $C_{10}H_{22}O$, mol wt. 158.286							
Hagemeyer and Hudson [1958]	208–209	760		0.8286		1.43561	
Hagemeyer, Wright, and Bobo [1958]	112	20					
Selected value [1967]	^{e}98.±2.	10					
Antoine constants: A 9.2165, B 3048., C 273.	dt/dp at 760 mmHg, ^{e}0.043 °C/mmHg						
4-Methyl-2-isopropyl-1-hexanol, $C_{10}H_{22}O$, mol wt. 158.286							
Hagemeyer and Hudson [1958]	201–202	760					

Isomeric Decanols—Continued

5-Methyl-2-isopropyl-1-hexanol, $C_{10}H_{22}O$, mol wt. 158.286

Investigators		Vapor Pressures and Boiling Points		Freezing Point	Density, d g cm^{-3}		Refractive Index, n_D	
		°C	mmHg	t_m, °C	20 °C	25 °C	20 °C	25 °C
Terentieff	[1925]	210–213	760		0.8322		1.4380	
von Braun and Manz	[1934]	92–95	11					
Schinz and Schappi	[1947]	96–97	12		.8342		1.4377	
Selected value	[1967]	^{e}213. ±3. ^{e}92. ±3.	760 10		^{b}.833 ±.002	^{c}0.829 ±0.003	^{b}1.438 ±0.002	^{c}1.436 ±0.002

Antoine constants: *A* 8.5629, *B* 2762., *C* 273. *dt/dp* at 760 mmHg, ^{e}0.049 °C/mmHg

2,4-Diethyl-1-hexanol, $C_{10}H_{22}O$, mol wt. 158.286

Investigators		Vapor Pressures and Boiling Points		Freezing Point	Density, d g cm^{-3}		Refractive Index, n_D	
		°C	mmHg	t_m, °C	20 °C	25 °C	20 °C	25 °C
Fourneau and Matti	[1931]	123–125	43					

5,5-Dimethyl-2-ethyl-1-hexanol, $C_{10}H_{22}O$, mol wt. 158.286

Investigators		Vapor Pressures and Boiling Points		Freezing Point	Density, d g cm^{-3}		Refractive Index, n_D	
		°C	mmHg	t_m, °C	20 °C	25 °C	20 °C	25 °C
Gol'dfarb and Konstantinov	[1956]	92–93	13		0.8386		1.4350	
Selected value	[1967]	^{f}90. ±2.	10					

2,3,4,4-Tetramethyl-2-hexanol, $C_{10}H_{22}O$, mol wt. 158.286

Investigators		Vapor Pressures and Boiling Points		Freezing Point	Density, d g cm^{-3}		Refractive Index, n_D	
		°C	mmHg	t_m, °C	20 °C	25 °C	20 °C	25 °C
Stehman	[1947]	195	760				1.4500	
Stehman, Cook, Percival, and Whitmore	[1950]	180–185	760				1.4490	
Selected value	[1967]	^{f}190. ±5.	760				^{b}1.450 ±0.001	^{c}1.448 ±0.002

3,3,5,5-Tetramethyl-2-hexanol, $C_{10}H_{22}O$, mol wt. 158.286

Investigators		Vapor Pressures and Boiling Points		Freezing Point	Density, d g cm^{-3}		Refractive Index, n_D	
		°C	mmHg	t_m, °C	20 °C	25 °C	20 °C	25 °C
Hickinbottom, Hyatt, and Sparke	[1954]	87–87.5	27				1.4458	
Selected value	[1967]	^{f}70. ±2.	10					

2-Methyl-3-isopropyl-3-hexanol, $C_{10}H_{22}O$, mol wt. 158.286

Investigators		Vapor Pressures and Boiling Points		Freezing Point	Density, d g cm^{-3}		Refractive Index, n_D	
		°C	mmHg	t_m, °C	20 °C	25 °C	20 °C	25 °C
George, R. S.	[1943]	131.6	125		0.8554			
		140.8	170					
Cadwallader, Fookson, Mears, and Howard	[1948]	90–95	22		0.8504			
Lewis and Wright	[1952]	119–120	90					1.4413
Selected value	[1967]	^{e}192. ±2. ^{e}69. ±2.	760 10		^{a}0.850 ±0.002	^{c}0.846 ±0.003		

Antoine constants: *A* 8.1109, *B* 2433., *C* 273. *dt/dp* at 760 mmHg, ^{e}0.051 °C/mmHg

Isomeric Decanols—Continued

Investigators	Vapor Pressures and Boiling Points		Freezing Point	Density, d g cm^{-3}		Refractive Index, n_D	
	°C	mmHg	t_m, °C	20 °C	25 °C	20 °C	25 °C
2,2-Dimethyl-4-ethyl-3-hexanol, $C_{10}H_{22}O$, mol wt. 158.286							
Haller and Bauer [1913]	187	760					
Whitmore, Whitaker, Mosher, Breivik, Wheeler, Miner, Sutherland, Wagner, Clapper, Lewis, Lux, and Popkin [1941]	80 131–132 123–124	20 150 100		0.8339		1.4375 to 1.4378	
Selected value [1967]	[e] 187.±1. [e] 65.±2.	760 10				[a] 1.438 ±0.002	[c] 1.436 ±0.002
Antoine constants: A 8.1171, B 2406., C 273.							dt/dp at 760 mmHg, [e] 0.050 °C/mmHg
2,4-Dimethyl-4-ethyl-3-hexanol, $C_{10}H_{22}O$, mol wt. 158.286							
Sokolova [1953]	109.5–111.0	50		0.8606		1.4463	
5,5-Dimethyl-3-ethyl-3-hexanol, $C_{10}H_{22}O$, mol wt. 158.286							
Stahly [1934]				0.8422		1.4410	
Whitmore, Popkin, Whitaker, Mattil, and Zech [1938]	62–64	10		0.8352		1.4390 to 1.4400	
Whitmore and Forster [1942]	54	5		0.845		1.4394 to 1.4403	
Selected value [1967]	[a] 62.±3.	10		[b] 0.840 ±0.005	[c] 0.836 ±0.005	[b] 1.440 ±0.001	[c] 1.438 ±0.002
2,2,3,4-Tetramethyl-3-hexanol, $C_{10}H_{22}O$, mol wt. 158.286							
Nazarov [1937]	190–193	760		0.859		1.447	
Stehman [1947]	200	760				1.4470	
Stehman, Cook, Percival, and Whitmore [1950]	191.8	760		0.8584		1.4469	
Selected value [1967]	[b] 192.±2.	760		[a] 0.858 ±0.002	[c] 0.854 ±0.003	[b] 1.447 ±0.001	[c] 1.445 ±0.002
2,2,3,5-Tetramethyl-3-hexanol, $C_{10}H_{22}O$, mol wt. 158.286							
Petrov [1955]	84.6–84.8	25		0.8393		1.4368	
Petrov, Sushchinskii, and Konoval'Chikov [1955]	84.6–84.8	25		.8383		1.4368	
Selected value [1967]	[f] 70.±2.	10		[b] .839 ±.001	[c] 0.835 ±0.002	[b] 1.437 ±0.002	[c] 1.435 ±0.002
2,2,4,4-Tetramethyl-3-hexanol, $C_{10}H_{22}O$, mol wt. 158.286, state at 25 °C liq.							
Haller and Bauer [1913]	187–188	760					
Stahly [1934]	190	760	4	0.8549		1.4465	
Selected value [1967]	[a] 190.±3.	760					

Isomeric Decanols—Continued

Investigators		Vapor Pressures and Boiling Points		Freezing Point	Density, *d* g cm⁻³		Refractive Index, n_D	
		°C	mmHg	t_m, °C	20 °C	25 °C	20 °C	25 °C
2,2,5,5-Tetramethyl-3-hexanol, $C_{10}H_{22}O$, mol wt. 158.286, state at 25 °C crystal								
Bouveault and Locquin	[1906]	173–174	760	52–53				
Whitmore and Heyd	[1938]	167–173	760	49.4				
Whitmore, Whitaker, Mosher, Breivik, Wheeler, Miner, Sutherland, Wagner, Clapper, Lewis, Lux, and Popkin	[1941]			51–52				
Hickinbottom, Hyatt, and Sparke	[1954]			50–51				
Logan and Flautt	[1960]			52.5–53.0				
Selected value	[1967]	[b] 170. ±3.	760	[b] 52. ±1.				
2,3,4,4-Tetramethyl-3-hexanol, $C_{10}H_{22}O$, mol wt. 158.286								
Nazarov	[1937]	197–199	760		0.873		1.4574	
Mosher	[1940]				.8694		1.4532	
Stehman	[1947]	219	760					
Stehman, Cook, Percival, and Whitmore	[1950]	200.6	760		0.8745		1.4530	
Selected value	[1967]	[a] 201. ±1.	760		[a] .874 ±.002	[c] 0.870 ±0.003	[b] 1.453 ±0.001	[c] 1.451 ±0.002
2,3,5,5-Tetramethyl-3-hexanol, $C_{10}H_{22}O$, mol wt. 158.286								
Moersch	[1942]	76	20		0.8378		1.4367	
Selected value	[1967]	[f] 62. ±2.	10					
2,4,4,5-Tetramethyl-3-hexanol, $C_{10}H_{22}O$, mol wt. 158.286								
Hickinbottom, Hyatt, and Sparke	[1954]	85–86	16				1.4492	
Selected value	[1967]	[f] 76. ±2.	10					
3,4,4,5-Tetramethyl-3-hexanol, $C_{10}H_{22}O$, mol wt. 158.286 at								
Stehman	[1947]	190	760				1.4533	
Stehman, Cook, Percival, and Whitmore	[1950]	201.9	760		0.8742		1.4533	
Selected value	[1967]	[a] 202. ±2.	760				[b] 1.453 ±0.002	[c] 1.451 ±0.002
3,4,5,5-Tetramethyl-3-hexanol, $C_{10}H_{22}O$, mol wt. 158.286								
Stehman	[1947]	180	760				1.4490	
Stehman, Cook, Percival, and Whitmore	[1950]	194.6	760		0.8623		1.4490	
Selected value	[1967]	[a] 195. ±2.	760				[b] 1.449 ±0.002	[c] 1.447 ±0.002

Isomeric Decanols—Continued

4-Methyl-2-isobutyl-1-pentanol, $C_{10}H_{22}O$, mol wt. 158.286

Investigators		Vapor Pressures and Boiling Points		Freezing Point	Density, *d* g cm^{-3}		Refractive Index, n_D	
		°C	mmHg	t_m, °C	20 °C	25 °C	20 °C	25 °C
Bouveault and Blanc	[1904c]	204	760		0.846 (4 °C)			
Freylon	[1910]	101–103	17		.846 (0 °C)			
Selected value	[1967]	^{e} 204. ±2. ^{e} 91. ±3.	760 10		^{f} .83 ±.01	^{f} 0.83 ±0.01		

Antoine constants: *A* 8.9484, *B* 2894., *C* 273. *dt/dp* at 760 mmHg, ^{e} 0.045 °C/mmHg

4,4-Dimethyl-3-isopropyl-1-pentanol, $C_{10}H_{22}O$, mol wt. 158.286

Investigators		Vapor Pressures and Boiling Points		Freezing Point	Density, *d* g cm^{-3}		Refractive Index, n_D	
		°C	mmHg	t_m, °C	20 °C	25 °C	20 °C	25 °C
Hickinbottom, Hyatt, and Sparke	[1954]	91	13				1.4623	
Selected value	[1967]	^{f} 88. ±3.	10					

3,4-Dimethyl-3-isopropyl-2-pentanol, $C_{10}H_{22}O$, mol wt. 158.286

Investigators		Vapor Pressures and Boiling Points		Freezing Point	Density, *d* g cm^{-3}		Refractive Index, n_D	
		°C	mmHg	t_m, °C	20 °C	25 °C	20 °C	25 °C
Hickinbottom, Hyatt, and Sparke	[1954]	100	16				1.4619	
Selected value	[1967]	^{f} 94. ±3.	10					

2,4-Dimethyl-3-*n*-propyl-3-pentanol, $C_{10}H_{22}O$, mol wt. 158.286

See also table 187

Investigators		Vapor Pressures and Boiling Points		Freezing Point	Density, *d* g cm^{-3}		Refractive Index, n_D	
		°C	mmHg	t_m, °C	20 °C	25 °C	20 °C	25 °C
Stas	[1926]	184	760		0.8552		1.4427	
Whitmore and George	[1942]	132	125				1.4445	
Lewis and Wright	[1952]	119–120	90					1.4413
Selected value	[1967]	^{e} 185. ±2. ^{e} 66. ±2.	760 10		^{d} 0.8552 ±0.001	^{d} 0.8518 ±0.001	^{a} 1.444 ±0.002	^{c} 1.442 ±0.002

Antoine constants: *A* 10.9478, *B* 5058., *C* 442. *dt/dp* at 760 mmHg, ^{e} 0.043 °C/mmHg

Isomeric Decanols—Continued

2,4-Dimethyl-3-isopropyl-3-pentanol, $C_{10}H_{22}O$, mol wt. 158.286, state at 25 °C liq.

See also table 187

Investigators	Vapor Pressures and Boiling Points °C	Vapor Pressures and Boiling Points mmHg	Freezing Point t_m, °C	Density, d g cm^{-3} 20 °C	Density, d g cm^{-3} 25 °C	Refractive Index, n_D 20 °C	Refractive Index, n_D 25 °C
Young and Roberts [1944]	106.6–108	50				1.4476 to 1.4480	
Bartlett and Schneider [1945]	105	50				1.4478	
Vavon and Collin [1946]	77–79	13		0.8612		1.4474	
Howard, Mears, Fookson, Pomerantz, and Brooks [1947]	194.5	760	−14.7	.8632	0.8591	1.4480	1.4458
	109	50					
Frank and Foster [1954]	94–95	30				1.4479	
Zook, March, and Smith [1959]	190.5–192	721					1.4456 to 1.4461
Selected value [1967]	[e] 194.5±0.2	760	[a] −14.7±0.5	[a] 0.8632 ±0.0010	[a] 0.8591 ±0.0010	[a] 1.4480 ±0.0010	[a] 1.4458 ±0.0010
	[e] 73.9±0.5	10					

Antoine constants: *A* 6.3781, *B* 1206., *C* 150.4. *dt/dp* at 760 mmHg, [e] 0.051 °C/mmHg

2,2,4-Trimethyl-3-ethyl-3-pentanol, $C_{10}H_{22}O$, mol wt. 158.286

Investigators	Vapor Pressures and Boiling Points °C	Vapor Pressures and Boiling Points mmHg	Freezing Point t_m, °C	Density, d g cm^{-3} 20 °C	Density, d g cm^{-3} 25 °C	Refractive Index, n_D 20 °C	Refractive Index, n_D 25 °C
Nazarov [1936]	188–191	760		0.8620		1.4485	
Cadwallader, Fookson, Mears, and Howard [1948]	93–97	35		0.862		1.4479	
Smith and Creitz [1951]	93–97	35		0.862		1.4479	
Mosher [1954]	41	4		0.8628		1.4480	
	125	107					
Selected value [1967]	[e] 191.±3.	760		[b] 0.862 ±0.001	[c] 0.858 ±0.002	[b] 1.4480 ±0.0010	[c] 1.446 ±0.002
	[e] 67.±3.	10					

Antoine constants: *A* 8.0150, *B* 2383., *C* 273. *dt/dp* at 760 mmHg, [e] 0.052 °C/mmHg

2,2,3,4,4-Pentamethyl-3-pentanol, $C_{10}H_{22}O$, mol wt. 158.286, state at 25 °C crystal

See also table 188

Investigators	Vapor Pressures and Boiling Points °C	Vapor Pressures and Boiling Points mmHg	Freezing Point t_m, °C	Density, d g cm^{-3} 20 °C	Density, d g cm^{-3} 25 °C	Refractive Index, n_D 20 °C	Refractive Index, n_D 25 °C
Conant and Blatt [1929]	184–191	760	34–41				
Whitmore and Laughlin [1933]	122.5–123	100	41.5–42				
Whitmore and Stahly [1933]			42				
Nazarov [1936]	172–176	760					
Howard, Mears, Fookson, Pomerantz, and Brooks [1947]	194.4	760	42.1				
Newman, Arkell, and Fukunaga [1960]	78–82	17	42.0–42.7				
Petrov, Sokolova, and Kao [1960]	104–106	57	37–38				
Selected value [1967]	[e] 194.6±0.5	760	42.1±0.1				
	[e] 70.±1	10					

Antoine constants: *A* 5.8559, *B* 956.5, *C* 126.9. *dt/dp* at 760 mmHg, [e] 0.055 °C/mmHg

2,3-Dimethyl-2-*tert*-butyl-1-butanol, $C_{10}H_{22}O$, mol wt. 158.286, state at 25 °C crystal

Investigators	Vapor Pressures and Boiling Points °C	Vapor Pressures and Boiling Points mmHg	Freezing Point t_m, °C	Density, d g cm^{-3} 20 °C	Density, d g cm^{-3} 25 °C	Refractive Index, n_D 20 °C	Refractive Index, n_D 25 °C
Newman, Arkell, and Fukunaga [1960]	105–110	29	54 to 55				
Selected value [1967]	[f] 90.±5.	10					

1-Undecanol

Properties of the Liquid Phase at Various Temperatures

Refractive Index

Observed values of the refractive index at 20 and 25 °C are shown in table 190. Since the agreement among these values is poor and none of them can be considered particularly accurate, the selected values were obtained by the best compromise, and the uncertainty is correspondingly large. Vogel [1948] reported the refractive index at 20 °C for four wavelengths from 6563 to 4861 Å. His value at the sodium D-line is appreciably lower than those of most of the other investigators. Vil'shan and Gavrilova [1963] measured n_D at 50 °C. Selected values above 25 °C reported in table 189 were obtained by a linear interpolation between the value selected for 25 °C and the value of Vil'shan and Gavrilova.

Density

Densities measured at 20 and 25 °C are listed in table 190. In addition, Verkade and Coops [1927] measured the density at 34.6 °C and Kuss [1956] measured the density at temperatures from 20 to 85 °C. Constants in the Francis equation were calculated from these values and from the ones underlined in table 190. Since the range of temperature was not sufficient to determine the value of E, a value of 600 was assumed. The selected values listed in tables 189 and 190 were calculated from the Francis equation.

Vapor Pressure and Boiling Point

Since there have been no systematic measurements of vapor pressure, the selected values are based on scattered boiling point measurements which have been reported in the literature. The only boiling point in the vicinity of 1 atm which has been reported is the one by Vogel [1948]. All the others are in the range of 6 to 30 mm Hg. The set of Antoine constants obtained from a direct least squares fit to these data are, $A = 5.48749$, $B = 729.7$ and $C = 36.2$. However, since the data are not adequate for determining a meaningful value of C, the selected values in tables 189 and 190 were calculated from constants obtained by setting $C = 100$, and adjusting B and C to minimize the sum of the square of the deviations. This set of constants fits the data as well as the first set, and probably gives a more reliable estimate of the boiling points from 30 to 760 mm Hg. They are listed in table 189.

Solid-Solid Phase Equilibrium

Transition Temperature

On the basis of the examination of x-ray diffraction lines obtained during the heating and cooling of samples of 1-undecanol, Tanaka, Seto, and Hayshida [1957] identified the α- and β-forms described in appendix E. On heating they obtained the α to β transition temperature of 11.7 °C, and on cooling of 10 °C. Thus the crystal which is stable at the melting point is the α-form. They also found some additional diffraction lines which seemed to indicate the presence of a third crystalline form which did not correspond to any crystal found in any of the other alcohols.

Solid-Liquid Phase Equilibrium

Melting Point

Several reported values of the normal melting point are listed in table 190. The selection was based on the three underlined ones. The selected value was close to the value of Meyer and Reid [1933] since they seem to have used the most accurate thermometry. However, since their value was a few tenths of a degree below the other two, their sample may have been less pure.

TABLE 189. 1-Undecanol. Selected values. Physical and thermodynamic properties

Temp. °C	Refractive Index, n_D	Density g cm^{-3}	Vapor Pressure, mmHg
20	1.4402	0.8324	
25	1.4386	.8291	
30	1.437	.8257	
40	1.434	.8189	
50	1.431	.8121	
60		.8052	
70		.7983	
80		.7913	
90		.7842	
125			9.4
126.2			10
130			12.4
135			16.1
140			20.8
145			27.
150			34.
155			42.
160			52.
165			65.
170			79.
175			96.
176.			100.
180			116.
185			138.
190			165.
195			195.
196.			200
200			229.
205			268.
210			312.
215			362.
218.			400
220			418.
225			480.
230			549.
235			625.
240			709.
242.8			760
245			801.

Data For Phase Transitions

Initial	Final	Temp. °C	dt/dP deg mm^{-1}	Pressure mmHg	ΔH kcal mol^{-1}	$d\Delta H/dt$ cal deg^{-1} mol^{-1}	ΔS cal deg^{-1} mol^{-1}	ΔC_p cal deg^{-1} mol^{-1}
c,II	c,I	11.7±1						
c,I	liq	15.9±0.2						
liq	g	242.8±1	0.0537	760				

Condensed Phase Heat Capacity			Properties of the Saturated Real Gas			
State	Temp. °C	C_p	Temp. °C	H^r-H^0	S^r-S^0	$C_p^r-C_p^0$
		cal deg^{-1} mol^{-1}		cal mol^{-1}	cal deg^{-1} mol^{-1}	cal deg^{-1} mol^{-1}

Data for the Standard States at 25 °C

State	Heat of Combustion ΔH_c^0 kcal mol^{-1}	Heat of Formation ΔH_f^0 kcal mol^{-1}	Entropy S^0 cal deg^{-1} mol^{-1}	Gibbs Energy of Formation ΔG_f^0 kcal mol^{-1}	Heat Capacity, C_p cal deg^{-1} mol^{-1}

Critical Constants

Temp. °C, K	Pressure atm	Density g cm^{-3}

Constants in Vapor Pressure and Density Equation

Antoine Equation				Francis Equation				
Temp. Range	A	B	C	Temp. Range	A	$B\times10^3$	C	E
120 to 243 °C	6.5271	1250.0	100.0	20 to 85 °C	0.92501	0.5281	47.57	600

TABLE 190. 1-Undecanol. Reported values. Simple physical properties

Investigators		Vapor Pressures and Boiling Points		Freezing Point	Density, d g cm^{-3}		Refractive Index, n_D	
		°C	mmHg	t_m, °C	20 °C	25 °C	20 °C	25 °C
1-Undecanol, $C_{11}H_{22}O$, mol wt. 172.31 state at 25 °C liq.								
Jeffreys	[1899]	131	15	19				
Blaise and Guerin	[1903]	146	30	11		0.8321		1.4384
Levene, West, Allen, and van der Scheer	[1915]	147	25					
Robinson	[1924]	130	12	14.3				
Verkade and Coops	[1927]	120.0–120.2	7.0	16.3				
Meyer and Reid	[1933]			15.85				
Muller	[1942]				0.8338		1.4410	
Harwood and Ralston	[1947]			16.2				
Vogel	[1948]	243.5	769		0.8298		1.43918	
Sackmann and Sauerwald	[1950]			24.3		0.8293		
Ziegler and Gellert	[1950]			12.5				
Lumb and Smith	[1952]	140–141	21				1.4403	
McKenna, Tartar, and Lingafelter	[1953]			16.5				1.4380
Gol'dfarb and Kirmalova	[1955]	118–120	6					1.4396
Kuss	[1955]				0.8332	0.8298		
Gol'dfarb and Konstantinov	[1956]	130–131	15		0.8368			1.4392
Tanaka, Seto, and Hayashida	[1957]			13				
Vil'shan and Gavrilova	[1963]			16.0				
Selected value	[1967]	242.8±1. 126.2±0.5	760 10	15.9±0.2	0.8324 ±0.0005	0.8291 ±0.0005	1.4402 ±.001	1.4386 ±0.001

Antoine constants: A 6.5271, B 1250.0, C 100.0. dt/dp at 760 mmHg, 0.0537 °C/mmHg

Isomeric Undecanols

Observed values of boiling points, melting points, and density and refractive indices at 20 and 25 °C are summarized in the following unnumbered tables. There have been no measurements of refractive index outside this temperature range, and additional density data have been reported for only three compounds. Pickard and Kenyon [1911] and [1912] reported densities over a range of temperatures for 2-undecanol and 3-undecanol and Owen, Quayle, and Beavers [1930] reported values at 0, 25 and 65 °C for 4-methyl-4-decanol. The constants A, B, and C in the Francis equation have been fitted to the data for 2- and 3-undecanol, with the assumption of $E = 500$. The corresponding calculated densities are shown in table 191. Densities of 4-methyl-4-decanol have been expressed as a linear function of temperature.

Smoothed boiling points calculated from the Antoine equation are shown in tables 191 and 192. These are all based on scattered boiling point measurements. The data were sufficient to determine a meaningful value of C only for 2,5-dimethyl-3-isopropyl-3-hexanol and for 2,2,4-trimethyl-3-isoprophy-3-pentanol. A value of 100 was assumed for the other compounds.

TABLE 191. Isomeric Undecanols. Selected values. Physical properties of the liquid

2-Undecanol				3-Undecanol				6-Undecanol			
Temp. °C	Refractive Index, n_D	Density g cm^{-3}	Vapor Pressure, mmHg	Temp. °C	Refractive Index, n_D	Density g cm^{-3}	Vapor Pressure, mmHg	Temp. °C	Refractive Index, n_D	Density g cm^{-3}	Vapor Pressure, mmHg
10		0.8340		10		0.836		20	1.437	0.833	
20	1.439	.8268		20	1.4367	.8289		25	1.434		
25	1.435	.8233		25		.8253		109.			10
30		.8197		30		.8217		110			10.7
40		.8124		40		.8144		120			18.3
50		.8049		50		.8069		130			30.
60		.7974		60		.7993		140			46.
70		.7897		70		.7915		150			70.
80		.7818		80		.7836		160			102.
90		.7738		90		.7754		170			144.
100		.7656		100		.7671		180			199.
110		.7656		108.			10	190			270.
114.8			10	110		.7585		200			357.
120		.7487	13.4	120		.7406		204.			400
130		.7399	22.8	130		.731		210			465.
140		.731	37.					220			596.
150			58.					230			752.
160			87.					230.5			760
164.			100								
170			127.								
180			181.								
190			251.								
200			341.								
205.			400								
210			455.								
220			595.								
230.			760								

Constants	Temp. Range	*A*	*B*	*C*	*E*	Constants	Temp. Range	*A*	*B*	*C*	*E*	Constants	Temp. Range	*A*	*B*	*C*	*E*
Antoine eq	114–230 °C	6.3965	1159.	100.		Antoine eq						Antoine eq	112–230 °C	6.1045	1065.4	100.	
Francis eq	14–132 °C	0.96005	0.4553×10^{-3}	59.55	500	Francis eq	17–128 °C	0.98423	4.050×10^{-4}	70.67	500	Francis eq					

TABLE 192. Isomeric Undecanols. Selected values. Physical properties of the liquid

4-Methyl-4-decanol

Temp. °C	Refractive Index, n_D	Density g cm^{-3}	Vapor Pressure, mmHg
0		0.8436	
10		.8357	
20		.8278	
25	1.4375	.8238	
30		.8199	
40		.8120	
50		.8041	
60		.7962	
70		.7883	

Constants	Temp. Range	A	B	C	E
Antoine eq					
Francis eq	0–65 °C	0.8436	7.9×10^{-4}		

2,5-Dimethyl-3-isopropyl-3-hexanol

Temp. °C	Refractive Index, n_D	Density g cm^{-3}	Vapor Pressure, mmHg
20	1.4429	0.8480	
25	1.4402	.844	
60			3.6
65			4.8
70			6.5
75			8.6
78			10
80			11.3
85			14.6
90			18.7
95			23.8
100			30.0
105			37.0
110			46.
115			57.
120			70.
125			84.
130			102.
135			122.
140			145.
145			171.
150			202.
155			236.
160			275.
165			320.
170			369.
173			400.
175			424.
180			487.
185			556.
190			632.
195			716.
197			760.
200			809.

Constants	Temp. Range	A	B	C	E
Antoine eq	48–185 °C	6.7859	1414.5	168.3	
Francis eq					

2,2,4-Trimethyl-3-isopropyl-3-pentanol

Temp. °C	Refractive Index, n_D	Density g cm^{-3}	Vapor Pressure, mmHg
20	1.4550	0.869	
25	1.453	.867	
60			2.2
65			3.1
70			4.4
75			6.1
80			8.2
83.5			10
85			10.9
90			14.3
95			18.
100			24.
105			30.
110			37.
115			46.
120			56.
125			68.
130			81.
135			97.
136.			100
140			114
145			134.
150			157.
158.			200
160			210.
165			241.
170			275.
175			313.
180			353.
185			398.
190			447.
195			499.
200			555.
205			615.
210			681.
215			750.
215.7			760
220			824.

Constants	Temp. Range	A	B	C	E
Antoine eq	48–185 °C	5.4886	823.	100.	
Francis eq					

Isomeric Undecanols

Investigators		Vapor Pressures and Boiling Points		Freezing Point	Density, *d* g cm^{-3}		Refractive Index, n_D	
		°C	mmHg	t_m, °C	20 °C	25 °C	20 °C	25 °C
2-Undecanol, $C_{11}H_{24}O$, mol wt. 172.31, state at 25 °C liq.								
See also table 191								
Giesecke	[1870]	228–229	760		0.8261			
Power and Lees	[1902]	231–233	760					
Thoms and Mannich	[1903]				.8249			
Mannich	[1902]	120	14					
Houben	[1902]	115 120	10 14					
Haller and Lassieur	[1910]	228–233	760			0.826		1.4328
Pickard and Kenyon	[1911]	119	12	12	.8270		1.4369	
Pickard and Kenyon	[1912]	228	760					
Müller	[1942]						1.4387	
Dreger, Keim, Miles, Shedlovsky, and Ross	[1944]	136	27	0				
Jasperson and Jones	[1947]	228–234	760				1.4402 1.4475	
Zeiss and Tsutsui	[1953]	130–131	28					1.4358
Selected value	[1967]	[e] 230. ±2 [e] 114.8±1	760 10		[d] .8269 ±.0005	[d] .8233 ±.0005	[b] 1.349 ±0.002	[b] 1.435 ±0.002
Antoine constants: *A* 6.3965, *B* 1159., *C* 100.						*dt*/*dp* at 760 mmHg, 0.0537 °C/mmHg		
3-Undecanol, $C_{11}H_{24}O$, mol wt. 172.31, state at 25 °C liq.								
See also table 191								
Pickard and Kenyon	[1913]	117 229	16 760	17	0.8295		1.4367	
Selected value	[1967]	[c] 108±2	10		[d] .8289 ±.001	[d] 0.8253 ±.001		
5-Undecanol, $C_{11}H_{24}O$, mol wt. 172.31								
Protiva, Exner, Borovicka, and Pliml	[1952]	94–96	2.5					
6-Undecanol, $C_{11}H_{24}O$, mol wt. 172.31, state at 25 °C liq.								
Hess and Bappert	[1925]	111 117 235	12 16 754	16	0.8334		1.4370	
Union Carbide Corporation	[1936]	228–229	760	24.2				
Wicket and Freure	[1937]	228–229	760					
Komarewsky and Coley	[1941a]			15–16				
Dreger, Keim, Miles, Shedlovsky, and Ross	[1944]	92	1	20.5				
Zeiss and Tsutsui	[1953]	130–132	28					1.4334
Selected value	[1967]	[e] 230.5±1. [e] 109. ±2.	760 10	[a] 24.2				
Antoine constants: *A* 6.10, *B* 1065.4, *C* 100.						*dt*/*dp* at 760 mmHg, 0.0586 °C/mmHg		

Isomeric Undecanols—Continued

Investigators		Vapor Pressures and Boiling Points		Freezing Point	Density, d g cm^{-3}		Refractive Index, n_D	
		°C	mmHg	t_m, °C	20 °C	25 °C	20 °C	25 °C
2-Methyl-1-decanol, $C_{11}H_{24}O$, mol wt. 172.31								
Keil and Schiller	[1947]	122	13					
4-Methyl-1-decanol, $C_{11}H_{24}O$, mol wt. 172.31								
Cason, Brewer, and Pippen	[1948]	105–107	5					1.4383
5-Methyl-1-decanol, $C_{11}H_{24}O$, mol wt. 172.31								
Levene and Marker	[1933]	140	25			0.839		
2-Methyl-2-decanol, $C_{11}H_{24}O$, mol wt. 172.31								
Petrov and Kurbskii	[1944]	82–83	1–2					
Prevost and Singer	[1950]	118	23					
Urry, Stacey, Juveland, and		49	0.1				1.4359	
McDonnell	[1953]	50–52	0.2				1.4369	
Urry, Stacey, Huyser, and Juveland	[1954]	75	0.3				1.4368	
Selected value	[1967]	[c] 104±3.	10				[b] 1.4365 ±0.001	[c] 1.434 ±0.001
4-Methyl-2-decanol, $C_{11}H_{24}O$, mol wt. 172.31								
Cymerman, Heilbron, and Jones	[1944]	104	12				1.4328	
4-Methyl-3-decanol, $C_{11}H_{24}O$, mol wt. 172.31								
Gredy	[1935]	91	13			0.827	1.4354	
6-Methyl-3-decanol, $C_{11}H_{24}O$, mol wt. 172.31								
Levene and Marker	[1931d]	117	22			0.828		
2-Methyl-4-decanol, $C_{11}H_{24}O$, mol wt. 172.31								
Werner and Bogert	[1938]	123–125	12			0.8168		1.4310
4-Methyl-4-decanol, $C_{11}H_{24}O$, mol wt. 172.31								
See also table 192								
Owen, Quayle, and Beavers	[1930]					0.8236		
Whitmore and Orem	[1938]				0.8296			1.437
Selected value	[1967]				[d] 0.8278 ±0.001	[d] .8238 ±0.001		

Isomeric Undecanols—Continued

Investigators		Vapor Pressures and Boiling Points		Freezing Point	Density, *d* g cm^{-3}		Refractive Index, n_D	
		°C	mmHg	t_m, °C	20 °C	25 °C	20 °C	25 °C
2-Methyl-5-decanol, $C_{11}H_{24}O$, mol wt. 172.31								
Powell and Hagemann	[1944]	122.5–123	24		0.8266		1.4351	
5-Methyl-5-decanol, $C_{11}H_{24}O$, mol wt. 172.31								
Whitmore and Williams	[1933]	106–107	15			0.8262	1.4369	
Church, Whitmore, and McGrew	[1934]	104–105	15				1.4373	
Selected value	[1967]						[b] 1.4371 ±0.001	[c] 1.435 ±0.001
2-Ethyl-1-nonanol, $C_{11}H_{24}O$, mol wt. 172.31								
Bowden and Adkins	[1934]	126	19–20					
7-Ethyl-1-nonanol, $C_{11}H_{24}O$, mol wt. 172.31								
Thewalt and Rudloph	[1965]	142	5					1.4499 (30°)
3,3-Dimethyl-1-nonanol, $C_{11}H_{24}O$, mol wt. 172.31								
Mousseron and Bolle	[1956–1957]	122–124	15					
4,8-Dimethyl-1-nonanol, $C_{11}H_{24}O$, mol wt. 172.31								
von Braun and Kaiser	[1923]	110–113 117–120	14 15		0.833			
Sax and Stross	[1957]						1.4385	
4-Ethyl-2-nonanol, $C_{11}H_{24}O$, mol wt. 172.31								
Union Carbide Corporation	[1958]	225.4	760		0.8348			
5-Ethyl-2-nonanol, $C_{11}H_{24}O$, mol wt. 172.31								
Weissler	[1948]					0.8267 (30°)		1.4362 (30°)
Union Carbide Corporation	[1958]	225.4	760		0.8348			
6-Ethyl-3-nonanol, $C_{11}H_{24}O$, mol wt. 172.31								
Levene and Marker	[1931e]	127 114	15 16		0.832			

Isomeric Undecanols—Continued

Investigators	Vapor Pressures and Boiling Points		Freezing Point	Density, d g cm^{-3}		Refractive Index, n_D	
	°C	mmHg	t_m, °C	20 °C	25 °C	20 °C	25 °C
4-Ethyl-4-nonanol, $C_{11}H_{24}O$, mol wt. 172.31							
Powell and Nielsen [1948]	112–113	15		0.837 (16°)		1.4412 (16°)	
2,2-Dimethyl-4-nonanol, $C_{11}H_{24}O$, mol wt. 172.31							
Whitmore, Popkin, Whitaker, Mattil, and Zech [1938]	90–93 96	10 13		0.8225		1.4338	
Whitmore, Whitaker, Mattil, and Popkin [1938]	132	100				1.4340– 1.4347	
Selected value [1967]	[c] 92±2.	10				[b] 1.434 ±0.001	[c] 1.432 ±0.001
2,4-Dimethyl-4-nonanol, $C_{11}H_{24}O$, mol wt. 172.31							
Petrov and Zakharov [1959]	93–94	10		0.8285		1.4362	
3,4-Dimethyl-4-nonanol, $C_{11}H_{24}O$, mol wt. 172.31							
Shine and Turner [1949]	68–69	2				1.4430	
4,8-Dimethyl-4-nonanol, $C_{11}H_{24}O$, mol wt. 172.31							
Escourrou [1928]	105–106	16		0.8458 (11°)		1.44917 (11°)	
5-Ethyl-5-nonanol, $C_{11}H_{24}O$, mol wt. 172.31							
Church, Whitmore, and McGrew [1934]	100–102	15				1.4411	
Whitmore and Woodburn [1933]	102.6–103.6 113.6–114.2	15.5 15		0.8376	0.8345	1.4400	
Protiva, Exner, Borovicka, and Pliml [1952]	78–81	5					
Selected value [1967]	[c] 93±2.	10				[b] 1.4405 ±0.001	[c] 1.439 ±0.001
2,6-Dimethyl-5-nonanol, $C_{11}H_{24}O$, mol wt. 172.31							
Bjelous [1912]	98–99	11			0.8126		1.42956
5,7-Dimethyl-5-nonanol, $C_{11}H_{24}O$, mol wt. 172.31							
Thaker and Vasi [1960]	118–125	20		0.8264 (28°)			1.433
5-*n*-Propyl-1-octanol, $C_{11}H_{24}O$, mol wt. 172.31							
Keil and Schiller [1947]	129–130	20					

Isomeric Undecanols—Continued

Investigators	Vapor Pressures and Boiling Points		Freezing Point	Density, d g cm^{-3}		Refractive Index, n_D	
	°C	mmHg	t_m, °C	20 °C	25 °C	20 °C	25 °C
3-n-Propyl-2-octanol, $C_{11}H_{24}O$, mol wt. 172.31, state at 25 °C Liq.							
Guerbet [1912b]	234–235	760	5	0.828			
3,7,7-Trimethyl-3-octanol, $C_{11}H_{24}O$, mol wt. 172.31							
Gutman and Hickinbottom [1951]	101–103	21				1.4342	
4-n-Propyl-4-octanol, $C_{11}H_{24}O$, mol wt 172.31							
Whitmore and Woodburn [1938]	101.4–102.4	15		0.8351	0.8319	1.4390	
4-Isopropyl-4-octanol, $C_{11}H_{24}O$, mol wt. 172.31							
Nazarov and Kakhniashvilli [1954c]	69–70	3		0.840		1.445	
2,2,4-Trimethyl-4-octanol, $C_{11}H_{24}O$, mol wt. 172.31							
Whitmore, Popkin, Whittaker, Mattil, and Zech [1938]	78–79	9				1.4400	
Moersch and Whitmore [1949]	137.1	100		0.835		1.4405	
	79.8	8					
Selected value [1967]	^{c}83±2	10				^{b}1.4402 ±0.001	^{c}1.438 ±0.001
2,4,7-Trimethyl-4-octanol, $C_{11}H_{24}O$, mol wt. 172.31							
Meyer and Tuot [1933]	100	17		0.8235		1.4359	
3,3,6,6-Tetramethyl-1-heptanol, $C_{11}H_{24}O$, mol wt. 172.31, state at 25 °C							
Brandstrom, A [1959]	103–108	8					
3-n-Butyl-2-heptanol, $C_{11}H_{24}O$, mol wt. 172.31							
Hess and Bappert [1925]	108–109	16				1.44042 (18.2°)	
2-Methyl-3-isopropyl-3-heptanol, $C_{11}H_{24}O$, mol wt. 172.31							
Connant and Blatt [1929]	115–118	45		0.8487		1.4435	
George [1943]	157.2	170		0.8557		1.4471	
	148.1	125					
Nazarov and Pinkira [1949]	85	10		0.8490		1.4455	
Selected value [1967]	^{e}85±1.	10		^{b}0.851 ±0.003	^{c}0.847 ±0.003	^{b}1.446 ±0.0015	^{c}1.444 ±0.002

Antoine constants: *A* 4.660, *B* 532., *C* 60.

Isomeric Undecanols—Continued

Investigators	Vapor Pressures and Boiling Points		Freezing Point	Density, *d* g cm^{-3}		Refractive Index, n_D	
	°C	mmHg	t_m, °C	20 °C	25 °C	20 °C	25 °C
2,2,3,4-Tetramethyl-3-heptanol, $C_{11}H_{24}O$, mol wt. 172.31							
Nazarov [1937]	212.5	760		0.866 (9°)		1.4530 (13°)	
2,2,3,6-Tetramethyl-3-heptanol, $C_{11}H_{24}O$, mol wt. 172.31							
Petrov, Sushchinskii, Zakharov, and Rogozhnikova [1957]	69.2–71.3	3		0.8506		1.4387	
2,3,4,4-Tetramethyl-3-heptanol, $C_{11}H_{24}O$, mol wt. 172.31							
Nazarov [1937]	215–217	760		0.870		1.4580	
2,2,6,6-Tetramethyl-3-heptanol, $C_{11}H_{24}O$, mol wt. 172.31, state at 25 °C crystal							
Whitmore, Whitaker, Mosher, Breivik, Wheeler, Miner, Sutherland, Wagner, Clapper, Lewis, Lux, and Popkin [1941]			58–59				
2-Methyl-4-*n*-propyl-4-heptanol, $C_{11}H_{24}O$, mol wt. 172.31							
Halse [1914]	86–88	12		0.833		1.43908 (13°)	
3,5-Diethyl-4-heptanol, $C_{11}H_{24}O$, mol wt. 172.31							
Zerner [1911]	99–101	13					
2,6-Dimethyl-4-ethyl-4-heptanol, $C_{11}H_{24}O$, mol wt. 172.31							
Casey [1959]	72–73	6				1.4368	
3,3-Dimethyl-5-ethyl-4-heptanol, $C_{11}H_{24}O$, mol wt. 172.31							
Whitmore, Whitaker, Mosher, Breivik, Wheeler, Miner, Sutherland, Wagner, Clapper, Lewis, Lux, and Popkin [1941]	150–152	150		0.8530 .8496		1.4435– 1.4440	
2,2,4,6-Tetramethyl-4-heptanol, $C_{11}H_{24}O$, mol wt. 172.31							
Moersch and Whitmore [1949]	64.0	7		0.828		1.4368	

Isomeric Undecanols—Continued

Investigators		Vapor Pressures and Boiling Points		Freezing Point	Density, *d* g cm^{-3}		Refractive Index, n_D	
		°C	mmHg	t_m, °C	20 °C	25 °C	20 °C	25 °C
2,2,5,5-Tetramethyl-4-heptanol, $C_{11}H_{24}O$, mol wt. 172.31								
Ansell, Hickinbottom, and Hyatt	[1955]	85	14				1.4410	
3,3,5,5-Tetramethyl-4-heptanol, $C_{11}H_{24}O$, mol wt. 172.31								
Haller and Bauer	[1913]	210–212	760					
5-Methyl-3-isobutyl-2-hexanol, $C_{11}H_{24}O$, mol wt. 172.31								
Freylon	[1910]	105	18		0.844(4°)			
2,2-Dimethyl-3-*n*-propyl-3-hexanol, $C_{11}H_{24}O$, mol wt. 172.31								
Leroide	[1921]	90	20		0.851		1.4447	
2,4-Dimethyl-3-isopropyl-3-hexanol, $C_{11}H_{24}O$, mol wt. 172.31								
Young and Roberts	[1944]	120.7–121.5	50				1.4518–1.4520	
2,5-Dimethyl-3-isopropyl-3-hexanol, $C_{11}H_{24}O$, mol. wt. 172.31								
See also table 192								
Murat and Amouroux	[1914]	102–105	40		0.8737 (16°)		1.448	
Whitmore and George	[1942]	140	125				1.4426	
		118.5	60					
George	[1943]	139.7	125		.8470		1.4426	
		149.0	170					
Cadwallader, Fookson, Mears, and Howard	[1948]	180–185 105–110	760 38		.8486		1.4430	
Zook, March, and Smith	[1959]	47–48	2					1.4402
Selected value	[1967]	[e] 197. ±3. [e] 78. ±2.	760 10		[b] .8480 ±0.0006	[c] 0.844 ± .001	[b] 1.4429 ±0.0005	[a] 1.4402 ±0.0007

Antoine constants: *A* 6.7486, *B* 1414.5, *C* 168.3. *dt/dp* at 760 mmHg, 0.0539 °C/mmHg

Investigators		°C	mmHg	t_m, °C	20 °C	25 °C	20 °C	25 °C
2,2,3-Trimethyl-4-ethyl-3-hexanol, $C_{11}H_{24}O$, mol. wt. 172.31								
Nazarov	[1937]	208–211	760		0.859		1.4518	

Isomeric Undecanols—Continued

Investigators		Vapor Pressures and Boiling Points		Freezing Point	Density, *d* g cm^{-3}		Refractive Index, n_D	
		°C	mmHg	t_m, °C	20 °C	25 °C	20 °C	25 °C
2,2,3,4,4-Pentamethyl-3-hexanol, $C_{11}H_{24}O$, mol. wt. 172.31								
Nazarov	[1937]	219–222	760		0.884		1.4661	
2,2,3,4,5-Pentamethyl-3-hexanol, $C_{11}H_{24}O$, mol. wt. 172.31								
Nazarov	[1937]	207–210	760		0.868 (12°)		1.4535 (13°)	
3,4,4,5,5-Pentamethyl-3-hexanol, $C_{11}H_{24}O$, mol. wt. 172.31								
Petrov, Kao, and Semenkin	[1960]	106–108	58		0.8778		1.4611	
2,2,4,5,5-Pentamethyl-4-hexanol, $C_{11}H_{24}O$, mol. wt. 172.31, state at 25 °C liq.								
Moersch and Whitmore	[1949]	124.1	100	11.4	0.841		1.4412	
		60.2	7					
Selected value	[1967]	[c] 67±2.	10					
2,4-Dimethyl-3-*n*-butyl-3-pentanol, $C_{11}H_{24}O$, mol. wt. 172.31								
Young and Roberts	[1944]	121	50		0.860		1.4479	
2,2,4-Trimethyl-3-isopropyl-3-pentanol, $C_{11}H_{24}O$, mol. wt. 172.31, state at 25 °C liq.								
See also table 192								
Bartlett and Schneider	[1945]	103–104	27				1.4562	
Vavon and Collin	[1946]	88.5–91	10		0.869		1.4556	
Cadwallader, Fookson, Mears, and Howard	[1948]	105–107	35				1.4550	
Smith and Creitz	[1951]	215.4	760	−18.3	0.8758		1.4574	
Zook, March, and Smith	[1959]	48	1					1.4560
Petrov, Sokolova, and Kao	[1960]	121–121.5	55		0.8661		1.4517	
Selected value	[1967]	[e] 215.7±1. [e] 83±2.	760 10		[b] 0.869 ±0.002	[c] 0.867 ±0.002	[a] 1.4550 ±0.001	[c] 1.453 ±0.001

Antoine constants: *A* 5.4886, *B* 823., *C* 100.

dt/*dp* at 760 mmHg, 0.0692 °C/mmHg

1-Dodecanol

Properties of the Liquid Phase at Various Temperatures

Refractive Index

Reported values of the refractive index at 20 and 25 °C are listed in table 194. Values at higher temperatures, up to 80 °C, have been published by Weissler [1948], Spizzichino [1956], Rathmann, Curtis, McGeer, and Smyth [1956], and Vil'shan and Gavrilova [1963]. Except for the value of Vil'shan and Gavrilova the values fall fairly close to a linear function of temperature. The selected values given in tables 193 and 194 are taken from a smoothed curve through these data. The value given by Zaar [1931] at 25 °C has been carefully measured and the selected value is close to his. The data at 20 °C refer to the undercooled liquid.

Density

Densities were calculated from the Francis equation, using constants reported in table 193. The Constants were adjusted by the least-squares criteria to fit the data underlined in table 194 at 20 and 25 °C, and to fit the data of Weissler [1948], Geiseler, Quitzsch, Hesselbach, and Huttig [1962], and Costello and Bowden [1958] at higher temperatures. Most of these agree to within about 0.001 g cm^{-3} with the calculated values.

Vapor Pressures and Boiling Points

Table 194 lists a number of experimental boiling point values in the range of 2 to 135 mmHg. Most of these are the result of only rough measurements. There is no reported value for the boiling point at 760 mmHg. The most accurate values of the vapor pressure have been published by Rose, Papahronis, and Williams [1958] who measured this property in an equilibrium still from 138 to 214 °C along with vapor liquid equilibrium data for two binary alcohol mixtures. Their Antoine constants were selected for this range and reported in table 193. In addition there have been several studies of the vapor pressure of solid and liquid dodecanol at lower temperatures. Spizzichino [1956] measured the vapor pressure of the liquid by a direct static method from 27 to 64 °C; Hoyer and Peperle [1958] determined the sublimation pressure of the solid by a torsion method; Geiseler, Quitzsch, Hesselbach, and Huttig [1962] reported data from 30 to 90 °C; and Davies and Kybett [1965] measured the sublimation pressure from 12 to 21 °C, and the vapor pressure of the liquid from 24 to 40 °C by the Knudsen effusion method. Davies and Kybett did not report the experimental values directly but gave the equations, $\log P(\mathrm{mmHg}) = 19.694 - 6794/T$ for the solid and $\log P(\mathrm{mmHg}) = 13.633 - 4981/T$ for the liquid as representing their measurements. Hoyer and Peperle and Geiseler, Quitzsch, Hesselbach, and Huttig also gave similar equations in addition to the experimental points. Spizzichino calculated the constants in the Rankine vapor pressure equation. However, the vapor pressures calculated from this equation did not match the experimental measurements very closely and the origin of these constants was not fully explained in the paper. The data of Geiseler et al. were reasonably consistent with the equation of Davies and Kybett in the region of overlap, and their equation gives reasonable values at higher temperatures. However, there are no reliable experimental data to check its accuracy from 90 to 135°C. The sublimation pressures measured by Hoyer and Peperle are appreciably higher than those of Davies and Kybett, although the slopes are similar. The values of Spizzichino agree fairly well the those of Davies and Kybett at the low temperature end of the range, but become progressively higher at higher temperatures. Although the method of measurement of Spizzichino should be reliable, the slope of her data gives rise to an unreasonably large heat of vaporization. The Antoine constants for the low temperature range reported in table 193 were based mainly on the data of Geiseler et al. and of Davies and Kybett, with some adjustment to correspond to the higher temperature data.

Solid-Gas Phase Equilibria

Sublimation Pressure

Vapor pressures of the solid phase have been measured by Davies and Kybett [1965] by the Knudsen effusion method, and by Hoyer and Peperle [1958] by a torsion method. Hoyer and Peperle represented their data by $\log P(\mathrm{mmHg}) = 21.29 - 7205/T$. The equation obtained by Davies and Kybett was given in the previous section. The data of Davies and Kybett are judged to be more reliable. The solid phase consists of the β-crystal, as described in Appendix E.

Heat of Sublimation

The vapor pressure equation of Hoyer and Peperle [1958] gives a heat of sublimation of 33.0 kcal mol^{-1}, while that of Davies and Kybett [1965] gives 31.1 kcal mol^{-1}. The latter value was selected.

Solid-Liquid and Solid-Solid Phase Equilibria

Melting Points and Transition Temperatures

1-Dodecanol exists in two solid forms, the α- and the β-phases. A general discussion of polymorphism in the higher alcohols is given in Appendix E. The preponderance of evidence favors identification of the stable phase which crystallizes from the liquid at 23.8 °C as the β-phase. Phillips and Mumford [1934] report that the α-phase melts at 21.6 °C. This indicates that the α-phase is metastable at all temperatures and therefore would

TABLE 193. 1-Dodecanol. Selected values. Physical and thermodynamic properties

Temp. °C	Refractive Index, n_D	Density g cm^{-3}	Vapor Pressure, mmHg
20	* 1.4428	* 0.8243	
25	1.4413	.8308	0.00084
30	1.4398	.8273	.00159
40	1.4357	.8204	.00522
50	1.4320	.8134	.0153
60	1.4283	.8063	.0406
70	1.4246	.7991	.0993
80	1.4208	.7919	.225
90		.7846	.478
100		.7773	
110		.7698	
120		.7623	
130		.7547	
135			8.53
138.2			10
140		.7470	10.9
145			13.9
150		.7392	17.5
155			21.9
160		.7314	27.2
165			33.6
170		.7234	41.2
175			50.3
180		.7153	61.0
185			73.6
190		.7071	88.3
193.5			100
195			105.
200		.6988	125.
205			148.
210		.6904	174.
214.3			200
215			205.
220		.6819	239.
225			278.
230		.6732	322.
240		.6644	
250		.6554	
260		.6463	
270		.6370	
280		.6275	
290		.6080	
300		.5979	

Data For Phase Transitions

Initial	Final	Temp. °C	dt/dP deg mm^{-1}	Pressure mmHg	ΔH kcal mol^{-1}	$d\Delta H/dt$	ΔS	ΔC_p
						cal deg^{-1} mol^{-1}		
c,u	liq	21.6±1						
c	liq	23.8±0.2		0.00071	7.5±1.5		25.±4	
c	g	23.8±0.2		.00071	31.1±1		105.±3	
liq	g	25	9030.	.00084	23.3±1		78.±3	

Condensed Phase Heat Capacity

State	Temp. °C	C_p
		cal deg^{-1} mol^{-1}

Properties of the Saturated Real Gas

Temp. °C	H^r-H^0	S^r-S^0	$C_p{}^r-C_p{}^0$
	kcal mol^{-1}	cal deg^{-1} mol^{-1}	

Data for the Standard States at 25 °C

State	Heat of Combustion $\Delta H_c{}^0$ kcal mol^{-1}	Heat of Formation $\Delta H_f{}^0$ kcal mol^{-1}	Entropy S^0 cal deg^{-1} mol^{-1}	Gibbs Energy of Formation $\Delta G_f{}^0$ kcal mol^{-1}	Heat Capacity, C_p cal deg^{-1} mol^{-1}

Critical Constants

Temp. °C, K	Pressure atm	Density g cm^{-3}

Constants in Vapor Pressure and Density Equation

Antoine Equation

Temp. Range	A	B	C
24 to 90 °C	7.5421	1968.7	160.4
138 to 214 °C	7.53986	2003.29	168.13

Francis Equation

Temp. Range	A	$B\times10^3$	C	E
20 to 300 °C	1.0113	0.4729	130.74	800

* Undercooled liquid.

TABLE 194. 1-Dodecanol. Reported values. Simple physical properties

Investigators		Vapor Pressures and Boiling Points		Freezing Point	Density, d g cm^{-3}		Refractive Index, n_D	
		°C	mmHg	t_m, °C	20 °C	25 °C	20 °C	25 °C
1-Dodecanol, $C_{12}H_{26}O$, mol. wt. 186.34, state at 25 °C liq.								
Scheuble and Loebl	[1904]	150	20	22.6				
Marvel and Tanenbaum	[1922]	143–146	18					
Verkade and Coops	[1927]	130.3–130.4	7.0	23.8		0.8298		
Biltz, Fischer, and Wunnenberg	[1930b]			23.4				
Ford and Marvel	[1930]	143–146	18					
		198–200	135					
Zaar	[1931]	114	2	21.6		.8312		1.44149
		120–121	3.5					
Schrauth, Schenck, and Stickdorn	[1931]	145–148	18	21–22				
Meyer and Reid	[1933]			23.87				
Mumford and Phillips	[1933]			23.5				
Phillips and Mumford	[1934]			23.8				
Palfray and Sabetay	[1936]	140–145	8	26		.8273	1.4415	
		131–133	13					
Strating and Backer	[1936]			24.0–24.2				
Whitmore, Whitaker, Mosher, Breivik, Wheeler, Miner, Sutherland, Wagner, Clapper, Lewis, Lux, and Popkin	[1941]	150	22	24				
		153.5	25					
Palfray	[1940b]	131–140		26				
Halasz	[1940]	141–142	15	24				
Muller	[1942]			24	0.8329		1.4455	
Hsu	[1943]	143.5	15	23.5	0.8302		1.4425	
Reid, Ruhoff, and Burnett	[1943]	192.5–193.5	100					
		151–152	21					
Asinger	[1944]	123–124	4.6					
Hoerr, Harwood, and Ralston	[1944]			23.95				
Stoll and Rouve	[1944]			24–25	0.8340			
Parks and Rowe	[1946]	150 155	21	17.3				
Grundmann	[1948]	138–139	12	23				
Hoffman and Smyth	[1949]			23.5				
Walker	[1949]			23.4				
Sackmann and Sauerwald	[1950]			23.8		0.8297		
Winsor	[1950]			23			1.4409	
Heyding and Winkler	[1951]	160–162	30	21				
Smith and Creitz	[1951]			23.5				
Broughton, Bowman, and Ames	[1952]			23.5				
Colonge and Berthoux	[1952]	144–146	16.5					
McKenna, Tartar, and Lingafelter	[1953]	145–146	18					1.4396
Epstein, Wilson, Jakob, Conroy, and Ross	[1954]	133	3.5					1.4410
Petrov, Sushchinskii, and Konoval'chikov	[1955]				0.8536		1.4547	
Spizzichino	[1956]			23.8				
Rathmann, Curtis, McGreer, and Smyth	[1956]			23.5				
Tanaka, Seto, and Hayachida	[1957]			22–23				
Costello and Bowden	[1958]	114	20	24				
Geiseler, Quitzsch, Hesselbach, and Huttig	[1962]			23.6	.8346	0.8312		1.4424
Mil'shan and Gavrilova	[1963]			23.0				
Blood and Hagemeyer	[1964]				.8345			
Davies and Kybett	[1965a]			22.3–23.6				
Rose, Papahronis, and Williams	[1958]	138.1	9.9					1.44098
Selected value	[1967]			23.8±0.2	.8343	0.8308	1.4428	1.4413
		138.2±0.3	10		±.0005	±0.0005	±0.0005	±0.0005

Antoine constants: A 7.53986, B 2003.29, C 168.13.

place dodecanol in Class 1 of Appendix E. This interpretation is also verified by studies of the dielectric constant and loss factors of long chain alcohols reported by Hoffman and Smyth [1949]. On the other hand Tanaka, Seto, and Hayashida [1957] found that the α-phase first crystallizes from the melt on cooling and then converts to the β-phase at 18 °C. However, it seems probable that the $\alpha \rightarrow \beta$ transition which they observed is not an equilibrium one, and that the α-phase is metastable. The fact that they did not observe the $\beta \rightarrow \alpha$ transition on heating confirms this interpretation.

Heat of Fusion

The heat of fusion at 23.8 °C was calculated from the selected values of the heat of sublimation and the heat of vaporization.

Liquid-Vapor Equilibrium at 25 °C

Vapor Pressure

The vapor pressure was calculated from the Antoine constants listed for the low temperature range in table 193.

Heat of Vaporization

No calorimetric values have been reported. The heats of vaporization calculated from the vapor pressure equations of Spizzichino [1956], Geiseler, Quitzsch, Hesselbach, and Huttig [1962], Davies and Kybett [1965a], and the selected Antoine constants are 23.3, 19.9, 22.8, and 23.3 kcal mol^{-1} respectively. Although the heat of vaporization calculated from the equation given by Spizzichino agrees with that calculated from the Antoine constants in table 193, her equation does not agree very closely with her observed vapor pressures. The value given by the Antoine constants was selected. The heat of vaporization at 23.8 °C, used to calculate the heat of fusion, is calculated to be 23.6 kcal mol^{-1}.

Isomeric Dodecanols

The reported values of the simple physical properties of the isomeric dodecanols are summarized in the following unnumbered tables. A few scattered values of density and refractive index at temperatures other than 20 and 25 °C are also included. Geiseler, Quitzsch, Hesselbach, and Huttig [1962] measured the density, as well as the viscosity and surface tension, of 1-dodecanol and the five secondary straight chain dodecanols from 20 to 90 °C. They also measured the vapor pressure from about 20 to 70 °C and gave the constants in the equation $\log P(\text{mmHg}) = A - B/T$. Since the vapor can be considered an ideal gas at these low pressures, the average heat of vaporization for this range of temperature can be calculated from B. The results of these calculations are shown in table 195.

The constants in the Francis equation, and the corresponding calculated densities from 20 to 130 °C for 2-decanol in table 195, are derived from the experimental values of Pickard and Kenyon [1911] and [1913] and from Geiseler, Quitzsch, Hesselbach, and Huttig [1962]. The Antoine constants and vapor pressures at 130 °C and above are based on the scattered boiling points listed in the unnumbered table for 2-decanol. The density data of Pickard and Kenyon [1913] and of Geiseler et al. were the basis of the selected densities of 3-dodecanol in table 196.

The selected densities of 2-methyl-3-undecanol in table 197 were based on the measurements of Pickard and Kenyon [1912]. The Antoine constants and corresponding vapor pressures of 2-n-butyl-1-octanol in table 198 were calculated from available boiling points, with the assumption of $C = 60$. The only other available measurements of physical properties over a range of temperature are the densities of Owen, Quayle and Beavers [1930] for 5-methyl-5-undecanol from 0 to 65 °C, which can be represented by $d = 0.8444 - 0.000768t$, and the densities of Quayle and Smart [1944] for 5-ethyl-5-decanol from 25 to 55 °C, which can be represented by $d = 0.8564 - 0.000830t$.

TABLE 195. Isomeric Dodecanols. Heats of vaporization calculated from vapor pressure data from 20 to 70 °C

Compound	ΔH_v, kcal mol^{-1}
2-Dodecanol	20.3
3-Dodecanol	18.7
4-Dodecanol	19.3
5-Dodecanol	19.0
6-Dodecanol	19.5

TABLE 196. Isomeric Dodecanols. Selected values. Physical properties of the liquid

2-Dodecanol			
Temp. °C	Refractive Index, n_D	Density g cm^{-3}	Vapor Pressure, mmHg
20	1.442	0.8297	0.00102
25	1.4401	.8262	.00183
30		.8227	.00322
40		.8155	.00944
50		.8083	.0259
60		.8009	.0671
70		.7934	.164
80		.7858	.382
90		.7779	
100		.7700	
120		.7535	
129.			10
130		.745	10.7
135			14.2
140			18.6
145			24.
150			31.
155			39.
160			48.
165			60.
170			74.
175			89.
178.			100
180			108.
185			129.
190			153.
195			181.
198.			200
200			212.
205			247.
210			286.
215			330.
220			378.
222.			400
225			431.
230			490.
235			554.
240			625.
245			701.
249.			760
250			784.

Constants	Temp. Range	*A*	*B*	*C*	*E*
Antoine eq	20–70	12.16	4442.	273.2	
Antoine eq	127–249	5.8477	915.6	60	
Francis eq	20–123	1.02632	0.3676×10^{-3}	109.8	600

3-Dodecanol			
Temp. °C	Refractive Index, n_D	Density g cm^{-3}	Vapor Pressure, mmHg
20		0.8313	0.00305
25	1.4402	.8278	.00523
30		.8243	.00881
40		.8171	.0238
50		.8097	.0603
60		.8021	.145
70		.7942	.330
80		.7861	.717
90		.7778	.717
100		.7691	
110		.7602	
120		.7509	
124			10
130		.741	

Constants	Temp. Range	*A*	*B*	*C*	*E*
Antoine eq	20–70	11.44	4091	273.2	
Francis eq	20–124	1.04208	0.2627×10^{-3}	98.7	500

4-Dodecanol			
Temp. °C	Refractive Index, n_D	Density g cm^{-3}	Vapor Pressure, mmHg
20	1.441	0.8291	0.00247
25	1.4390	.8256	.00429
30		.8219	.00734
40		.8146	.0204
50		.8072	.0531
60		.7996	.131
70		.7919	.305
80		.7841	.678
90		.7761	.678
100		.768	
122			10

Constants	Temp. Range	*A*	*B*	*C*	*E*
Antoine eq	20–70	11.75	4209	273.2	
Francis eq	20–90	1.01598	0.4073×10^{-3}	103.6	600

TABLE 197. Isomeric Dodecanol. Selected values. Physical properties of the liquid

5-Dodecanol				6-Dodecanol				2-Methyl-3-undecanol			
Temp. °C	Refractive Index, n_D	Density g cm^{-3}	Vapor Pressure, mmHg	Temp. °C	Refractive Index, n_D	Density g cm^{-3}	Vapor Pressure, mmHg	Temp. °C	Refractive Index, n_D	Density g cm^{-3}	Vapor Pressure, mmHg
20	1.4388	0.8296	0.00238	25	* 1.4386	* 0.8239	* 0.00412	0		0.8482	
25	1.4388	.8260	.00411	30		.8202	.00709	10		.8402	
30		.8225	.00698	40		.8128	.0199	20		.8322	
40		.8152	.0191	50		.8054	.0524	25		.8282	
50		.8078	.0491	60		.7978	.130	30		.8242	
60		.8003	.119	70		.7902	.307	40		.8161	
70		.7926	.275	80		.7824	.689	50		.8080	
80		.7846	.604	90		.7745		60		.7999	
90		.7766		100		.766		70		.7917	
100		.768		110			4.9	80		.7835	
123.			10	120			9.5	90		.7752	
				121.			10	100		.7669	
				130			17.	110		.7586	
				140			28.	120		.7502	
								130		.7418	
								140		.7333	
								150		.7247	
								160		.7160	
								170		.7073	
								180		.6985	
								190		.6896	

Constants	Temp. Range	A	B	C	E	Constants	Temp. Range	A	B	C	E	Constants	Temp. Range	A	B	C	E
Antoine eq	20–70 °C	11.53	4149	273.2		Antoine eq	30–70 °C	11.89	4256	273.2		Antoine eq					
Francis eq	20–90 °C	1.06546	0.3070×10^{-3}	133.3	600	Francis eq	30–90 °C	0.93060	0.5319×10^{-3}	44.4	500	Francis eq	0–190 °C	0.87857	0.7366×10^{-3}	15.2	500

* Undercooled liquid.

TABLE 198. Isomeric Dodecanols. Selected values. Physical properties of the liquid

2-*n*-Butyl-1-octanol

Temp. °C	Refractive Index, n_D	Density g cm^{-3}	Vapor Pressure, mmHg
15	1.444	0.837	
20	1.442	.8340	
25	1.4400	.832	
127.			10
130			12.1
140			20.5
150			33.
160			51.
170			75.
178.			100
180			108.
190			151.
199.			200
200			205.
210			273.
220			355.
224.			400
230			455.
240			572.
250			709.
253.4			760

Constants	Temp. Range	*A*	*B*	*C*	*E*
Antoine eq	130–252 °C	5.6501	868.	60.	
Francis eq					

Constants	Temp. Range	*A*	*B*	*C*	*E*
Antoine eq					
Francis eq					

Constants	Temp. Range	*A*	*B*	*C*	*E*
Antoine eq					
Francis eq					

Isomeric Dodecanols

2-Dodecanol, $C_{12}H_{26}O$, mol. wt. 186.34, state at 25 °C liq.

See also table 196

Investigators	Vapor Pressures and Boiling Points °C	Vapor Pressures and Boiling Points mmHg	Freezing Point t_m, °C	Density, d g cm^{-3} 20 °C	Density, d g cm^{-3} 25 °C	Refractive Index, n_D 20 °C	Refractive Index, n_D 25 °C
Pickard and Kenyon [1911]	140	15	5	0.8315		1.4423	
	146	24	18.7				
Pickard and Kenyon [1912]	245	760					
Baumgarten [1942]	125	9	18–19				
Smolin [1955]	250	760					
Geiseler, Quitzsch, Hesselbach, and Hüttig [1962]	129	11					1.4401
Selected value [1967]	249.±1	760	19.±1	.8297 ±.0005	.8262 ±.0005		
	129.±2	10					

Antoine constants: A 5.8477, B 915.6, C 60.

dt/dp at 760 mmHg, 0.0596 °C/mmHg

3-Dodecanol, $C_{12}H_{26}O$, mol. wt. 186.34, state at 25 °C liq.

Investigators	Vapor Pressures and Boiling Points °C	Vapor Pressures and Boiling Points mmHg	Freezing Point t_m, °C	Density, d g cm^{-3} 20 °C	Density, d g cm^{-3} 25 °C	Refractive Index, n_D 20 °C	Refractive Index, n_D 25 °C
Pickard and Kenyon [1913]	130	15	25				
Baumgarten [1942]	123	9	12				
Geiseler, Quitzsch, Hesselbach, and Hüttig [1962]	127	11		0.8316	0.8280		1.4402
Selected value [1967]	[c] 124±1.	10	[a] 25±2.	[d] .8313 ±.0003	[d] .8278 ±.0003		

4-Dodecanol, $C_{12}H_{26}O$, mol. wt. 186.34

Investigators	Vapor Pressures and Boiling Points °C	Vapor Pressures and Boiling Points mmHg	Freezing Point t_m, °C	Density, d g cm^{-3} 20 °C	Density, d g cm^{-3} 25 °C	Refractive Index, n_D 20 °C	Refractive Index, n_D 25 °C
Baumgarten [1942]	120	9					
Urry, Stacey, Juveland, and McDonnell [1943]	83–84	1				1.4409	
Urry, Stacey, Huyser, and Juveland [1954]	83–84	1				1.4409	
Geiseler, Quitzsch, Hesselbach, and Hüttig [1962]	124	11		0.8292	0.8255		1.4390
Selected value [1967]	[c] 122±1.	10		[d] .8291 ±.0005	[d] .8255 ±.0005	[b] 1.441 ±0.001	[a] 1.439 ±0.001

5-Dodecanol, $C_{12}H_{26}O$, mol. wt. 186.34

See also table 197

Investigators	Vapor Pressures and Boiling Points °C	Vapor Pressures and Boiling Points mmHg	Freezing Point t_m, °C	Density, d g cm^{-3} 20 °C	Density, d g cm^{-3} 25 °C	Refractive Index, n_D 20 °C	Refractive Index, n_D 25 °C
Baumgarten [1942]	121	9					
Geiseler, Quitzsch, Hesselbach, and Hüttig [1962]	133	16		0.8295	0.8260		1.4388
Selected value [1967]	[c] 123±1.	10		[d] 0.8296 ±0.0005	[d] 0.8260 ±0.0005		

Isomeric Dodecanols—Continued

Investigators		Vapor Pressures and Boiling Points		Freezing Point	Density, *d* g cm^{-3}		Refractive Index, n_D	
		°C	mmHg	t_m, °C	20 °C	25 °C	20 °C	25 °C
6-Dodecanol, $C_{12}H_{26}O$, mol. wt. 186.34, state at 25 °C crystal								
See also table 197								
Bouveault and Locquin	[1906]	119	9	30				
Baumgarten	[1942]	120	9					
Griess	[1955]	126	12					
Geiseler, Quitzsch, Hasselbach, and Hüttig	[1962]	125	12	29.0				* 1.4386
Studt, P.	[1966]	137	26					
Selected value	[1967]	[c] 121±1.	10	[a] 29.0±1.		[d] * 0.823		
* Undercooled liquid.								
2-Methyl-1-undecanol, $C_{12}H_{26}O$, mol. wt. 186.34								
Mousseron and Bolle	[1956–1957]	129	12					
3-Methyl-1-undecanol, $C_{12}H_{26}O$, mol. wt. 186.34								
Prout, Cason, and Ingersoll	[1948]	117	2		0.8341	0.8309		1.4409
9-Methyl-1-undecanol, $C_{12}H_{26}O$, mol. wt. 186.34								
Lardicci, Salvador, and Pino	[1962]	138–139	17			0.8316		1.4413
10-Methyl-1-undecanol, $C_{12}H_{26}O$, mol. wt. 186.34								
Milburn and Truter	[1954]	147–149	18				1.4412	
2-Methyl-2-undecanol, $C_{12}H_{26}O$, mol. wt. 186.34								
Houben	[1902]	117–118	12.5					
Barbier and Locquin	[1913]	123–127	13					
Behal	[1919]	134–135	15		0.8349 (13°)		1.43968 (13°)	
Prevost and Singer	[1950]	115	14					
Mauge, Malen, and Boissier	[1956]	98–104	20					
Selected value	[1967]	[c] 100±1.	10					
2-Methyl-3-undecanol, $C_{12}H_{26}O$, mol. wt. 186.34								
See also table 197								
Pickard and Kenyon	[1912]	236	760		0.8327		1.4405	

Isomeric Dodecanols—Continued

Investigators		Vapor Pressures and Boiling Points		Freezing Point	Density, *d* g cm^{-3}		Refractive Index, n_D	
		°C	mmHg	t_m, °C	20 °C	25 °C	20 °C	20 °C
3-Methyl-3-undecanol, $C_{12}H_{26}O$, mol. wt. 186.34								
Urry, Stacey, Juveland, and McDonnell	[1953]	58–60 63	0.2 0.025				1.4416–1.4418	
Urry, Stacey, Huyser, and Juveland	[1954]	63 58–60	0.1 0.1				1.4416–1.4418	
Selected value	[1967]						^{b}1.4417 ±0.001	^{c}1.440 ±0.001
2-Methyl-4-undecanol, $C_{12}H_{26}O$, mol. wt. 186.34								
Koch and Schauerte	[1965]	131.5	20				1.4369	
2-Methyl-5-undecanol, $C_{12}H_{26}O$, mol. wt. 186.34								
Powell and Hageman	[1944]	132–133	24		0.8266		1.4346	
Petrov and Ol'dekop	[1949]	128–130	20		0.8251		1.436	
Selected value	[1967]				^{b}0.826 ±0.001	^{c}0.822 ±0.001	^{b}1.435 ±0.001	^{c}1.433 ±0.001
3-Methyl-5-undecanol, $C_{12}H_{26}O$, mol. wt. 186.34								
Levene and Harris	[1935]	113	12			0.8264		1.4367
4-Methyl-5-undecanol, $C_{12}H_{26}O$, mol. wt. 186.34								
Koch and Schauerte	[1965]	131.5	20				1.4417	
5-Methyl-5-undecanol, $C_{12}H_{26}O$, mol. wt. 186.34								
See also table 197								
Owen, Quayle, and Beavers	[1930]					0.8247		
Griess	[1955]	126	10					
Selected value	[1967]				^{d}0.8291 ±0.0007	^{d}0.8252 ±0.0007		
6-Methyl-6-undecanol, $C_{12}H_{26}O$, mol. wt. 186.34								
Whitmore and Williams	[1933]	80–83	2.0			0.8271	1.4392	
Church, Whitmore, and McGrew	[1934]	117–120	15				1.4395	
Frank and Foster	[1954]	78–83	1.5–2.0				1.4386	
Selected value	[1967]						^{b}1.4391 ±0.0007	^{c}1.437 ±0.001

Isomeric Dodecanols—Continued

Investigators		Vapor Pressures and Boiling Points		Freezing Point	Density, d g cm^{-3}		Refractive Index, n_D	
		°C	mmHg	t_m, °C	20 °C	25 °C	20 °C	25 °C
2-Ethyl-1-decanol, $C_{12}H_{26}O$, mol. wt. 186.34								
von Braun and Teuffert	[1929]	135–137	12					
2,2-Dimethyl-1-decanol, $C_{12}H_{26}O$, mol. wt. 186.34, state at 25 °C liq.								
Blondeau	[1928]	134	19					
Blood and Hagemeyer	[1964]	244	760	−44	0.8345			1.4408
Selected value	[1967]	^{c} 122±2.	10					
3,3-Dimethyl-1-decanol, $C_{12}H_{26}O$, mol. wt. 186.34								
Mousseron and Bolle	[1956]	135–137	15					
3-Ethyl-3-decanol, $C_{12}H_{26}O$, mol. wt. 186.34								
Colonge and Berthoux	[1952]	88–91	3					
6-Ethyl-3-decanol, $C_{12}H_{26}O$, mol. wt. 186.34								
Powell and Baldwin	[1936]	119–120	18			0.8364 (28°)		1.4435 (28°)
Union Carbide Corporation	[1936]	115–118	10					
Wicket and Freure	[1937]	225	760					
Selected value	[1967]	^{c} 118±2.	10					
3-Ethyl-4-decanol, $C_{12}H_{26}O$, mol. wt. 186.34								
Mousseron and Bolle	[1956]	90–93	5					
2,4-Dimethyl-4-decanol, $C_{12}H_{26}O$, mol. wt. 186.34								
Petrov and Zakharov	[1959]	87–89	2		0.8284		1.4390	
3,3-Dimethyl-4-decanol, $C_{12}H_{26}O$, mol. wt. 186.34								
Koch and Schauerte	[1965]	126	20				1.4447	

Isomeric Dodecanols—Continued

Investigators	Vapor Pressures and Boiling Points		Freezing Point	Density, *d* g cm^{-3}		Refractive Index, n_D	
	°C	mmHg	t_m, °C	20 °C	25 °C	20 °C	25 °C
5-Ethyl-5-decanol, $C_{12}H_{26}O$, mol. wt. 186.34							
See also table 197							
Grimshaw and Shorlemmer [1873]	112	13					
Quayle and Smart [1944]					0.8357	1.4424	1.4401
Rabjohn and Latina [1954]	119–120	20				1.4428	
Selected value [1967]				^{d}0.8399 ±0.0007	^{d}.8357 ±.0007	^{b}1.4426 ±0.0007	^{a}1.4401 ±0.001
6,6-Dimethyl-5-decanol, $C_{12}H_{26}O$, mol. wt. 186.34							
Whitmore and Krueger [1933]	112–112	15		0.845		1.4469	
2,6-Dimethyl-6-decanol, $C_{12}H_{26}O$, mol. wt. 186.34							
Escourro [1928]	115	14		0.8526 (11°)		1.45537 (12°)	
6,8-Dimethyl-6-decanol, $C_{12}H_{26}O$, mol. wt. 186.34							
Thaker and Vasi [1960]	143–155	20			0.82770 (28°)		1.440
2-*n*-Propyl-1-nonanol, $C_{12}H_{26}O$, mol. wt. 186.34							
von Braun and Kroper [1929]	132–133	14					
3-Methyl-2-ethyl-1-nonanol, $C_{12}H_{26}O$, mol. wt. 186.34							
Fieser, Berlinger, Bondhus, Chang, Dauben, Ettlinger, Fawaz, Fields, Heidelberger, Heymann, Vaughan, Wilson, Wilson, Wu, Leffler, Hamlin, Matson, Moore, Moore, and Zaugg [1948]	65	0.1					1.4447
2-Methyl-5-ethyl-3-nonanol, $C_{12}H_{26}O$, mol. wt. 186.34							
Petrov, Nefedov, and Grigor'ev [1957]	81–82	2.5		0.8471		1.4412	
7-Methyl-5-ethyl-3-nonanol, $C_{12}H_{26}O$, mol. wt. 186.34							
Guerbet [1912d]	250–253	760		0.9210 (0°)			

Isomeric Dodecanols—Continued

Investigators	Vapor Pressures and Boiling Points		Freezing Point	Density, d g cm^{-3}		Refractive Index, n_D	
	°C	mmHg	t_m, °C	20 °C	25 °C	20 °C	25 °C
3,7,7-Trimethyl-3-nonanol, $C_{12}H_{26}O$, mol. wt. 186.34							
Gutman and Hickinbottom [1951]	62–73	0.6				1.4430	
4-*n*-Propyl-4-nonanol, $C_{12}H_{26}O$, mol. wt. 186.34							
Whitmore and Williams [1933]	75–76	1.4			0.8324	1.4406	
Church, Whitmore, and McGrew [1934]	88–90	4				1.4413	
Selected value [1967]						^{b}1.4410 ±0.001	^{c}1.439 ±0.001
2,2,4-Trimethyl-4-nonanol, $C_{12}H_{26}O$, mol. wt. 186.34							
Whitmore, Popkin, Whitaker, Mattil, and Zech [1938]	92	8				1.4425	
2,6,8-Trimethyl-4-nonanol, $C_{12}H_{26}O$, mol. wt. 186.34, state at 25 °C liq.							
Union Carbide Corporation [1958]	225.2	760	−60 (glass)	0.8179			
5-*n*-Propyl-5-nonanol, $C_{12}H_{26}O$, mol. wt. 186.34							
Church, Whitmore, and McGrew [1934]	110–112	12				1.4427	
Whitmore and Woodburn [1938]				0.8370	0.8340	1.4419	
Protiva, Exner, Borovička, and Pliml [1952]	104–106	7					
Meshcheryakov, Erzyutova, and Kuo [1961]	113.6–114	15		.8399		1.4420	
Selected value [1967]	^{c}109±2.	10		^{b}.838 ±.001	^{a}.834 ±.001	^{b}1.4422 ±0.0007	^{c}1.440 ±0.001
5-Isopropyl-5-nonanol, $C_{12}H_{26}O$, mol. wt. 186.34							
Whitmore and Kreuger [1933]	75.0–75.5	2		0.844		1.4446	
	110–113	16					
Selected value [1967]	^{c}102±2.	10					
2,5,8-Trimethyl-5-nonanol, $C_{12}H_{26}O$, mol. wt. 186.34							
Halse [1914]	105–106	12					
Yur'ev and Belyakova [1959]	100–101	9		0.8289		1.4385	

Isomeric Dodecanols—Continued

Investigators		Vapor Pressures and Boiling Points		Freezing Point	Density, *d* g cm^{-3}		Refractive Index, n_D	
		°C	mmHg	t_m, °C	20 °C	25 °C	20 °C	25 °C
2-*n*-Butyl-1-octanol, $C_{12}H_{26}O$, mol. wt. 186.34, state at 25 °C liq.								
See also table 198								
von Braun and Kroper	[1929]	131–133	12					
Mastagli	[1938]	132	15		0.8371 (16.5°)		1.4435 (16°)	
Bolle and Bourgeois	[1951]	137	4					
Union Carbide Corporation	[1953]	253.3	760	−80	.8340			
Pratt and Kubler	[1954]							1.4400
Griess	[1955]	126	10					
Mousseron and Bolle	[1956]	114–117	10					
Selected value	[1967]	^{e}253.4±0.5	760		^{a}.8340 ±.0007	^{c}0.832 ±.001	^{c}1.442 ±0.001	^{a}1.4400 ±0.001
		^{e}127±1.	10					
4-*n*-Butyl-1-octanol, $C_{12}H_{26}O$, mol. wt. 186.34								
Levene and Cretcher	[1918]	139	15					
Levene and Allen	[1916]	139	15		0.838			
Levene and Taylor	[1922b]	127–130	8					
Selected value	[1967]	^{c}132±2.	10					
2,4-Diethyl-1-octanol, $C_{12}H_{26}O$, mol. wt. 186.34								
Miller and Bennett	[1961]	106–108	4		0.840			1.4482
2,5,7,7-Tetramethyl-2-octanol, $C_{12}H_{26}O$, mol. wt. 186.34								
Turner and Turner	[1951]	85.5–88	5					1.4360
2-Methyl-3-isopropyl-3-octanol, $C_{12}H_{26}O$, mol. wt. 186.34								
George	[1943]	165.2	125		0.8537		1.4484	
		174.8	170					
2,2-Dimethyl-4-ethyl-3-octanol, $C_{12}H_{26}O$, mol. wt. 186.34								
Whitmore, Whitaker, Mosher, Breivik,		105	17		0.8409		1.4420	
Wheeler, Miner, Sutherland, Wagner,		162	150					
Clapper, Lewis, Lux, and Popkin	[1941]							
Selected value	[1967]	^{c}95±2.	10					
5-Methyl-5-*n*-propyl-4-octanol, $C_{12}H_{26}O$, mol. wt. 186.34								
Leroide	[1921]	109–112	18		0.8455 (16.5°)		1.4421 (16.5°)	

Antoine constants (2-*n*-Butyl-1-octanol): *A* 5.6501, *B* 867.8, *C* 60. *dt*/*dp* at 760 mmHg, 0.0647 °C/mmHg

Isomeric Dodecanols—Continued

Investigators	Vapor Pressures and Boiling Points		Freezing Point	Density, *d* g cm^{-3}		Refractive Index, n_D	
	°C	mmHg	t_m, °C	20 °C	25 °C	20 °C	25 °C
2,2,7,7-Tetramethyl-4-octanol, $C_{12}H_{26}O$, mol. wt. 186.34, state at 25 °C crystal							
Cook [1943]			37.3				
4-Methyl-2-*n*-butyl-1-heptanol, $C_{12}H_{26}O$, mol. wt. 186.34							
Hagemeyer and Hudson [1958]	232	760					
2-Isobutyl-6-methyl-1-heptanol, $C_{12}H_{26}O$, mol. wt. 186.34							
Mousseron and Bolle [1956]	112–114	10					
3-Methyl-3-*n*-butyl-2-heptanol, $C_{12}H_{26}O$, mol. wt. 186.34							
Hess and Bappert [1925]				0.8375			
Whitmore and Krueger [1933]	112.0–112.5	14		.850		1.4492	
2,2-Dimethyl-3-isopropyl-3-heptanol, $C_{12}H_{26}O$, mol. wt. 186.34							
Nazarov and Kotlyarevskii [1950]	79	6		0.8565		1.4578	
2,6-Dimethyl-3-isopropyl-3-heptanol, $C_{12}H_{26}O$, mol. wt. 186.34							
Murat and Amouroux [1914]	137–140	65		0.8606 (16°)		1.442	
2,2,3,4,4-*Pentamethyl-3-heptanol*, $C_{12}H_{26}O$, *mol. wt.* 186.34							
Nazarov [1937]	233–235	760		0.885 (13°)		1.4628	
2,2,3,6,6-Pentamethyl-3-heptanol, $C_{12}H_{26}O$, mol. wt. 186.34, state at 25 °C crystal							
Cook [1943]			32.5				
2,2,4,6,6-Pentamethyl-3-heptanol, $C_{12}H_{26}O$, mol. wt. 186.34							
Whitmore, Whitaker, Mosher, Breivik, Wheeler, Miner, Sutherland, Wagner, Clapper, Lewis, Lux, and Popkin [1941]	102–106	22		0.8380		1.4400–1.4416	
Davis and Hickinbottom [1957]	100–102	21				1.4420	
Selected value [1967]						^{b}1.442 ±0.001	^{c}1.440 ±0.001

Isomeric Dodecanols—Continued

Investigators		Vapor Pressures and Boiling Points		Freezing Point	Density, *d* g cm^{-3}		Refractive Index, n_D	
		°C	mmHg	t_m, °C	20 °C	25 °C	20 °C	25 °C
2,2,5,6,6-Pentamethyl-3-heptanol, $C_{12}H_{26}O$, mol. wt. 186.34								
Colonge	[1935]	107	20		0.843		1.4477 (16°)	
2,2-Dimethyl-4-*n*-propyl-4-heptanol, $C_{12}H_{26}O$, mol. wt. 186.34								
Whitmore, Popkin, Whitaker, Mattil, and Zech	[1938]	94–96	10		0.8376		1.4429	
Whitmore and Forster	[1942]	67	3		0.8386		1.4423– 1.4428	
Selected value	[1967]				^{b}0.838 ±0.001	^{c}0.834 ±0.001	^{b}1.4425 ±0.001	^{c}1.441 ±0.001
2,6-Dimethyl-4-isopropyl-4-heptanol, $C_{12}H_{26}O$, mol. wt. 186.34								
Shine and Turner	[1949]	48–49	1				1.4448	
3,4,5-Trimethyl-3-ethyl-4-heptanol, $C_{12}H_{26}O$, mol. wt. 186.34								
Nazarov	[1937]				0.885 (13°)		1.4613	
2,2,3,3,4-Pentamethyl-4-heptanol, $C_{12}H_{26}O$, mol. wt. 186.34								
Petrov, Kao, and Semenkin	[1960]	153–154	85		0.8772		1.4608	
3,3,4,5,5-Pentamethyl-4-heptanol, $C_{12}H_{26}O$, mol. wt. 186.34								
Nazarov	[1937]	243–246	760		0.9004 (16°)			
5-Methyl-2-(3-methylbutyl)-1-hexanol, $C_{12}H_{26}O$, mol. wt. 186.34								
von Braun and Kurtz	[1937]	122–124	14		0.8340			
5,5-Dimethyl-4-tert-butyl-1-hexanol, $C_{12}H_{26}O$, mol. wt. 186.34								
Petrov, Sokolova, and Kao	[1961]				0.8652			
2,5-Dimethyl-3-isobutyl-2-hexanol, $C_{12}H_{26}O$, mol. wt. 186.34								
Freylon	[1910]	93–94	7					

Isomeric Dodecanols—Continued

Investigators		Vapor Pressures and Boiling Points		Freezing Point	Density, d g cm^{-3}		Refractive Index, n_D	
		°C	mmHg	t_m, °C	20 °C	25 °C	20 °C	25 °C
2,2-Dimethyl-3-tert-butyl-3-hexanol, $C_{12}H_{26}O$, mol. wt. 186.34, state at 25 °C liq.								
Cadwallader, Fookson, Mears, and Howard	[1948]	117	22	−10.1	0.8595		1.4563	
Smith and Creitz	[1951]	117	22		.8595		1.4563	
Petrov, Sokolova, and Chin-Lan	[1957]	101	22		.8652		1.4542	
Petrov, Sokolova, and Kao	[1960]						1.4542	
Selected value	[1967]				[b] .8595 ±0.0005	[c] 0.856 ±0.001	[b] 1.4563 ±0.0007	[c] 1.454 ±0.001
2-Methyl-4-ethyl-3-isopropyl-3-hexanol, $C_{12}H_{26}O$, mol. wt. 186.34								
George	[1943]	157.5 167.9	125 170		0.8528		1.4477	
Selected value	[1967]	[c] 95±2.	10					
2,2,5-Trimethyl-3-isopropyl-3-hexanol, $C_{12}H_{26}O$, mol. wt. 186.34								
Petrov, Sushchinskii, Zakharov, and Rogozhnikova	[1957]	65.6–66.5	2		0.8552		1.4505	
2,5,5-Trimethyl-3-isopropyl-3-hexanol, $C_{12}H_{26}O$, mol. wt. 186.34								
Whitmore and George	[1942]	127	60				1.4472	
Zook, March, and Smith	[1959]	52–54	1					1.4459
Selected value	[1967]	[c] 86±2	10					
2,2-Dimethyl-4,4-diethyl-3-hexanol, $C_{12}H_{26}O$, mol. wt. 186.34								
Haller and Bauer	[1913]	226–228	760					
2,2,3,4-Tetramethyl-4-ethyl-3-hexanol, $C_{12}H_{26}O$, mol. wt. 186.34								
Nazarov	[1937]	237–240	760		0.890		1.4702	
2,2,3,4,4,5-Hexamethyl-3-hexanol, $C_{12}H_{26}O$, mol. wt. 186.34								
Nazarov	[1937]	235–238	760		0.893 (13°)		1.4668	
2,2,4,4,5,5-Hexamethyl-3-hexanol, $C_{12}H_{26}O$, mol. wt. 186.34								
Favorskii and Nazarov	[1933]	99	15		0.8481 (15°)			
Bartlett and Stiles	[1955]	130–135	70					1.4547
Selected value	[1967]	[c] 92±2	10					

Isomeric Dodecanols—Continued

Investigators	Vapor Pressures and Boiling Points		Freezing Point	Density, d g cm^{-3}		Refractive Index, n_D	
	°C	mmHg	t_m, °C	20 °C	25 °C	20 °C	25 °C
2,3,4,4,5,5-Hexamethyl-3-hexanol, $C_{12}H_{26}O$, mol. wt. 186.34							
Petrov, Kao, and Semenkin [1960]				0.8886		1.4667	
4,4-Dimethyl-2-(2,2-dimethyl-1-propyl)-1-pentanol, $C_{12}H_{26}O$, mol. wt. 186.34, state at 25 °C crystal							
Whitmore, Whitaker, Mosher, Breivik, Wheeler, Miner, Sutherland, Wagner, Clapper, Lewis, Lux, and Popkin [1941]	108	17	44				
2,4,4-Trimethyl-2-*tert*-butyl-1-pentanol, $C_{12}H_{26}O$, mol. wt. 186.34							
Whitmore, Whitaker, Mosher, Breivik, Wheeler, Miner, Sutherland, Wagner, Clapper, Lewis, Lux, and Popkin [1941]	113-114 118-120 126.5	16 25 28		0.8748		1.4610	
2,4,4-Trimethyl-3-*tert*-butyl-2-pentanol, $C_{12}H_{26}O$, mol. wt. 186.34, state at 25 °C lig.							
Petrov, Sokolova, and Kao [1961]			24				
2,2,4,4-Tetramethyl-3-isopropyl-3-pentanol, $C_{12}H_{26}O$, mol. wt. 186.34							
Bartlett and Schneider [1945]	120-122	30					1.4625
Cadwallader, Fookson, Mears, and Howard [1948]	113	37				1.4655	
Smith and Creitz [1951]	234.0	760		0.8889		1.4646	
Petrov, Sokolova, and Chin-Lan [1957]	78	4		0.8853		1.4655	
Selected value [1967]	^{a}234±1. ^{c}95±4.	760 10		^{b}0.8875 ±0.001	^{c}0.884 ±0.001	^{b}1.4650 ±0.0007	^{a}1.4625 ±0.001

Tridecanols

The physical property data for the tridecanols have been given in the following unnumbered tables. Tanaka, Seto, and Hayashida [1957] have determined that the stable form of 1-tridecanol at the melting point is the α-crystal. They report the α to β transition temperature is 25 °C. Meyer and Reid [1933] previously reported a more accurate value of 23.85 °C for this temperature. The boiling point of 201–204 at 750mmHg reported by Hill, Senter, Haynes, and Hill [1954] for 1-tridecanol appears unreasonably low, and since no other measurement has been reported, no selection of the normal boiling point was made. The experimental data are insufficient to permit the calculation of either density or vapor pressure as functions of temperature.

Eykman [1919] investigated several physical properties of 4-*n*-propyl-4-decanol and 5-*n*-butyl-5-nonanol. Besides the properties listed in the corresponding unnumbered tables he obtained a density of 0.7670 g cm^{-3} for 4-*n*-propyl-4-decanol at 79.2 °C and 0.7689 g cm^{-3} as for 5-*n*-butyl-5-nonanol at 78.7 °C. He also measured the refractive indices at several wavelengths and at two temperatures near 20 and 80 °C. These data, converted to standard temperatures and wavelengths, are shown in table 199.

The densities of 2-tridecanol and 3-tridecanol listed in table 200 are calculated from data reported by Pickard and Kenyon [1911], [1912], and [1913]. The densities of 6-methyl-6-dodecanol are based on the values of Owen, Quayle, and Beavers [1939].

For the most part the Antoine constants and vapor pressures of the highly branched isomers in table 201 were calculated from the data of Mosher [1954].

TABLE 199. Isomeric Tridecanols. Selected values. Refractive index at various temperatures and wavelengths

Symbol	Wavelength, angstroms	Refractive index			
		4-*n*-Propyl-4-decanol		5-*n*-Butyl-5-nonanol	
		20 °C	80 °C	20 °C	80 °C
He_{red}	6678.1	1.4411	1.4148	1.4424	1.4142
H_c	6562.8	1.4414	1.4151	1.4427	1.4151
Na_D	5892.6	1.4436	1.4170	1.4448	1.4165
Hg_e	5460.7	1.4455	1.4188	1.4467	1.4183
He_{blue}	5015.7	1.4481	1.4211	1.4493	1.4207
H_F	4861.3	1.4491	1.4223	1.4504	1.4217
Hg_g	4358.3	1.4533	1.4262	1.4546	1.4257
$H_{G'}$	4340.5	1.4536	1.4264	1.4548	1.4258

TABLE 200. Isomeric tridecanols. Selected values. Density of the liquids at various temperatures

Temperature °C	2-Tridecanol	3-Tridecanol	6-Methyl-6-dodecanol	5-*n*-Propyl-5-decanol	5-*n*-Butyl-5-nonanol
	Density, g cm^{-3}				
0			0.8452		
10			.8382		
20			.8310	0.8360	0.8417
25	0.8282		.8273	.8320	.8355
30	.8244	0.826	.8236	.8280	.8293
40	.8168	.8183	.8159	.8200	.8169
50	.8092	.8110	.8080	.8121	.8045
60	.8015	.8034	.7998	.8041	.7921
70	.7937	.7957	.7913		.7797
80	.7858	.7878			
90	.7779	.7797			
100	.7699	.7713			
110	.7618	.7627			
120	.7536	.7539			
130	.7453	.7448			
140	.7369	.735			
150	.728				

Francis Constants

Temp. Range, °C	34–145	43–128	0–65	25–55	20–79
A	0.9032	1.0015	1.0936	0.8519	0.8665
$B\times10^3$	.630	0.361	0.194	.797	1.240
C	28.1	77.6	124.2		
E	500	500	500		

TABLE 201. Isomeric tridecanols. Selected values. Vapor pressure of the liquids at various temperatures

Temperature °C	2,2-Dimethyl-3-tert-butyl-3-heptanol	3,3,5,5-tetramethyl-4-ethyl-4-heptanol	3,3,6-Trimethyl-4-isopropyl-4-heptanol	3,3,6-Trimethyl-4-*n*-propyl-4-heptanol	2,2,5-Trimethyl-3-*tert*-butyl-3-hexanol
	Vapor pressures mmHg				
104.					10
108.	10		10		
110	11.0		11.0	10	13.5
118.		10			
120	17.6	10.9	17.9	16.4	21.5
130	27.	16.7	28.	26.	33.
140	41.	25.	42.	39.	49.
150	60.	37.	62.	58.	70.
160	85.	53.	89.	84.	100
164.	100		100		
165.				100	
170	119.	75.	124.	118.	136.
179.		100			
180	163.	104.	169.	161.	182.
183.					200
186.	200		200		
187.				200	
190	218.	142.	226.	217.	239.
200	288.	192.	298.	287.	310.
201.		200			
210	373.	256.	386.	374.	395.
211.					400
212.			400		
213.	400			400	
220	478.	336.	492.	478.	496.
227.		400			
230	603.	437.	619.	604.	614.
239.4			760		
240	753.	562.	770.	754.	752.
240.3				760	
240.4	760				
240.5					760
250		716.			
252.6		760			
	Antoine Constants				
Temp. Range	106–240	120–253	108–239	110–240	104–240
A	6.4890	7.8864	6.2978	6.3071	5.9308
B	1394.	2467.	1264.	1261.	1091.
C	145.8	240.2	130.7	127.5	117.3

Isomeric Tridecanols

Investigators		Vapor Pressures and Boiling Points		Freezing Point	Density, d g cm^{-3}		Refractive Index, n_D	
		°C	mmHg	t_m, °C	20 °C	25 °C	20 °C	20 °C
1-Tridecanol, $C_{13}H_{28}O$, mol. wt. 200.37, state at 25 °C crystal								
Blau	[1905]	155–156	15	30.5		0.8263 (31°)		
Levene, West, and Vander Scheer	[1915]	117	0.5					
Meyer and Reid	[1933]			30.63				
Turkiewiez	[1939]	152	14	30.5				
Ziegler and Gellert	[1950]			32				
Broughton, Bowman, and Ames	[1952]	116	0.6	29.5				
Hill, Senter, Haynes, and Hill	[1954]	201–204	750					
Sörensen and Sörensen	[1956]			26.5–26.7				
Tanaka, Seto, and Hayashida	[1957]			29–30				
Vil'shan and Gavrilova	[1963]			30–33		0.8165 (50°)		1.4351 (50°)
Selected value	[1967]	[c] 148.±3.	10	30.6±0.2				
2-Tridecanol, $C_{13}H_{28}O$, mol. wt. 200.37, state at 25 °C crystal								
See also table 200								
Pickard and Kenyon	[1911]	151	11	30		0.8279		
		156–157	17					
Pickard and Kenyon	[1912]	265	760					
Dreger, Keim, Miles, Shedlovsky, and Ross	[1944]	161	30	17				
Selected value	[1967]	[c] 146±3.	10	[a] 30±3.		[d] .8282 ±.001		
3-Tridecanol, $C_{13}H_{28}O$, mol. wt. 200.37, state at 25 °C crystal								
Pickard and Kenyon	[1913]	139	12	32				
4-Tridecanol, $C_{12}H_{28}O$, mol. wt. 200.27								
Petrov and Ol'dekep	[1948]	165–166	33		0.8234		1.438	
7-Tridecanol, $C_{13}H_{28}O$, mol. wt. 200.37, state at 25 °C crystal								
Tischer	[1939]			51				
Komarewsky and Coley	[1941a]			40.0–40.5				
Dreger, Keim, Miles, Shedlovsky, and Ross	[1944]			43				
Coley and Komarewsky	[1946]			40.0–40.5				
Rust, Seubold, and Vaughan	[1948]			40.5–41				
Gastambide	[1954]			43–43.5				
Selected value	[1967]			[b] 43±2.				

Isomeric Tridecanols—Continued

Investigators	Vapor Pressures and Boiling Points		Freezing Point	Density, d g cm^{-3}		Refractive Index, n_D	
	°C	mmHg	t_m °C	20 °C	25 °C	20 °C	25 °C
2-Methyl-1-dodecanol, $C_{13}H_{28}O$, mol. wt. 200.37							
Levene and Mikeska [1929]	105	1.4			0.844		
10-Methyl-1-dodecanol, $C_{13}H_{28}O$, mol. wt. 200.37, state at 25 °C							
Milburn and Truter [1954]	145–150	15				1.4550	
2-Methyl-2-dodecanol, $C_{13}H_{28}O$, mol. wt. 200.37							
Robinson [1924]	145	10					
Prevost and Singer [1950]	130	15					
6-Methyl-6-dodecanol, $C_{13}H_{28}O$, mol. wt. 200.37							
See also table 200							
Owen, Quayle, and Beavers [1939]					0.8274		
Selected value [1967]				^{d}0.8310 ±0.0007	^{d}0.8273 ±0.0007		
2-Ethyl-1-undecanol, $C_{13}H_{28}O$, mol. wt. 200.37							
Stoll [1947]	135–140	12		0.8404		1.4445	
3-Ethyl-3-undecanol, $C_{13}H_{28}O$, mol. wt. 200.37							
Masson [1901]	250	760					
6-Ethyl-6-undecanol, $C_{13}H_{28}O$, mol. wt. 200.37							
Whitmore and Williams [1933]	87–89	2.0			0.8348	1.4438	
Church, Whitmore, and McGrew [1934]	104–106	3				1.4424	
Selected value [1967]						^{b}1.443 ±0.001	^{c}1.441 ±0.001
3,5-Dimethyl-5-undecanol, $C_{13}H_{28}O$, mol. wt. 200.37							
Thaker and Vasi [1960]	160–170	20			0.8304		1.442

Isomeric Tridecanols—Continued

Investigators		Vapor Pressures and Boiling Points		Freezing Point	Density, *d* g cm^{-3}		Refractive Index, n_D	
		°C	mmHg	t_m, °C	20 °C	25 °C	20 °C	25 °C
4-*n*-Propyl-4-decanol, $C_{13}H_{28}O$, mo.l wt. 200.37								
See also table 199								
Eykman	[1919]	92	1		0.8387 (15.6°)		1.4436	
		107	3					
		118–119	9					
Selected value	[1967]	^{c} 122±2.	10				^{c} 1.4436 ±0.001	^{c} 1.4412 ±0.001
5-*n*-Propyl-5-decanol, $C_{13}H_{28}O$, mol. wt. 200.37								
See also table 200								
Quayle and Smart	[1944]					0.8320	1.4420	1.4397
Selected value	[1967]				^{d} 0.836 ±.0015	^{d} .8320 ±.001		
2,5,9-Trimethyl-5-decanol, $C_{13}H_{28}O$, mol. wt. 200.37								
Escourrou	[1928]	131–133	20		0.8444 (11°)		1.45007 (11°)	
2-*n*-Butyl-1-nonanol, $C_{13}H_{28}O$, mol. wt. 200.37								
Levene and Taylor	[1922b]	112–114	0.5		0.8359		1.4430	
3,6,8,8-Tetramethyl-3-nonanol, $C_{13}H_{28}O$, mol. wt. 200.37								
Turner and Turner	[1951]	85–88	2.8					1.4408
3,3-Dimethyl-5-ethyl-4-nonanol, $C_{13}H_{28}O$, mol. wt. 200.37								
Whitmore, Whitaker, Mosher, Breivik, Wheeler, Miner, Sutherland, Wagner, Clapper, Lewis, Lux, and Popkin	[1941]	125–137	25		0.8512		1.4482– 1.4490	

Isomeric Tridecanols—Continued

Investigators	Vapor Pressures and Boiling Points		Freezing Point	Density, d g cm^{-3}		Refractive Index, n_D	
	°C	mmHg	t_m, °C	20 °C	25 °C	20 °C	25 °C
5-n-Butyl-5-nonanol, $C_{13}H_{28}O$, mol. wt. 200.37, state at 25 °C liq							
See also tables 200 and 199							
Eykman [1919]	102 108	3 5	23.5		0.8333	1.4451	
Bourgom [1924]	177–178	15					
Moyer and Marvel [1931]	129–131	20					
Church, Whitmore, and McGrew [1934]	118–120	17				1.4445	
Whitmore and Woodburn [1938]	125.0 99.8–100.0	15 4		0.8408	.8368	1.4434	
Protiva, Exner, Borovicka, and Pliml [1952]	109–117	7					
Zook and Goldey [1953]	138	19				1.4449	
Challenger and Pantony [1954]	126–127 114–115	15 10					
Desgrandchamps, Deluzarche, and Maillard [1961]	148–150	15				1.4440	
Mescheryakov, Erzyutova, and Kuo [1961]	124–125	12		0.8442		1.4440	
Selected value [1967]	^{c} 119±3.	10		^{d} .8417 ±.001	^{d} 0.8355 ±0.001	^{b} 1.4448 ±0.0005	^{c} 1.4464 ±0.0007
2,8-Dimethyl-5-ethyl-5-nonanol, $C_{13}H_{28}O$, mol. wt. 200.37							
Halse [1914]	119–120	17		0.8677		1.44602 (15°)	
5,7,7-Trimethyl-3-ethyl-3-octanol, $C_{13}H_{28}O$, mol. wt. 200.37							
Turner and Turner [1951]	92	7					1.4431
2,2,3,3,4-Pentamethyl-4-octanol, $C_{13}H_{28}O$, mol. wt. 200.37							
Petrov, Kao, and Semenkin [1960]	124–126	15		0.8763		1.4616	
2,2-Dimethyl-3-n-butyl-3-heptanol, $C_{13}H_{28}O$, mol. wt. 200.37							
Whitmore, Popkin, Whitaker, Mattil, and Zech [1938]	105.5–107	11		0.8498		1.4488	

Isomeric Tridecanols—Continued

Investigators		Vapor Pressures and Boiling Points		Freezing Point	Density, d g cm^{-3}		Refractive Index, n_D	
		°C	mmHg	t_m, °C	20 °C	25 °C	20 °C	25 °C
2,2-Dimethyl-3-*tert*-butyl-3-heptanol, $C_{13}H_{28}O$, mol. wt. 200.37								
See also table 201								
Mosher	[1954]	**106**	9		0.8606		1.4546	
		140	41					
		240	753					
Petrov, Sokolova, and Kao	[1960]	121.5–123	24		.8596		1.4540	
Selected value	[1967]	[e] 240.4±1.	760		[b] .8602	[c] 0.856	[b] 1.4544	[c] 1.452
		[e] 108.1±1.	10		±.0007	±0.001	±0.0005	±0.001
Antoine constants: *A* 6.4890, *B* 1393.5, *C* 145.8.								*dt*/*dp* at 760 mmHg, 0.0612 °C/mmHg
2,2,3-Trimethyl-4-*n*-propyl-3-heptanol, $C_{13}H_{28}O$, mol. wt. 200.37, state at 25 °C								
Nazarov	[1937]	103–103.5	10		0.859 (12°)		1.4510 (17°)	
		234–237.5	760					
2,6-Dimethyl-4-isobutyl-4-heptanol, $C_{13}H_{28}O$, mol. wt. 200.37, state at 25 °C								
Shine and Turner	[1949]	72–73	2				1.4340	
3,3,6-Trimethyl-4-*n*-propyl-4-heptanol, $C_{13}H_{28}O$, mol. wt. 200.37								
See also table 201								
Mosher	[1954]	**110**	10		0.8598		1.4538	
		141	41					
		240	754					
Selected value	[1967]	[e] 240.4±1.	760					
		[e] 110.0±1.	10					
Antoine constants: *A* 6.3071, *B* 1260.5, *C* 127.5.								*dt*/*dp* at 760 mmHg, 0.0614 °C/mmHg
3,3,6-Trimethyl-4-isopropyl-4-heptanol, $C_{13}H_{28}O$, mol. wt. 200.37								
See also table 201								
Mosher	[1954]	**108**	10		0.8648		1.4550	
		141	44					
		239	754					
Selected value	[1967]	[e] 239.4±1	760					
		[e] 108.0±1	10					
Antoine constants: *A* 6.2978, *B* 1264.5, *C* 130.7.								*dt*/*dp* at 760 mmHg, 0.0619 °C/mmHg

Isomeric Tridecanols—Continued

Investigators	Vapor Pressures and Boiling Points		Freezing Point	Density, d g cm^{-3}		Refractive Index, n_D	
	°C	mmHg	t_m, °C	20 °C	25 °C	20 °C	25 °C
3,3,5-Triethyl-4-heptanol, $C_{13}H_{28}O$, mol. wt. 200.37							
Zerner [1911]	125–127	18					
3,3,5,5-Tetramethyl 4 ethyl-4 heptanol, $C_{13}H_{28}O$, mol. wt. 200.37							
Mosher [1954]	119.5 170.5 253	10.7 76 768		0.8928		1.4698	
Selected value [1967]	^{e}252.6±1. ^{e}118.0±1.	760 10					
Antoine constants: A 7.8864, B 2466.7, C 240.2.				dt/dp at 760 mmHg, 0.0562 °C/mmHg			
2,3,3,5,5,6-Hexamethyl-4-heptanol, $C_{13}H_{28}O$, mol. wt. 200.37, state at 25 °C							
Haller and Bauer [1913]	115–117	13					
5,5-Dimethyl-2-neopentyl-1-hexanol, $C_{13}H_{28}O$, mol wt. 200.37							
Gol'dfarb and Konstantinov [1956]	125–126	27		0.8475		1.4488	
3,5,5-Trimethyl-3-tert-butyl-2-hexanol, $C_{13}H_{28}O$, mol. wt. 200.37							
George [1943]	119–124	17				1.4684– 1.4690	
2,2,5-Trimethyl-3-tert-butyl-3-hexanol, $C_{13}H_{28}O$, mol. wt. 200.37							
See also table 201							
Mosher [1954]	104 138 240	10 44 753		0.8668		1.4578	
Petrov, Sokolova, and Kao [1960]	133–134	40		0.8676		1.4573	
Selected value [1967]	^{e}240.5±1 ^{e}104.0±1	760 10		^{b}0.8670 ±0.0007	^{c}0.863 ±0.001	^{b}1.4576 ±0.0005	^{c}1.455 ±0.001
Antoine constants: A 5.9308, B 1091.4, C 117.3.				dt/dp at 760 mmHg, 0.0670 °C/mmHg			
2,2,3-Trimethyl-4,4-diethyl-3-hexanol, $C_{13}H_{28}O$, mol. wt. 200.37							
Nazarov [1939]				0.906 (10°)		1.4762 (14°)	
2,2,4,4-Tetramethyl-*tert*-butyl-3-pentanol, $C_{13}H_{28}O$, mol. wt. 200.37, state at 25 °C crystal							
Bartlett and Schneider [1945]	138–140	28	94–95				

1-Tetradecanol

Properties of the Liquid Phase at Various Temperatures

Refractive Index

1-Tetradecanol is normally a solid at 25 °C and only a few values of the refractive index, measured above the melting point, are available. These are listed in table 203. The selected values at temperatures from 40 to 80 °C, listed in table 202, are taken from a straight line drawn through a plot of these data. This was determined largely by the two values, at 40 and 80 °C observed by Rathmann, Curtiss, McGeer, and Smyth [1956]. No data at wavelengths other than the sodium D-line were found.

Density

A few observed values of the density at several temperatures are shown in table 203. Data at 20 °C refer to the undercooled liquid. In addition Costello and Bowden [1958] measured the density at temperatures for 40 to 300 °C. The constants in the Francis equation were obtained by at least squares fit to these data. The calculated densities are listed in table 202. Nearly all of the experimental points are within 0.001 g cm^{-3} of the calculated ones.

Boiling Points and Vapor Pressures

As for the other higher alcohols, the measured vapor pressure data fall within two distinct ranges. Davies and Kybett reported the vapor pressure of the liquid from 40 to 53 °C as $\log P(\text{mmHg}) = 14.259 - 5440/T$. Spizzichino [1956] measured the vapor pressure from 44 to 85 °C using the same procedure that she used for 1-dodecanol. Although the vapor pressures obtained by Spizzichino were of the same order of magnitude as those calculated from the equation of Davies and Kybett in the 40 to 53 °C range, the slope of the pressures plotted against temperature was much greater for Spizzichino's values. Similar results have been found for the other higher normal alcohols. The Antoine constants selected for this range were obtained by using points calculated from the equation of Davies and Kybett up to 55 °C, the experimental points of Spizzichino from 55 to 85 °C, and the vapor pressure calculated from the Antoine constants at the high range at 130 °C.

There have been no systematic studies of the vapor pressure of 1-tetradecanol above 85 °C. The Antoine constants for the temperatures from 130 to 264 °C were calculated from the scattered boiling point data underlined in table 203. The vapor pressures calculated from these are only approximate. Only two values of the normal boiling point have been reported. The one obtained from the Union Carbide Corporation was given more weight.

Solid-Gas Phase Equilibria

Sublimation Pressure

Hoyer and Peperle [1958] reported the vapor pressure of the solid to be represented by $\log P(\text{mmHg}) = 24.08 - 8484/T$ as obtained from a torsion method. Davies and Kybett [1965] obtained $\log P(\text{mmHg}) = 20.919 - 7526/T$ for the solid from 20 to 34 °C from the Knudsen effusion method. Littlewood [1957] measured a vapor pressure of 1.03×10^{-5} mmHg at 20 °C also by the Knudsen effusion method. The equation of Hoyer and Peperle gives 1.38×10^{-5} mmHg at 20 °C, and that of Davies and Kybett gives 1.77×10^{-5} mmHg. The measurements of Davies and Kybett are considered more reliable. The sublimation pressure given by their equation is 4.75×10^{-5} mmHg at 25 °C.

Heat of Sublimation

The vapor pressure equation of Hoyer and Peperle [1958] implies a heat of sublimation of 38.8 kcal mol^{-1}, while that of Davies and Kybett [1965] gives 34.4 kcal mol^{-1}. The latter value was selected.

Solid-Liquid and Solid-Solid Phase Equilibria

Melting Points and Transition Temperatures

The polymorphism of 1-tetradecanol places it in class 4, as described in Appendix E. The stable solid phase is the γ-phase. The α- and β-phases are metastable at all temperatures. Melting points of the γ-phase are listed in table 203. The value of 37.8 °C was selected. According to Tanaka, Seto, and Hayshida [1957] the α-phase melts at 37.9 °C, which was 0.1 °C below their value for the melting point of the γ-phase. They also observed a partial transformation from the α- to the γ-phase, which would indicate that the α-phase is metastable, and therefore its melting point should be lower than that of the γ-phase. Thus the melting point of the α-phase is selected to be 37.7 ± 0.2 °C. The temperature for the transition from α- to the β-phase has been reported by Meyer and Reid [1933], Garner and Rushbrooke [1927], Phillips and Mumford [1934] and Tanaka, Seto, and Hayashida [1957] is 34.95, 34, 35.0, and 32–37.5 °C respectively. The value 35.0 ± 2 °C was selected for this transition.

Heat of Fusion

The heat of fusion was taken as the difference between the selected heat of sublimation and heat of vaporization of the liquid.

TABLE 202. 1-Tetradecanol. Selected values. Physical and thermodynamic properties

Temp. °C	Refractive Index, n_D	Density g cm^{-3}	Vapor Pressure, mmHg
20		* 0.836	
25		* .833	
30		* .829	
40	1.440	.8322	0.00070
50	1.4358	.8151	.00285
60	1.4320	.8081	.0094
70	1.4283	.8009	.0258
80	1.4246	.7937	.0620
90		.7864	.133
100		.7791	
110		.7718	
120		.7644	
130		.7569	
140		.7494	2.9
150		.7418	5.9
158.			10
160		.7342	11.1
170		.7264	20.
180		.7186	34.
190		.7108	55.
200		.7028	86.
204.			100
210		.6948	129.
220		.6867	190.
221.			200
230		.6785	271.
240		.6702	378.
242.			400
250		.6618	516.
240		.6532	689.
263.5			760

Data For Phase Transitions

Initial	Final	Temp. °C	dt/dP deg mm^{-1}	Pressure mmHg	ΔH kcal mol^{-1}	$d\Delta H/dt$	ΔS	ΔC_p
						cal deg^{-1} mol^{-1}		
c	g	25		4.8×10^{-5}	34.4±1		115.±3	
c	liq	37.8±0.2		760	9.5±1.5		31.±4	
liq	g	37.8±0.2		0.0049	24.9±1		80.±4	
liq	g	263.5±1		760				

Condensed Phase Heat Capacity

State	Temp. °C	C_p cal deg^{-1} mol^{-1}

Properties of the Saturated Real Gas

Temp. °C	H^r-H^0 kcal mol^{-1}	S^r-S^0 cal deg^{-1} mol^{-1}	$C_p^r-C_p^0$ cal deg^{-1} mol^{-1}

Data for the Standard States at 25 °C

State	Heat of Combustion ΔH_c^0 kcal mol^{-1}	Heat of Formation ΔH_f^0 kcal mol^{-1}	Entropy S^0 cal deg^{-1} mol^{-1}	Gibbs Energy of Formation ΔG_f^0 kcal mol^{-1}	Heat Capacity, C_p cal deg^{-1} mol^{-1}

Critical Constants

Temp °C, K	Pressure atm	Density g cm^{-3}

Constants in Vapor Pressure and Density Equation

Antoine Equation

Temp. Range	A	B	C
40 to 85 °C	4.0417	775.6	67.8
130 to 264 °C	6.6741	1204.5	54.0

Francis Equation

Temp. Range	A	$B\times10^3$	C	E
20 to 300 °C	0.96230	0.5495	89.74	800

* Undercooled liquid.

TABLE 203. 1-Tetradecanol. Reported values. Simple physical properties

Investigators		Vapor Pressures and Boiling Points		Freezing Point	Density, d g cm^{-3}		Refractive Index, n_D	
		°C	mmHg	t_m, °C	20 °C	25 °C	20 °C	25 °C
1-Tetradecanol, $C_{14}H_{30}O$, mol. wt. 214.40, state at 25 °C crystal								
Krafft	[1883]	167	15	38		0.8236 (38°)		
Krafft	[1890]	165–166	14	38				
Marvel and Tanenbaum	[1922]	170–173	20	39–39.5				
Andre and Francois	[1926]			38				
Garner and Rushbrooke	[1927]			37.7				
Ford and Marvel	[1930]	170–173	20	39–39.5				
Malkin	[1930]			38.0				
Adkins and Folkers	[1931]			37.5–38				
Meyer and Reid	[1933]			37.62				
Phillips and Mumford	[1933]			37.7				
Drake and Marvel	[1937]	140	4	36–38				
Krewson	[1939]	131.5–132.5	6	37.3–37.5				
Niemann and Wagner	[1942]	128–132	3	38.5				
Hoerr, Harwood, and Ralston	[1944]			38.26				
Trapeznikov	[1945]			36.7				
Adkins and Burks	[1938]	111–113	0.1	38				
Hoffman and Smyth	[1949]			36.4				
Othmer, Savitt, Krisher, Goldberg, and Markowitz	[1949]	260.0	760					
Tsvetkov and Marinin	[1949]					0.824 (38.4°)		
Baldacci	[1950]			36–37				
Kakiuchi, Sakurai, and Suzuki	[1950]			31.5				
Bergmann, Feeney, and Swift	[1951]	132–135	2	38–38.5				
Stahl and Pessen	[1952]			37.7				
Epstein, Wilson, Jakob, Conroy, and Ross	[1954]	143	3					1.4350 (50°)
Rathmann, Curtiss, McGreer, and Smyth	[1956]			36.4		0.822 (40°)		1.4320 (60°)
Spizzichino	[1956]			38.3				1.4330 (60°)
Tanaka, Seto, and Hayashida	[1957]			37–38				
Costello and Bowden	[1958]	170	20	39		0.8227 (40°)		
Union Carbide Corporation	[1958]	264.3	760		0.8340			
Petrov, Sokolova, and Kao	[1960]				0.8202			
Petrov, Kao, and Semenkin	[1960]				0.8751			
Vil'shan and Gavrilova	[1963]			35.6		0.8161 (50°)		1.4370 (70°)
Davies and Kybett	[1965]			36.7–37.1				
Selected value	[1967]	263.5±1. 158.±2.	760 10	37.8±0.2	0.836* ±0.002	0.833* ±0.002		

Antoine constants: A 6.6741, B 1204.5, C 54.0.

dt/dp at 760 mmHg, 0.0478 °C/mmHg

* Undercooled liquid.

Liquid-Vapor Equilibrium at the Triple Point

The vapor pressure equation reported by Spizzichino [1956] gives a heat of vaporization of 24.2 kcal mol^{-1} at 40 °C. However, this equation does not fit the slope of her vapor pressure measurements in this region. The equation of Davies and Kybett [1965] for the liquid gives 24.9 kcal mol^{-1}, and the selected Antoine constants for the low pressure region, listed on table 202, gives 30.0 kcal mol^{-1} at 40 °C. Although these Antoine constants give vapor pressures which agree with the equation of Davies and Kybett from 40 to 53 °C within the experimental accuracy, the slope of the vapor pressure versus temperature is probably too high at the low end of the range. Thus the heat of vaporization derived from the equation of Davies and Kybett is considered more reliable, and was therefore selected.

Isomeric Tetradecanols

The reported values of physical properties have been collected in the following unnumbered tables. Duplicate measurements by different investigators have been made in only a few cases so there are few checks to establish the reliability of these data. The smoothed values of refractive index of 2-methyl-2-tridecanol and 4-methyl-4-tridecanol in table 204 were based on the work of Eykman [1919].

TABLE 204. Isomeric Tetradecanols. Selected values. Refractive index at various temperatures and wavelengths

Symbol	Wavelength, angstroms	2-Methyl-2-tridecanol		4-Methyl-4-tridecanol
		20 °C	80 °C	25 °C
He_{red}	6678.1	1.4410	1.4157	1.4405
H_c	6562.8	1.4413	1.4160	1.4409
Na_D	5892.6	1.4435	1.4180	1.4430
Hg_e	5460.7	1.4454	1.4198	1.4449
He_{blue}	5015.7	1.4480	1.4223	1.4475
H_F	4861.3	1.4491	1.4233	1.4486
Hg_g	4358.3	1.4533	1.4273	1.4528
$H_{G'}$	4340.5	1.4536	1.4275	1.4530

TABLE 205. Isomeric Tetradecanols. Selected values. Density of the liquids at various temperatures

Temperature °C	3-Tetradecanol	2-Methyl-3-tridecanol	5-*n*-Butyl-5-decanol
	Density, g cm^{-3}		
20		0.8381	0.8414
25		.8340	.8370
30		.8299	.8325
40		.8217	.8235
50	0.8119	.8135	.8146
60	.8042	.8053	.806
70	.7964	.7971	
80	.7886	.7889	
90	.7807	.7807	
100	.7728	.7725	
110	.7648	.7643	
120	.7569	.7561	
130	.7488	.7479	
140	.7407	.7397	
150	.7326	.7315	
160		.7233	
170		.7151	
	Francis Constants		
Temperature Range °C	53–147	20–170	20–55
A	0.8784	0.8524	0.8593
$B \times 10^3$	.704	.825	.894
C	14.05	−1.30	
E	500	600	

The constants in the Francis equation and the calculated densities in table 205 for 3-tetradecanol and 2-methyl-3-tridecanol were calculated from the data of Pickard and Kenyon [1912] and [1913]. The smoothed values for 5-*n*-butyl-5-decanol were calculated from the densities in the unnumbered table plus values obtained by Quayle and Smart [1944] at 45 and 55 °C. Mosher [1954] reported the boiling points of a series of highly branched tetradecanols at pressures of about 760, 40 and 10 mmHg. The Antoine constants and the corresponding boiling points and vapor pressures calculated from his data are given in table 206.

TABLE 206. Isomeric Tetradecanols. Selected values. Vapor pressure of the liquids at various temperatures

Temperature °C	3,3-Dimethyl-4-isobutyl-4-octanol	3,3-Dimethyl-4-tert-butyl-4-octanol	3,3,6-Trimethyl-4-isobutyl-4-heptanol	3,3,6-Trimethyl-4-*tert*-butyl-4-heptanol
112.			10	
116.	10			
119.				10
120	11.7		14.5	10.5
126.		10		
130	17.7	12.0	22.5	16.1
140	26.	18.5	34.	24.
150	38.	28.	50.	35.
160	55.	41.	72.	51.
169.			100	
170	79.	59.	103.	71.
177.	100			
180	110.	83.	143.	98.
181.				100
186.		100		
190	152.	115.	195.	133.
191.			200	
199.	200			
200	207.	157.	263.	177.
204.				200
208.		200		
210	280.	211.	350.	232.
215.			400	
220	374.	279.	458.	301.
222.	400			
230	493.	364.	593.	385.
232.				400
234.		400		
240	645.	469.		486.
240.1			760	
246.3	760			
250		597.		608.
260				753.
260.4		760		760
	Antoine Constants			
Temperature Range, °C	114–246	126–260	112–240	119–260
A	9.2238	7.2858	7.5272	6.8866
B	3602.	1979.	2065.	1773.
C	321.6	188.8	204.4	182.3

Isomeric Tetradecanols

Investigators		Vapor Pressures and Boiling Points		Freezing Point	Density, *d* g cm^{-3}		Refractive Index, n_D	
		°C	mmHg	t_m, °C	20 °C	25 °C	20 °C	25 °C
2-Tetradecanol, $C_{14}H_{30}O$, mol. wt. 214.40, state at 25 °C crystal								
Breusch and Sokulla	[1953]			33–34				1.4216 (80°)
3-Tetradecanol, $C_{14}H_{30}O$, mol. wt. 214.40, state at 25 °C crystal								
See also table 205								
Pickard and Kenyon	[1913]	146	10	38				
4-Tetradecanol, $C_{14}H_{30}O$, mol. wt. 214.40, state at 25 °C crystal								
Petrov and Ol'dekop	[1948]	146–148	7	32–33		0.8272		1.442 (32°)
5-Tetradecanol, $C_{14}H_{30}O$, mol. wt. 214.40, state at 25 °C crystal								
Komarewsky and Coley	[1941]			28.5				
6-Tetradecanol, $C_{14}H_{30}O$, mol. wt. 214.40								
Studt	[1966]	128–130	1					
11-Methyl-1-tridecanol, $C_{14}H_{30}O$, mol. wt. 214.40								
Lardicci, Salvadori, and Pino	[1962]	163–164	15			0.8344		1.4455
12-Methyl-1-tridecanol, $C_{14}H_{30}O$, mol. wt. 214.40								
Milburn and Truter	[1954]	161–163	11					1.4464
2-Methyl-2-tridecanol, $C_{14}H_{30}O$, mol. wt. 214.40, state at 25 °C liq.								
See also table 204								
Eykman	[1919]			16.3	0.8279		1.4435	
Prevost and Singer	[1950]	125	2					

Isomeric Tetradecanols—Continued

Investigators	Vapor Pressures and Boiling Points		Freezing Point	Density, *d* g cm^{-3}		Refractive Index, n_D	
	°C	mmHg	t_m, °C	20 °C	25 °C	20 °C	25 °C
2-Methyl-3-tridecanol, $C_{14}H_{30}O$, mol. wt. 214.40							
See also table 205							
Pickard and Kenyon [1912]	274	760		0.8390		1.4460	
Selected value [1967]				^{d} .8381 ±.001	^{d} 0.8340 ±.001		
2-Methyl-4-tridecanol, $C_{14}H_{30}O$, mol. wt. 214.40							
Pratt and Kubler [1954]	147–148	14					1.4404
4-Methyl-4-tridecanol, $C_{14}H_{30}O$, mol. wt. 214.40							
See also table 204							
Eykman [1919]	108–111	1			0.8284		1.4430
6-Methyl-6-tridecanol, $C_{14}H_{30}O$, mol. wt. 214.40							
Griess [1955]	142	15					
2,2-Dimethyl-1-dodecanol, $C_{14}H_{30}O$, mol. wt. 214.40, state at 25 °C liq.							
Blood and Hagemeyer [1964]	272	760	−18	0.8363			
4,10-Dimethyl-1-dodecanol, $C_{14}H_{30}O$, mol. wt. 214.40							
Crombie, Manzoor-i-Khuda, and Smith [1957]	92	0.03				1.4464	
3,10,10-Trimethyl-3-undecanol, $C_{14}H_{30}O$, mol. wt. 214.40							
Gutman and Hickinbottom [1951]	97	0.8				1.4438	
2-Methyl-7-ethyl-4-undecanol, $C_{14}H_{30}O$, mol. wt. 214.40							
Union Carbide Corporation [1953]	264.1	760		0.8340			
Union Carbide Corporation [1958]	264.3	760		.8340			
Othmer, Savitt, Krisher, Goldberg, and Markowitz [1949]	260.0	760					
Selected value [1967]	^{a} 264.3±0.5	760					

Isomeric Tetradecanols—Continued

Investigators	Vapor Pressures and Boiling Points		Freezing Point	Density, *d* g cm^{-3}		Refractive Index, n_D	
	°C	mmHg	t_m, °C	20 °C	25 °C	20 °C	20 °C
6-*n*-Propyl-6-undecanol, $C_{14}H_{30}O$, mol. wt. 214.40							
Whitmore and Williams [1933]	81–82	0.4			0.8336	1.4452	
Church, Whitmore, and McGrew [1934]	135–138	14				1.4453	
Selected value [1967]	[c] 93±3.	10				[b] 1.4453 ±0.001	
6-Isopropyl-6-undecanol, $C_{14}H_{30}O$, mol. wt. 214.40							
Huston and Bailey [1946]	104–1–6	2		0.8425		1.4477	
2,2,6-Trimethyl-6-undecanol, $C_{14}H_{30}O$, mol. wt. 214.40							
Gutman and Hickinbottom [1951]	126–128	11				1.4418	
5-*n*-Butyl-5-decanol, $C_{14}H_{30}O$, mol. wt. 214.40							
See also table 205							
Whitmore and Williams [1933]	90–92	1.2			0.8345	1.4450	
Church, Whitmore, and McGrew [1934]	98–100	2				1.4450	
Quayle and Smart [1944]					0.8348	1.4458	1.4434
Protiva, Exner, Borovicka, and Pliml [1952]	135–140	5					
Meshcheryakov, Erzyutova, and Kuo [1961]	139–141	15		0.8454		1.4420	
Selected value [1967]	[c] 120±3.	10		[d] 0.8414 ±0.001	[d] 0.8370 ±0.001	[a] 1.4458 ±0.001	[a] 1.4434 ±0.001
2-*n*-Pentyl-1-nonanol, $C_{14}H_{30}O$, mol. wt. 214.40							
Guerbet [1901b]	151.5–152.5 286–289	13 760		0.8405 (15°)			
Guerbet [1902]	240	760					
von Braun and Manz [1934]	148–152	10					
Mastagli [1938]	154	13			0.8370	1.4464	
Griess [1955]	142	15					
Selected value [1967]	[a] 240±5. [c] 150±4.	760 10					
2-Methyl-4-isobutyl-4-nonanol, $C_{14}H_{30}O$, mol. wt. 214.40							
Frank and Foster [1954]	77–78	0.2					
2,2,3,3,4-Pentamethyl-4-nonanol, $C_{14}H_{30}O$, mol. wt. 214.40							
Petrov, Kao, and Semenkin [1960]	130–132	18		0.8751		1.4644	

Isomeric Tetradecanols—Continued

Investigators	Vapor Pressures and Boiling Points		Freezing Point	Density, d g cm^{-3}		Refractive Index, n_D	
	°C	mmHg	t_m, °C	20 °C	25 °C	20 °C	25 °C
4,4,5,6,6-Pentamethyl-5-nonanol, $C_{14}H_{30}O$, mol. wt. 214.40							
Nazarov [1937]	266–269	760		0.8876 (15°)		1.4700	
7,7-Dimethyl-6-*tert*-butyl-1-octanol, $C_{14}H_{30}O$, mol. wt. 214.40							
Petrov, Sokolova, and Kao [1960]						1.4212	
2,2-Dimethyl-4-*n*-butyl-4-octanol, $C_{14}H_{30}O$, mol. wt. 214.40, state at 25 °C							
Whitmore, Popkin, Whitaker, Mattil, and Zech [1938]	**112–115**	8		0.8320		**1.4460**	
Whitmore and Forster [1942]	**83**	3		**0.8403**		**1.4462–1.4469**	
Selected value [1967]	[c] 120±3.	10		[a] 0.8403 ±0.002	[c] 0.836 ±0.002	[b] 1.4464 ±0.001	[c] 1.444 ±0.001
3,3-Dimethyl-4-isobutyl-4-octanol, $C_{14}H_{30}O$, mol. wt. 214.40							
Mosher [1954]	**114**	9		0.8568		1.4532	
	153	43					
	246	754					
Selected value [1967]	[e] 246±1.	760					
	[e] 116±1.	10					
Antoine constants: A 9.2238, B 3602.2, C 321.6.							dt/dp at 760 mmHg, 0.0511 °C/mmHg
3,3-Dimethyl-4-*tert*-butyl-4-octanol, $C_{14}H_{30}O$, mol. wt. 214.40							
See also table 206							
Mosher [1954]	**126**	10		0.8734		1.4624	
	160	41					
	260	753					
Selected value [1967]	[e] 260±1.	760					
	[e] 126±1.	10					
Antoine constants: A 7.2858, B 1978.8, C 188.8.							dt/dp at 760 mmHg, 0.0582 °C/mmHg
2,2,6-Trimethyl-4-isobutyl-4-heptanol, $C_{14}H_{30}O$, mol. wt. 214.40							
Whitmore and Forster [1942]	68.5	3		0.8317		1.4395–1.4410	
	69.5	2		0.8313		1.4375–1.4411	

Isomeric Tetradecanols—Continued

Investigators	Vapor Pressures and Boiling Points		Freezing Point	Density, *d* g cm^{-3}		Refractive Index, n_D	
	°C	mmHg	t_m, °C	20 °C	25 °C	20 °C	25 °C

3,3,6-Trimethyl-4-isobutyl-4-heptanol, $C_{14}H_{30}O$, mol. wt. 214.40, state at 25 °C

Mosher [1954]	112	10		0.8530		1.4515	
	146	43					
	240	759					
Selected value [1967]	^{e}240±1.	760					
	^{e}112±1.	10					

Antoine constants: *A* 7.2858, *B* 1978.8, *C* 204.4. *dt/dp* at 760 mmHg, 0.0630 °C/mmHg

3,3,6-Trimethyl-4-*tert*-butyl-4-heptanol, $C_{14}H_{30}O$, mol. wt. 214.40

See also table 206

Mosher [1954]	119	10		0.8794		1.4654	
	154	41					
	260	753					
Selected value [1967]	^{e}260±1.	760					
	^{e}119±1.	10					

Antoine constants: *A* 6.8866, *B* 1773.4, *C* 182.3. *dt/dp* at 760 mmHg, 0.0630 °C/mmHg

3,3,5,5-Tetramethyl-4-*n*-propyl-4-heptanol, $C_{14}H_{30}O$, mol. wt. 214.40

Mosher [1954]	160	44		0.8882		1.4692	

2,2-Di-*n*-butyl-1-hexanol, $C_{14}H_{30}O$, mol. wt. 214.40

Whitmore, Whitaker, Mosher, Breivik, Wheeler, Miner, Sutherland, Wagner, Clapper, Lewis, Lux, and Popkin [1941]	114–118	3				1.4532– 1.4535	

Pentadecanols

No thermodynamic data have been reported for the pentadecanols, and the data on even the simple physical properties are scarce. Properties reported for 1-pentadecanol are listed on table 207 and properties of the isomeric pentadecanols on the following unnumbered tables. The only tables of smoothed properties as functions of temperature are table 208 for density of 3-pentadecanol derived from the data of Pickard and Kenyon [1913] and table 209 for the vapor pressure of 3, 3, 5, 5-tetramethyl-4-*n*-butyl-4-heptanol based on the measurements of Mosher [1954] at three temperatures.

The melting point selected for 1-pentadecanol is for the α-form. The α to β transition has been observed by three sets of investigators. Meyer and Reid [1933] obtained the transition temperature of 37.33 °C, Phillips and Mumford obtained 38.9 °C, and Tanaka, Seto, and Hayashida [1957] obtained 35 and 39 °C. The selected transition temperature is 37.5 ± 0.5 °C. Additional discussion is given in Appendix E.

Except for the melting point of 1-pentadecanol, no accurate measurements have been made for the properties of any of the C_{15} alcohols. Most of these compounds melt above room temperature, and therefore values of the refractive index and density of the liquid at 25 °C are available for only a few of them. The data of Mosher [1954] are the only reliable boiling values available for this group of compounds.

TABLE 207. 1-Pentadecanol. Reported values. Simple physical properties

Investigators		Vapor Pressures and Boiling Points		Freezing Point	Density, d g cm^{-3}		Refractive Index, n_D	
		°C	mmHg	t_m, °C	20 °C	25 °C	20 °C	25 °C
1-Pentadecanol, $C_{15}H_{32}O$, mol. wt. 228.42, state at 25 °C crystal								
Simonini	[1893]			45–46				
Jeffreys	[1899]			45–46				
Gascard	[1921]			44				
Meyer and Reid	[1933]			43.84				
Phillips and Mumford	[1934]			43.9–44.0				
Tischer	[1939]			45–46				
Weinhaus and Mucke	[1942]			46				
Stoll	[1947]	122–125	0.35	45–46	* 0.8384		* 1.4477	
Dauben	[1948]	112–114	.2					
		118	.3					
Anker	[1952]			42–43				
Tanaka, Seto, and Hayashida	[1957]			40–42				
Vil'shan and Gavrilova	[1963]			44.2		0.8192 (50°)		1.4408 (50°)
Selected value	[1967]			[b] 43.9± 0.2	*[a] 0.838 ±0.001		*[a] 1.448 ±0.001	

* Undercooled liquid

2-Pentadecanol, $C_{15}H_{32}O$, mol. wt. 228.42, state at 25 °C crystal								
Baumgarten	[1943]	174	18	30–31				
Dreger, Keim, Miles, Shedlovsky, and Ross	[1944]	152	11	27				
Breusch and Sokullu	[1953]			35–36				
Selected value	[1967]	[c] 149±3.	10	[b] 32±2.				
3-Pentadecanol, $C_{15}H_{32}O$, mol. wt. 228.42, state at 25 °C crystal								
Pickard and Kenyon	[1913]	168	14	45				
Sparks and Knobloch	[1955]			33–34				
Selected value	[1967]	[c] 153±4.	10	[a] 45±2.				
4-Pentadecanol, $C_{15}H_{32}O$, mol. wt. 228.42, state at 25 °C crystal								
Dreger, Keim, Miles, Shedlofsky, and Ross	[1944]	143	1	34				

* Undercooled liquids.

6-Pentadecanol, $C_{15}H_{32}O$, mol. wt. 228.42, state at 25 °C crystal								
Dreger, Keim, Miles, Shedlovsky, and Ross	[1944]	159	10	36				
Studt	[1966]	122	0.2					

Pentadecanols—Continued

Investigators	Vapor Pressures and Boiling Points		Freezing Point	Density, d g cm^{-3}		Refractive Index, n_D	
	°C	mmHg	t_m, °C	20 °C	25 °C	20 °C	25 °C
8-Pentadecanol, $C_{15}H_{32}O$, mol. wt. 228.42, state at 25 °C crystal							
Komarewsky and Coley [1941]			49.0				
Asinger and Eckoldt [1943]	132.5–133	1.5	50				
Baumgarten [1943]			48.5–49				
Dreger, Keim, Miles, Shedlovsky, and Ross [1944]	137	1	52				
Tuot and Guyard [1947]	153	11	43.5				
Selected value [1967]	[c] 152±3.	10	[b] 49±1.				
2-Methyl-1-tetradecanol, $C_{15}H_{32}O$, mol. wt. 228.42, state at 25 °C crystal							
Linblad and Stenhagen [1941]	134	2	32.0–33.2				
12-Methyl-1-tetradecanol, $C_{15}H_{32}O$, mol. wt. 228.42, state at 25 °C liq.							
Milburn and Truter [1954]	170–175	15				1.4493	
2-Methyl-2-tetradecanol, $C_{15}H_{32}O$, mol. wt. 228.42, state at 25 °C liq.							
Prevost and Singer [1950]	119	0.5					
Urry, Stacey, Huyser, and Juveland [1954]	115–117	0.2				1.4437	
	104	0.1					1.4447
Foreman and Lankelma [1957]	102	1	21.5	0.838		1.4438	
Selected value [1967]						[b] 1.444 ±0.001	[c] 1.442 ±0.001
5-Methyl-5-tetradecanol, $C_{15}H_{32}O$, mol. wt. 228.42							
Protiva, Exner, Boroviska, and Pliml [1952]	141–142	4					
6,10-Dimethyl-2-tridecanol, $C_{15}H_{32}O$, mol. wt. 228.42							
Shvart and Petrov [1961]	144–145	10		0.8882		1.4472	
9-Ethyl-6-tridecanol, $C_{15}H_{32}O$, mol. wt. 228.42							
Union Carbide Corporation [1936]	143–144	7					
Wicket and Freure [1937]	276–277	760					
Selected value [1967]	[c] 147±3	10					
2,3,6-Trimethyl-1-dodecanol, $C_{15}H_{32}O$, mol. wt. 228.42							
Werner and Bogert [1938]	149–151	17			0.8351		1.4472

Pentadecanols—Continued

Investigators		Vapor Pressures and Boiling Points		Freezing Point	Density, *d* g cm^{-3}		Refractive Index, n_D	
		°C	mmHg	t_m, °C	20 °C	25 °C	20 °C	25 °C
3,7,11-Trimethyl-3-dodecanol, $C_{15}H_{32}O$, mol. wt. 228.42								
Nazarov, Gussev, and Gunar	[1958]	127–130	7		0.8387		1.4460	
2,6,10-Trimethyl-6-dodecanol, $C_{15}H_{32}O$, mol. wt. 228.42								
Sorm and Arient	[1950]	124–125	3.5					
2,7,10-Trimethyl-6-dodecanol, $C_{15}H_{32}O$, mol. wt. 228.42								
Sorm and Arient	[1950]	118–119	2.5					
5,7-Diethyl-4-undecanol, $C_{15}H_{32}O$, mol. wt. 228.42								
Union Carbide Corporation	[1936]	113–114	10					
Wicket and Freure	[1937]	264–265	760					
6-*n*-Butyl-6-undecanol, $C_{15}H_{32}O$, mol. wt. 228.42								
Whitmore and Williams	[1933]	99–102	1			0.8344	1.4460	
Church, Whitmore, and McGrew	[1934]	109–110	2				1.4482	
Selected value	[1967]						^{b}1.447 ±0.001	
6-Isobutyl-6-undecanol, $C_{15}H_{32}O$, mol. wt. 228.42								
Huston and Bailey	[1946]	116–118	3		0.8367		1.4464	
2,2-Dimethyl-3-*tert*-butyl-3-nonanol, $C_{15}H_{32}O$, mol. wt. 228.42								
Petrov, Sokolova, and Chin-Lan	[1957]	128	7.5		0.8603		1.4569	
Petrov, Sokalova, and Kao	[1960]	128	7.5		0.8603		1.4569	
2,8-Dimethyl-5-isobutyl-5-nonanol, $C_{15}H_{32}O$, mol. wt. 228.42								
Grignard	[1904]	126–129	15		0.8416 (19.4 °C)		1.44864 (10.4 °C)	
Selected value	[1967]				^{c}0.833 ±0.002		^{c}1.446 ±0.002	
3,3-Di-*n*-butyl-2-heptanol, $C_{15}H_{32}O$, mol. wt. 228.42								
Zeiss and Tsutsui	[1953]	99–99.5	0.5					1.4546

Pentadecanols—Continued

Investigators		Vapor Pressures and Boiling Points		Freezing Point	Density, d g cm^{-3}		Refractive Index, n_D	
		°C	mmHg	t_m, °C	20 °C	25 °C	20 °C	25 °C
3,3,5,5-Tetramethyl-4-n-butyl-4-heptanol, $C_{15}H_{32}O$, mol. wt. 228.42								
Mosher	[1954]	187.0	110		0.8849		1.4693	
		173.0	58					
		110.0	2.5					
Selected value	[1967]	^{e}136.7±1	10					
3,3,5,5-Tetraethyl-4-heptanol, $C_{15}H_{32}O$, mol. wt. 228.42								
Zerner	[1911]	159–161	18					

TABLE 208. Isomeric Pentadecanols. Selected values. Density of the liquid at various temperatures

Temperature °C	3-Pentadecanol
Density, g cm^{-3}	
50	0.8153
60	.8077
70	.8000
80	.7924
90	.7847
100	.7769
110	.7691
120	.7613
130	.7534
140	.745
Francis Constants	
Temperature Range, °C	55–132
A	0.8806
$B \times 10^3$	.691
C	13.84
E	500

TABLE 209. Isomeric Pentadecanols. Selected values. Vapor pressure at various temperatures

Temperature °C	3,3,5,5-Tetramethyl-4-n-butyl-4-heptanol
Pressure, mmHg	
110	2.5
120	4.6
130	8.
134.	10
140	14.
150	23.
160	35.
170	54.
180	81.
186.	100
190	117.
Antoine Constants	
Temperature Range, °C	110–105
A	6.9839
B	1549.
C	125.

1-Hexadecanol

Properties of the Liquid Phase at Various Temperatures

Refractive Index

Eykman [1919] has measured the refractive index over a range of wavelengths at 78.9 °C. The smoothed values in Table 211 were obtained by adjusting his values to 80 °C. The refractive indices for the sodium D-line given in table 210 were taken from a linear plot of the data of Eykman [1919], Hosman, Steenis, and Waterman [1949], Kremmling [1953], Rathmann, Curtis, McGeer, and Smyth [1956], Spizzichino [1956], and Bergmann, Cregiton, and Stokes [1956]. The refractive index reported by Vil'shan and Gavrilova [1963] at 60 °C is about 0.004 higher than the other available data. Volander and Selke [1927] report that crystalline hexadecanol at 25.5 °C is

TABLE 210. 1-Hexadecanol. Selected values. Physical and thermodynamic properties

Temp. °C	Refractive Index, n_D	Density g cm^{-3}	Vapor Pressure, mmHg
30		* 0.8327	
30		* .8257	
50	1.4391	.8187	0.00036
60	1.4355	.8116	.00135
70	1.4319	.8045	.00440
80	1.4283	.7974	.0128
90		.7903	.0337
100		.7831	.0815
110		.7758	.18
120		.7686	
130		.7613	
140		.7539	1.5
145			2.0
150		.7465	2.7
155			3.5
160		.7391	4.6
165			5.9
170		.7316	7.4
175			9.3
176.5			10
180		.7240	11.7
185			14.
190		.7164	18.
200		.7087	26.
210		.7010	
220		.6932	
230		.6854	
240		.6774	
250		.6694	
260		.6613	
270		.6532	
280		.6449	
290		.6366	
300		.6281	

Data For Phase Transitions

Initial	Final	Temp. °C	dt/dP deg mm^{-1}	Pressure mmHg	ΔH kcal mol^{-1}	$d\Delta H/dt$ cal deg^{-1} mol^{-1}	ΔS cal deg^{-1} mol^{-1}	ΔC_p cal deg^{-1} mol^{-1}
c,II	g	25		0.0000020	40.5±1		135.±3	
c,u	c,I	44.0±0.5		.000126	4.8±0.5		15.1±1.5	
c,II	c,I	49.1±0.5		.000307	5.7±0.5		17.7±1.5	
c,I	liq	49.3±0.2		.000331	7.8±0.5		24.2±1.5	
liq	g	49.3±0.2	16000	.000331	26.5±1		82.±3	

Condensed Phase Heat Capacity

State	Temp. °C	C_p cal deg^{-1} mol^{-1}

Properties of the Saturated Real Gas

Temp. °C	H^r-H^0 kcal mol^{-1}	S^r-S^0 cal deg^{-1} mol^{-1}	$C_p{}^r-C_p{}^0$ cal deg^{-1} mol^{-1}

Data for the Standard States at 25 °C

State	Heat of Combustion $\Delta H_c{}^0$ kcal mol^{-1}	Heat of Formation $\Delta H_f{}^0$ kcal mol^{-1}	Entropy S^0 cal deg^{-1} mol^{-1}	Gibbs Energy of Formation $\Delta G_f{}^0$ kcal mol^{-1}	Heat Capacity, C_p cal deg^{-1} mol^{-1}
c,II	−2502.8±1	−163.4±1	108.±2	−23.6±1	104.8±1
g	−2543.3±1.5	−122.9±1.5	204.±4	−11.7±2	

Critical Constants

Temp. °C, K	Pressure atm	Density g cm^{-3}

Constants in Vapor Pressure and Density Equation

Antoine Equation

Temp. Range	A	B	C
50–103 °C	7.2817	1909.7	128.1
145–190 °C	6.1586	1380.0	91.

Francis Equation

Temp. Range	A	$B\times10^3$	C	E
20–300 °C	0.9360	0.5863	66.00	800

* Undercooled liquid.

uniaxial positive with refractive indices $\omega = 1.4805$ and $\epsilon = 1.5285$ (ordinary and extraordinary rays respectively).

TABLE 211. 1-Hexadecanol. Selected values. Refractive index at various wavelengths at 80 °C

Symbol	Wavelength, angstroms	Refractive Index, n
He_{red}	6678.2	1.4259
H_C	6562.8	1.4262
Na_D	5892.6	1.4283
Hg_e	5460.7	1.4301
He_{blue}	5015.7	1.4326
H_F	4861.3	1.4348
Hg_g	4358.3	1.4379
$H_{G'}$	4340.5	1.4380

Density

There are about a dozen reports of the density of liquid hexadecanol. Costello and Bowden [1958] measured the density from 60 to 300 °C. Measurements over shorter temperature ranges have also been made by Krafft [1883], Delcourt [1931], and Boelhouwer, Nederbragt, and Verberg [1950]. These data, along with individual density values reported by Eykman [1893a], Tromp [1922], Baker and Smyth [1938], Hosman, Steenis, and Waterman [1949], Kremmling [1953], Rathmann, Curtis McGeer, and Smyth [1956], and a value for the undercooled liquid at 20 °C from Blood and Hagemeyer [1964] were used in the calculation of the Francis constants. The calculated densities are listed in table 210. Most of the measured values are within 0.001 g cm^{-3} of the calculated ones.

Vapor Pressure and Boiling Points

Antoine constants were calculated for hexadecanol in two different temperature ranges. From 145 to 190 °C only a few scattered boiling point measurements were available. These are summarized in table 212. The data were not suitable for direct determination of the C constant. Instead the values of A and B were calculated for the minimum sum of the squared deviations for several fixed values of C in the vicinity of 100. The set of constants which gave the best fit was selected and is given in table 210.

Vapor pressures at lower temperatures have been measured by Davies and Kybett]1965a] by the Knudsen effusion method and by Spizzichino [1956] by a static metod. Davies and Kybett expressed their results for the liquid from 50 to 62 °C by the equation $\log P\,(\mathrm{mmHg}) = 14.251 - 5717/T$. Spizzichino's measurements extended from 49 to 103 °C. The two sets of data agreed closely at 49 °C but Spizzichino obtained increasingly higher vapor pressures than Davies and Kybett at higher temperatures. The vapor pressures calculated from the Antoine constants for this range in table 210 are intermediate between these two sets of data in the region of overlap.

Solid-Gas Phase Equilibria

Sublimation Pressure

Hoyer and Peperle [1958] expressed their measurements as $\log P(\mathrm{mmHg}) = 23.47 - 8681/T$ for the solid from 40 to 50 °C and Davies and Kybett [1965a] gave $\log P(\mathrm{mmHg}) = 23.648 - 8736/T$ from 35 to 47 °C. Littlewood [1957] reported a single measurement of 3.06×10^{-6} mmHg at 30 °C. All these measurements were made by the Knudsen effusion method. The equations of Hoyer and Peperle and of Davies and Kybett gave pressures of 6.82×10^{-6} and 6.77×10^{-6} mmHg, respectively at 30 °C. The selected sublimation pressure at 25 °C was based on the equation of Davies and Kybett, and includes a relatively large uncertainty.

Heat of Sublimation

The equation for the sublimation pressure of Hoyer and Peperle gives a heat of sublimation of 39.7 kcal mol^{-1}, while that of Davies and Kybett [1965a] gives 40.0 ± 0.5 kcal mol^{-1}. The value selected for 25 °C in table 210 was obtained by applying an estimated correction to the value reported by Davies and Kybett in the 35 to 47 °C range. These enthalpies of sublimation refer to the crystal, II (γ-form).

Solid-Solid and Solid-Liquid Phase Equilibria

Transition Temperatures and Melting Point

As shown in table 212 many determinations of the melting point of hexadecanol have been reported. However, the condensed phase transitions are complex and the interpretation of various experimental observations is difficult. There is a general consensus that crystal I, the form stable at the melting point, is the α-form, which is described in Appendix E. The α-form changes more or less reversibly into the β-form at approximately 44 °C. This transition temperature has been reported by Smith, J. C. [1931], Meyer and Reid [1933], Phillips and Mumford [1933] and [1934], Baker and Smyth [1938], Kolp and Lutton [1951], Parks, Kennedy, Gates, Mosley, Moore, and Renquist [1956], and Tanaka, Seton, and Hayashida [1957] at values ranging from 32 to 45 °C. However both the α- and β-forms are metastable with respect to the γ-form over most or all of temperatures below the melting point. The transformation to the γ-form takes place slowly, however, so that the α- and β-forms can exist for a period of several days. Tanaka, Seto, and Hayashida [1957] report a γ- to α-phase transition temperature at 46 °C. However the vapor pressure data of Davies and Kybett [1965a] and other observations

TABLE 212. 1-Hexadecanol. Reported values. Simple physical properties

Investigators	Vapor Pressures and Boiling Points		Freezing Point	Density, d g cm^{-3}		Refractive Index, n_D	
	°C	mmHg	t_m, °C	20 °C	25 °C	20 °C	25 °C
1-Hexadecanol, $C_{16}H_{34}O$, mol. wt. 242.45, state at 25 °C crystal							
Krafft [1883]	189.5	15	49.5				
Krafft [1884]	189–190	15	49.2–49.3				
Stohmann [1884]			50				
Eykman [1893]					0.8176 (49.5°)		
Scheuble and Loeble [1904]			49.3				
Piutti [1906]			46.8–47.3				
Flaschner [1909]			48				
Power and Rogerson [1912]			50–51				
Eykman [1919]	189–190	15	49.7–50				
Gascard [1921]			49				
Tromp [1922]					0.8097 (64 °C)		
Adam [1922]			50				
Sanderens [1925]	340	760	50				
Ford and Marvel [1930]	178–182	12	48.5–49.5				
Biltz, Fischer, and Wünnenberg [1930]			45				
Malkin [1930]			49.0				
Delcourt [1931]			49.10				
Smith [1931]			49.27				
Phillips and Mumford [1931]			49.1				
Carey and Smith [1933]			49.22				
Meyer and Reid [1933]			49.27				
Phillips and Mumford [1934]			49.25				
Baker and Smyth [1938]	155–156	5	47.8		0.8886		
Higasi and Kubo [1939]	125–135	0.01	49.10–49.2				
Michel [1939]			49.10				
Tischer [1939]			51				
Bertrand, Baker, and Haack [1939]	189–190	15	45–46				
Niemand and Wagner [1942]	144–146	3	49.0				
Kind and Bergmann [1942]			49				
Asinger and Eckoldt [1943]			50.4				
Badin [1943]			49–50				
Hoerr, Harwood, and Ralston [1944]			49.62				
Trapeznikov [1945]			48.6				
Parks and Rowe [1946]			48–49				
Grundman [1948]			50				
deRooster [1948]			49				
Hosman, Steenis, and Waterman [1949]			47				
Weitzel and Wojahn [1950]	173	3	49.5–50.0				

TABLE 212. 1-Hexadecanol. Reported values. Simple physical properties—Continued

Investigators		Vapor Pressures and Boiling Points		Freezing Point	Density, d g cm^{-3}		Refractive Index, n_D	
		°C	mmHg	t_m, °C	20 °C	25 °C	20 °C	20 °C
1-Hexadecanol, $C_{16}H_{34}O$, mol. wt. 242.45, state at 25 °C crystal								
Boelhouwer, Nederbragt, and Verberg	[1950]			49.5–49.7				
Kakiuchi, Sakurai, and Suzuki	[1950]			48.2				
Meadow and Cavagnol	[1951]			48.5–49				
Meakins and Mulley	[1951]			48.5				
Kolp and Lutton	[1951]			49.1				
Bergmann, Feeney, and Swift	[1951]	186–188	15	49.2				
Bailey, Polgar, Tate, and Wilkinson	[1955]	166	2					
Parks Kennedy, Gates, Mosley, Moore, and Renquist	[1956]			50.6				
Rathmann, Curtis, McGreer, and Smyth	[1956]			48.9				
Spizzichino	[1956]			49.5				1.4363 (60°)
Tanaka, Seto, and Hayashida	[1957]			48.5–49				
Costello and Bowden	[1958]	190	20	49.2				
Vil'shan and Gavrilova	[1963]			48.5		0.8143 (60°)		1.4392 (60°)
Blood and Hagemeyer	[1964]				0.8400			
Davies and Kybett	[1965a]			48.7–48.9				
Davies and Kybett	[1965b]			48.0–49.7				
Selected value	[1967]	^{e}177.±3.	10	^{b}49.3±0.2				

seem to imply that this transition temperature, if it exists, is very close to the melting point. Thus the α-form has only a very short temperature range of stability. These conclusions place 1-hexadecanol in Class 3, as described in Appendix E. Crystal I is the α-form and crystal II is the γ-form, while the β-form is meatastable at all temperatures.

TABLE 213. 1-Hexadecanol. Reported values. Heats of transition and heats of fusion

Investigator	ΔH_{tr}, kcal mol^{-1}		ΔH_m, kcal mol^{-1}	
	c,u→c,I	c,II→c,I	c,I	c,II
Favre and Silbermann [1852]			7.08	
Tammann [1913]			8.19	
Fischer [1940]*			8.90	
Parks and Rowe [1946]		4.0		12.44
Kakiuchi, Sakurai, and Suzuki [1950]		5.92	7.73	
Davies and Kybett [1965a]				13.8
Davies and Kybett [1965b]	4.77	5.66		

* Reported by J. Timmermans, "Les Constantes Physiques des Composes Organiques Cristallises", Masson et Cie., Paris, 1953

Heats of Transition and Fusion

The reported values of heats of transition and fusion are given in table 213. The measurement of the heat of fusion will give ΔH_m for either the *c*, *I* or *c*, *II*, depending upon the method employed. Fischer [1940] calculated the heat of fusion from measurements of the depression of the freezing point by dissolved solutes, while the values of Favre and Silbermann [1852], Tamman [1913], and Kakiuchi, Sakurai, and Suzuki [1950] were obtained by direct calorimetric measurements. All of these refer to equilibrium between the solid and liquid phases and thus correspond to the fusion of crystal, I. Parks and Rowe [1946] measured the heat of solution of solid hexadecanol in liquid methanol, ethanol, 1-heptanol, and 1-dodecanol at 25 °C. They assumed that the extrapolation of these values to C_{16} would give the heat of fusion of 1-hexadecanol at 25 °C. They then estimated the effect of converting this to 49.3 °C, the melting point of 1-hexadecanol. Since the solid form of hexadecanol which they used in these experiments was the crystal II, this procedure gives the heat of fusion of this form. They also gave a rough measurement of the *c*, II-*c*, I heat of transition from a study of the temperature time heating curve. The heat of fusion reported by Davies and Kybett [1965a] was calculated from the heat of vaporization of the liquid and the heat of sublimation of the c, II, based on their vapor pressure data. The heats of transition obtained by Davies and Kybett [1965b] were calculated from the observed heats of solution of the three forms of 1-hexadecanol in benzene at 25 °C.

Properties of the Solid at 25 °C

Heat Capacity

The stable form at 25 °C is the γ-form, or crystal II. The heat capacity was taken from the calorimetric measurements of Parks, Kennedy, Gates, Mosley, Moore, and Renquist [1956]. Kakiuchi, Sakurai, and Suzuki [1950] also described some heat capacity measurements, but gave no numerical data.

Heat of Combustion

The experimental values are listed in table 214. The value obtained by Parks, Mosley and Peterson was selected.

Absolute Entropy

Parks, Kennedy, Gates, Mosley, Moore, and Renquist [1956] measured the heat capacity down to 80 K and calculated the entropy at 25 °C using the third law of theromodynamics. The result of their calculations was selected. The estimated uncertainty includes the effect of experimental errors in heat capacity and the extrapolation to O K.

TABLE 214. 1-Hexadecanol. Reported values. Heat of combustion of crystal II at 25 °C

Investigator	ΔH_c^0(c), kcal mol^{-1}
Stohmann [1885]	−2524.0
Beckers [1931]	−2500.4
Richardson and Parks [1939]	−2501.8
Parks, Mosley, and Peterson [1950]	−2502.8

Vapor-Liquid Equilibrium

Heat of Vaporization at the Melting Point

The vapor pressure of Davies and Kybett [1965a] gives a heat of vaporization of 26.2 kcal mol^{-1}, assuming an ideal gas but their measurements covered only a 12 °C range of temperature. Spizzichino [1956] calculated a heat of vaporization of 25.9 kcal mol^{-1} at 50 °C from her vapor pressure equation. However this equation did not match the slope of her measurements in the vicinity of 50 °C. The Antoine constants for the range 50 to 103 °C, reported in table 210, give a heat of vaporization of 28.9 kcal mol^{-1} at 50 °C. The high value reflects the effect of the vapor pressure of Spizzichino in this range. Since Spizzichino's data apparently have high pressure-temperature slopes for the other alcohols at the low temperature end, the selected heat of vaporization is closer to the value calculated by Davies and Kybett then to the one calculated from the Antoine constants.

Isomeric Hexadecanols

Reported values of the simple physical properties are summarized in the following unnumbered tables. Values of the normal boiling point have been found only for 2,2-dimethyl-1-tetradecanol and 5-methyl-9-ethyl-6-tridecanol. 6-*n*-Pentyl-6-undecanol is the only compound in this group for which the boiling point data was sufficient to allow calculation of the Antoine constants. However, these data are of low accuracy and cover only the range from 115 to 165 °C. A value of 100 was assumed for *C*. The smoothed values of refractive indices in table 215 were based on the measurements of Eykman [1919]. The densities in table 216 were calculated from the Francis constants listed or, when applicable, from a linear function of temperature. These constants were obtained from the least squares fit to the data for Pickard and Kenyon [1913] for 3-hexadecanol and, primarily, to the data of Bingham and Stephens [1933] for the other compounds.

TABLE 215. Isomeric hexadecanols. Selected values. Refractive index at various temperatures and wavelengths

Symbol	Wavelength, angstroms	2-Methyl-2-pentadecanol		3-Ethyl-3-tetradecanol	
		20 °C	80 °C	20 °C	80 °C
He_{red}	6687.1	1.4426	1.4198	1.4485	1.4221
H_c	6562.8	1.4429	1.4201	1.4488	1.4224
Na_D	5892.6	1.4452	1.4222	1.4511	1.4244
Hg_e	5460.7	1.4471	1.4240	1.4530	1.4262
He_{blue}	5015.7	1.4497	1.4265	1.4556	1.4287
H_F	4861.3	1.4508	1.4275	1.4567	1.4297
H_{gg}	4358.3	1.4551	1.4315	1.4610	1.4338
$H_{G'}$	4340.5	1.4553	1.4317	1.4612	1.4339

TABLE 216. Isomeric hexadecanols. Selected values. Density of the liquids at various temperatures

Temperature °C	3-Hexadecanol	2-Ethyl-1-tetradecanol	2-Propyl-1-tridecanol	2-Butyl-1-dodecanol	Temperature Range, °C	Francis Constants			
	Density, g cm^{-3}					67–153	20–100	20–100	20–100
10		0.847	0.846		*A*	1.0307	0.8929	0.8786	0.8521
20		.8405	.8387	0.8321	$B \times 10^3$	0.3063	.5944	.6253	.692
25		.8371	.8353	.8347	*C*	111.95	19.45	13.15	
30		.8337	.8320	.8313	*E*	600	500	500	
40		.8250	.8250	.8244					
50		.8200	.8181	.8174					
60	0.8050	.8130	.8112	.8105					
70	.7980	.8061	.8043	.8036					
80	.7909	.7909	.7990	.7967					
90	.7836	.7836	.7920	.7897					
100	.7762	.7848	.7832	.7828					
110	.7685	.7776	.7761						
120	.7607								
130	.7527								
140	.7444								
150	.7360								
160	.7273								

TABLE 216—continued

Temperature °C	2-Pentyl-1-undecanol	2-Hexyl-1-decanol	2-Heptyl-1-nonanol
	Density, g cm^{-3}		
10		0.844	0.844
20	0.8377	.8378	.8377
25	.8343	.8343	.8343
30	.8309	.8308	.8309
40	.8239	.8238	.8241
50	.8170	.8168	.8173
60	.8101	.8098	.8103
70	.8032	.8028	.8033
80	.7963	.7958	.7962
90	.7894	.7888	.7891
100	.7825	.7818	.7818
110			.7745
	Francis Constants		
Temperature Range, °C	20–100	16–100	20–100
A	0.8516	0.8518	0.9091
$B \times 10^3$	.690	.700	.5469
C			29.04
E			500

TABLE 217. Isomeric Hexadecanols. Selected values. Vapor pressure of the liquid at various temperatures

Temperature °C	6-n-Pentyl-6-undecanol
	Pressure, mmHg
120	1.9
130	3.5
140	6.0
150.	10
160	16.
170	24.
	Antoine Constants
Temperature Range, °C	116–165
A	6.2204
B	1307.
C	100.

Isomeric Hexadecanols—Continued

Investigators		Vapor Pressures and Boiling Points		Freezing Point	Density, d g cm^{-3}		Refractive Index, n_D	
		°C	mmHg	t_m, °C	20 °C	25 °C	20 °C	25 °C
2-Hexadecanol, $C_{16}H_{34}O$, mol. wt. 242.45, state at 25 °3 crystal								
Asinger and Eckoldt	[1943]	135	1	43–44				
Breusch and Sokulla	[1953]			42.2–45				1.4256 (80°)
Selected value	[1967]			[b] 44±2				
3-Hexadecanol, $C_{16}H_{34}O$, mol. wt. 242.45, state at 25 °C crystal								
See also table 216								
Pickard and Kenyon	[1913]	152	4	50		0.7907 (80°)		
Asinger and Eckoldt	[1943]	150	4	40				
Selected value	[1967]			[b] 45±5				
4-Hexadecanol, $C_{16}H_{34}O$, mol. wt. 242.45, state at 25 °C crystal								
Asinger and Eckoldt	[1943]	128	1	38–39				

Isomeric Hexadecanols—Continued

Investigators		Vapor Pressures and Boiling Points		Freezing Point	Density, d g cm^{-3}		Refractive Index, n_D	
		°C	mmHg	t_m, °C	20 °C	25 °C	20 °C	25 °C
5-Hexadecanol, $C_{16}H_{34}O$, mol. wt. 242.45, state at 25 °C crystal								
Asinger and Eckoldt	[1943]	134	1.5	36				
6-Hexadecanol, $C_{16}H_{34}O$, mol. wt. 242.45, state at 25 °C crystal								
Asinger and Eckoldt	[1943]	148	3.5	34–35				
7-Hexadecanol, $C_{16}H_{34}O$, mol. wt. 242.45, state at 25 °C crystal								
Asinger and Eckoldt	[1943]	155	3	32				
8-Hexadecanol, $C_{16}H_{34}O$, mol. wt. 242.45, state at 25 °C crystal								
Asinger and Eckoldt	[1943]	128	1.5	48				
14-Methyl-1-pentadecanol, $C_{16}H_{34}O$, mol. wt. 242.45, state at 25 °C crystal								
Milburn and Truter	[1954]			30				
2-Methyl-2-pentadecanol, $C_{16}H_{34}O$, mol. wt. 242.45, state at 25 °C crystal								
See also table 215								
Eykman	[1919]			31		0.8266	1.4452	
6-Methyl-6-pentadecanol, $C_{16}H_{34}O$, mol. wt. 242.45								
Davies, Dixon, and Jones	[1930]	199–200	50			0.8316		1.4446
9-methyl-7-pentadecanol mol. wt. 242.45								
Guerbet	[1912]	180	18		0.8351 (15°)			
Whitmore and Kreuger	[1933]	130–132	2				1.4478	
		102–104	0.2					
Selected value	[1967]	^{c} 165±3	10					
8-methyl-8-pentadecanol mol. wt. 242.45								
Birch and Robinson	[1942]	165	13					

Isomeric Hexadecanols—Continued

Investigators	Vapor Pressures and Boiling Points		Freezing Point	Density, d g cm^{-3}		Refractive Index, n_D	
	°C	mmHg	t_m, °C	20 °C	25 °C	20 °C	25 °C
2-Ethyl-1-tetradecanol, $C_{16}H_{34}O$, mol. wt. 242.45							
See also table 216							
Bingham and Stephens [1933] Selected value [1967]				0.8405 ^{d} .8405 ±.0005	^{d} 0.8371 ±.0005		
2,2-Dimethyl-1-tetradecanol, $C_{16}H_{34}O$, mol. wt. 242.45, state at 25 °C liq.							
Blood and Hagemeyer [1964]	293	760	2	0.8400			1.4475
2,2-Dimethyl-3-tetradecanol, $C_{16}H_{34}O$, mol. wt. 242.45							
Whitmore, Whitaker, Mosher, Breivik, Wheeler, Miner, Sutherland, Wagner, Clapper, Lewis, Lux, and Popkin [1941]	149	7		0.8356		1.4477– 1.4479	
3-Ethyl-3-tetradecanol, $C_{16}H_{34}O$, mol. wt. 242.45, state at 25 °C liq.							
See also table 215							
Eykman [1919]			3	0.8462 (15°)	0.772 (80°)	1.4511	
2-*n*-Propyl-1-tridecanol, $C_{16}H_{34}O$, mol. wt. 242.45							
See also table 216							
Bingham and Stephens [1933] Selected value [1967]				0.8384 ^{d} .8387 ±.0005	^{d} 0.8353 ±.0005		
5-*n*-Propyl-4-tridecanol, $C_{16}H_{34}O$, mol. wt. 244.45							
Petrov and Ol'dekop [1948]	152–153	10		0.8310 (15°)		1.442 (15°)	
5-Methyl-9-ethyl-6-tridecanol, $C_{16}H_{34}O$, mol. wt. 242.45							
Union Carbide Corporation [1936] Wicket and Freure [1937]	155–157 287–288	10 760					

Isomeric Hexadecanols—Continued

Investigators		Vapor Pressures and Boiling Points		Freezing Point	Density, d g cm^{-3}		Refractive Index, n_D	
		°C	mmHg	t_m, °C	20 °C	25 °C	20 °C	25 °C
2-*n*-Butyl-1-dodecanol, $C_{16}H_{34}O$, mol. wt. 242.45								
See also table 216								
Bingham and Stephens	[1933]				0.8379			
Selected value	[1967]				^{d} .8383 ±.0005	^{d} 0.8347 ±.0005		
2-*n*-Pentyl-1-undecanol, $C_{16}H_{34}O$, mol. wt. 242.45								
See also table 216								
Bingham and Stephens	[1933]				0.8381			
Selected value	[1967]				^{d} .8378 ±.0005	^{d} 0.8343 ±.0005		
6-*n*-Pentyl-6-undecanol, $C_{16}H_{34}O$, mol. wt. 242.45								
Moyer and Marvel	[1931]	160–164	19					
Whitmore and Williams	[1933]	115–117	1.5			0.8293	1.4470	
Church, Whitmore, and McGrew	[1934]	163–165	17					
Challenger and Pantony	[1954]	165–167	20					
		154–155	11					
Selected value	[1967]	^{e} 150±3	10					
Antoine constants: *A* 6.2204, *B* 1307., *C* 100.								
2,2,6,10,10-Pentamethyl-6-undecanol, $C_{16}H_{34}O$, mol. wt. 242.45, state at 25 °C crystal								
Gutman and Hickinbottom	[1951]	122–124	4	64.5				
2-*n*-Hexyl-1-decanol, $C_{16}H_{34}O$, mol. wt. 242.45								
See also table 216								
Bingham and Stephens	[1933]				0.8372			
Mastagli	[1938]	177	15		.8409 (16.5°)		1.4520 (16.5)	
Weizmann, Bergmann, and Sulzbacher	[1950]	170–180	24					
Bolle and Bourgeois	[1951]	165–170	4					
Selected value	[1967]	^{c} 172±5	10		^{d} .8378 ±.0005	^{d} 0.8343 ±.0005	^{d} 1.451 ±0.001	
2,4,6-Triethyl-1-decanol, $C_{16}H_{34}O$, mol. wt. 242.45								
Miller and Bennett	[1961]	133–140	3					1.4669

Isomeric Hexadecanols—Continued

Investigators	Vapor Pressures and Boiling Points		Freezing Point	Density, *d* g cm^{-3}		Refractive Index, n_D	
	°C	mmHg	t_m, °C	20 °C	25 °C	20 °C	25 °C
2-Heptyl-1-nonanol, $C_{16}H_{34}O$, mol. wt. 242.45							
Bingham and Stephens [1933]				0.8376 ^{d} .8377 ±.0005	^{d} 0.8343 ±.0005		
2,8-Dimethyl-5-(3-methylbutyl)-5-nonanol, $C_{16}H_{34}O$, mol. wt. 242.45							
Grignard [1904]	143–145	15					
2,2,6,6-Tetramethyl-4-(2,2-dimethyl-1-propyl)-3-heptanol, $C_{16}H_{34}O$, mol. wt. 242.45							
Whitmore, Whitaker, Mosher, Breivik, Wheeler, Miner, Sutherland, Wagner, Clapper, Lewis, Lux, and Popkin [1941]	97–101	5					

Heptadecanols

Of the theoretically possible 321,198 isomers of heptadecanol, physical property data were located for only 9 isomers. Most of these were melting points. No systematic measurements of properties as functions of temperature have been made. In accordance with the assignments made in Appendix E, the crystalline form of 1-heptadecanol stable at the melting point is the α-modification. The following β → α transition temperatures have been reported for 1-heptadecanol: Carey and Smith [1933], 43.5 °C; Meyer and Reid [1933], 45.7 °C; and Phillips and Mumford [1934], 47.3 °C. A temperature of 46. ± 2. °C was selected for this transition.

Heptadecanols

Investigators		Vapor Pressures and Boiling Points		Freezing Point	Density, *d* g cm^{-3}		Refractive Index, n_D	
		°C	mmHg	t_m, °C	20 °C	25 °C	20 °C	25 °C
1-Heptadecanol, $C_{17}H_{36}O$, mol. wt. 256.48, state at 25 °C crystal								
Levene, West, and Van der Scheer	[1915]			54				
Gascard	[1921]			54				
Heiduschke and Ripper	[1923]			54				
Carey and Smith	[1933]			53.8				
Meyer and Reid	[1933]			53.31				
Phillips and Mumford	[1934]			53.9				
Carey and Smith	[1935]			54.2				
Tischer	[1939]			54				
Union Carbide Corporation	[1958]	333	760		0.8382			
Tanaka, Seto, Watanabe, and Hayashida	[1959]			51–53				
Vil'shan and Gavrilova	[1963]			52.3		0.8153 (60°)		1.4392 (60°)
Selected value	[1967]			^{b} 53.8± 0.2				

Heptadecanols—Continued

Investigators		Vapor Pressures and Boiling Points		Freezing Point	Density, d g cm^{-3}		Refractive Index, n_D	
		°C	mmHg	t_m, °C	20 °C	25 °C	20 °C	25 °C
2-Heptadecanol, $C_{17}H_{36}O$, mol. wt. 256.48, state at 25 °C crystal								
Wilstätter, Schuppli, and Mayer	[1919]	176–177.5	10		0.837(0°)		1.45037	
Kuhn, Kohler, and Kohler	[1936]	140	0.5	34–35				1.4407 (37°)
Dreger, Keim, Miles, Shedlovsky, and Ross	[1944]	155	1	44.5				
Breusch and Sokullu	[1953]			44–44.5				
Selected value	[1967]			^{b}44.5±1				
8-Heptadecanol, $C_{17}H_{36}O$, mol. wt. 256.48, state at 25 °C crystal								
Dreger, Keim, Miles, Shedlovsky, and Ross	[1944]	144	1	60.5				
9-Heptadecanol, $C_{17}H_{36}O$, mol. wt. 256.48, state at 25 °C								
Petrov and Ol'dekop	[1948]	158–200	3					
14-Methyl-1-hexadecanol, $C_{17}H_{36}O$, mol. wt. 256.48, state at 25 °C liq.								
Murray and Schoenfeld	[1952]			18.4				
Milburn and Truter	[1954]			18.5–19			1.4530	
Selected value	[1967]			^{b}18.5±1				
3,3-Dimethyl-4-pentadecanol, $C_{17}H_{36}O$, mol. wt. 256.48								
Whitmore, Whitaker, Mosher, Breivik, Wheeler, Miner, Sutherland, Wagner, Clapper, Lewis, Lux, and Popkin	[1941]	190	25		0.8437		1.4252–1.4510	
6-Methyl-6-*n*-propyl-4-tridecanol, $C_{17}H_{36}O$, mol. wt. 256.48								
Desgrandchamps, Deluzarche, and Millard	[1961]	160–170	0.7					
3,9-Diethyl-6-tridecanol, $C_{17}H_{36}O$, mol. wt. 256.48								
Union Carbide Corporation	[1958]	309	760		0.8460			
8-Methyl-8-isobutyl-6-dodecanol, $C_{17}H_{36}O$, mol. wt. 256.48								
Desgrandchamps, Deluzarche, and Millard	[1961]	125–126	0.2		0.8461		1.4544	

1-Octadecanol

Properties of the Liquid Phase at Various Temperatures

Refractive Index

The selected values in table 218 were based on the measurements of Rathmann, Curtis, McGeer, and Smyth [1956] from 60 to 90 °C and on the single measurement of Spizzichino [1956] at 60 °C. Bergmann, Cregiton, and Stokes [1956] also reported a value of n_D at 70.5 °C, but it was lower than the value interpolated from the other data by 0.002 units. A linear extrapolation from this temperature range to the undercooled liquid at 25 °C gives a refractive index of 1.4523.

Density

The most extensive data on density of the liquid have published by Costello and Bowden [1958], who covered the range from 80 to 300 °C. Krafft [1883a] and [1884] reported densities at 59, 70, and 99.4 °C, and Rathmann, Curtis, McGeer, and Smyth [1956] reported values from 60 to 90 °C. The Francis constants in table 218 and the corresponding calculated densities were obtained from these data. Differences between observed and calculated densities were generally less than 0.001 g cm^{-3}. Tsvetkov and Marinin [1949] also reported a density value at 59.1 °C.

Vapor Pressure and Boiling Points

There are no measurements of vapor pressure or boiling points above 19 mmHg. The Antoine constants for the temperature range from 120 to 218 °C listed in table 218 were obtained by a least squares fit to scattered boiling point values reported by Krafft [1883a] and [1884]; Levene, West, and van der Scheer [1915); Higasi and Kubo [1939]; Backer and Strating [1940]; Paul and Joseph [1952]; and Costello and Bowden [1958]. Differences between calculated and observed temperatures range from 1 to 4 °C; thus, there is a large uncertainty associated with the tabulated values. In the low temperature range from 58 to 120 °C, there are two sources of data—Spizzichino [1956] and Davies and Kybett [1965a]. Davies and Kybett give the equation, $\log P(\mathrm{mmHg}) = 14.143 - 5928/T$, for the range 61 to 83 °C. The relationship between the two sets of experimental data is similar to the data for the other alcohols. They appear to approach each other at the low end, but the slope of the pressure with temperature is larger for the data from Spizzichino than it is for the data from Davies and Kybett. The Antoine constants for the low temperature range reflect a compromise between these two sets.

Solid-Gas Phase Equilibria

Sublimation Pressure

There are two sets of measurements of the vapor pressure of the solid phase. Both involve an effusion phenomenon. Hoyer and Peperle [1958] give the equation, $\log P(\mathrm{mmHg}) = 23.63 - 9075/T$, for the temperature range of about 45 °C to the triple point, and Davies and Kybett [1965] give the equation, $\log P(\mathrm{mmHg}) = 25.865 - 9787/T$, for similar temperatures. This range includes the *c*, I → *c*, II transition temperature. However, the accuracy of measurement and range of temperature were not adequate in either case to distinguish the change in slope of the vapor pressure at this temperature. Davies and Kybett stated that they started out with the c, II (γ-form) and therefore their sublimation pressure measurements refer to this form. Although it is probable that they had at least some of the c, I (α-form) present at temperatures above 54 °C, their data would reflect primarily the vapor pressures of c, II unless the transformation to c, I were complete. Comparison of the heat of sublimation calculated from these equations with that for 1-hexadecanol also indicates that these equations refer to c, II. The equation of Hoyer and Peperle [1958] gives a c-liq-gas triple point of 0.166×10^{-3} mmHg, and that of Davies and Kybett gives 0.202×10^{-3} mmHg.

Heat of Sublimation

The vapor pressure equation of Hoyer and Peperle [1958] gives a heat of sublimation of 41.5 kcal mol^{-1}, and that of Davies and Kybett [1965a] gives 44.8 ± 0.5 kcal mol^{-1}. The value derived from Davis and Kybett's measurements is judged to be more reliable and was selected. Presumably it refers to the vaporization of c,II (γ-form).

Solid-Solid and Solid-Liquid Phase Equilibria

Transition Temperature and Melting Point

Octadecanol shows a polymorphic behavior similar to that of hexadecanol. Thus, it belongs in Class 3 described in Appendix E. The form stable at the melting point, crystal I, is the α-form. In the α-phase, the molecules rotate about their long axes, and this results in a transparent appearance. The α-phase has only a short range of stability below the melting point. Melting point data have been summarized in table 219. Solid phase transitions have been observed by Meyer and Reid [1933], Phillips and Mumford [1933] and [1934], Hoffman and Smyth [1949], Kolp and Lutton [1951], Tanaka, Seto, and Hayashida [1957], and Tanaka, Seto, Watanabe, and

TABLE 218. 1-Octadecanol. Selected values. Physical and thermodynamic properties

Temp. °C	Refractive Index, n_D	Density g cm^{-3}	Vapor Pressure, mmHg
60	1.4388	0.8123	0.00022
70	1.4349	.8052	.00084
80	1.4311	.7981	.00263
90	1.4272	.7910	.0071
100		.7838	.0172
110		.7767	.0377
120		.7695	.070
130		.7622	.155
140		.7550	.322
150		.7477	.63
160		.7404	1.16
170		.7330	2.04
180		.7256	2.5
190		.7182	5.6
200		.7107	8.8
203.			10
210		.7032	13.5
220		.6956	20.
230		.6880	
240		.6803	
250		.6726	
260		.6648	
270		.6569	
280		.6490	
290		.6410	
300		.6329	

Data For Phase Transitions

Initial	Final	Temp. °C	dt/dP deg mm^{-1}	Pressure mmHg	ΔH kcal mol^{-1}	$d\Delta H/dt$ cal deg^{-1} mol^{-1}	ΔS cal deg^{-1} mol^{-1}	ΔC_p cal deg^{-1} mol^{-1}
c,u	c,I	53.5±1						
c,II	c,I	54±1.5						
c,I	liq	57.9±0.1		0.00017				
liq	g	57.9±0.1		.00017	27.1±1		81.±3	

Condensed Phase Heat Capacity

State	Temp. °C	C_p cal deg^{-1} mol^{-1}

Properties of the Saturated Real Gas

Temp. °C	H^r-H^0 kcal mol^{-1}	S^r-S^0 cal deg^{-1} mol^{-1}	$C_p^r-C_p^0$ cal deg^{-1} mol^{-1}

Data for the Standard States at 25 °C

State	Heat of Combustion ΔH_c^0 kcal mol^{-1}	Heat of Formation ΔH_f^0 kcal mol^{-1}	Entropy S^0 cal deg^{-1} mol^{-1}	Gibbs Energy of Formation ΔG_f^0 kcal mol^{-1}	Heat Capacity, C_p cal deg^{-1} mol^{-1}

Critical Constants

Temp. °C, K	Pressure atm	Density g cm^{-3}

Constants in Vapor Pressure and Density Equation

Antoine Equation

Temp. Range	A	B	C
58 to 120 °C	4.3809	1047.	70.4
120 to 218 °C	6.4616	1599.	90.

Francis Equation

Temp. Range	A	$B\times10^3$	C	E
60 to 300 °C	0.89397	0.6388	27.76	300.

TABLE 219. 1-Octadecanol. Reported values. Simple physical properties

Investigators		Vapor Pressures and Boiling Points		Freezing Point	Density, d g cm^{-3}		Refractive Index, n_D	
		°C	mmHg	t_m, °C	20 °C	25 °C	20 °C	25 °C
1-Octadecanol, $C_{18}H_{38}O$, mol. wt. 270.50, state at 25 °C crystal								
Krafft	[1883a]			59				
Krafft	[1883b]			59				
Krafft	[1884]	210	15	59				
Levene, West, and Van der Scheer	[1915]	210	15	58.5				
Gascard	[1921]			58.5				
Kind and Bergmann	[1924]			58				
Levene and Taylor	[1924]	153–154	0.27	58.5–59.5				
Andre and Francois	[1926]			61				
Jantzen and Tiedcke	[1930]			59				
Malkin	[1930]			59.0				
Schrauth, Schenck, and Stickdorn	[1931]	208–212	15	58.9				
Bleyberg and Ulrich	[1931]	195–205	0.2	59.4–59.8				
Smith	[1931]			57.95				
Meyer and Reid	[1933]			57.85				
Phillips and Mumford	[1933]			57.95				
Carey and Smith	[1933]			57.95				
Sauer and Adkins	[1937]			57–58				
Turpeinen	[1938]			57.5–58				
Higasi and Kubo	[1939]	160	0.9	57.6–57.75				
Backer and Strating	[1940]	170–171	2	58.3–58.5				
Komarewsky and Coley	[1941]			58.0				
Kind and Bergmann	[1942]	100–105	0.5					
Niemann and Wegner	[1942]			58.0				
Frewing	[1944]			58				
Hoerr, Harwood, and Ralston	[1944]			57.98				
Trapeznikov	[1945]			58.4				
Weaver and Kraus	[1948]			57.5–58.5				
Martin and Pink	[1948]			58.0				
Honn, Bezman, and Daubert	[1949]			56.5–58				
Greenhill	[1949]			58				
Hoffman and Smyth	[1949]			57.7				
Shreve, Heether, Knight, and Swern	[1950]			58				
Baldacci	[1950]			57–58				
Bergmann, Freeney, and Swift	[1951]			56.5				
Meakins and Mulley	[1951]			58.2				
Cockbain and McMullen	[1951]			58.5				
Kilp and Lutton	[1951]			57.9				
Clemo and Stevens	[1952]			55–56				

TABLE 219. 1-Octadecanol. Reported values. Simple physical properties—Continued

Investigators		Vapor Pressures and Boiling Points		Freezing Point	Density, *d* g cm^{-3}		Refractive Index, n_D	
		°C	mmHg	t_m, °C	20 °C	25 °C	20 °C	25 °C
1-Octadecanol, $C_{18}H_{38}O$, mol. wt. 270.50, state at 25 °C crystal								
Paul and Joseph	[1952]	156–158	0.8					
Tiedt and Truter	[1952]			57.1–58.5				
Umezawa	[1954]			59				
Brown, Mead, and Subba Rao	[1955]			58–59				
Rathmann, Curtis, McGreer, and Smyth	[1956]			57.6				
Spizzichino	[1956]			57.8				
Tanaka, Seto, and Hayashida	[1957]			55–57				
Costello and Bowden	[1958]	217	19	59				
Watanabe	[1960]			58				
Davies and Kybett	[1965]			58.0–58.2				
Selected value	[1967]	[e] 203.±3	10	[b] 57.9±0.1				

Antoine constants: *A* 6.4616, *B* 1599., *C* 90.

Hayashida [1959]. The investigations of Hoffman and Smyth included measurements of dielectric constants of the solid phases, and those of Tanaka et al. included x-ray diffraction measurements. As for hexadecanol, the interpretations of the observations given by the various investigators have not been in agreement. On cooling the α-phase a few degrees below the melting point, a reversible transformation to the β-phase is observed; however, the β-phase appears to be metastable since it slowly transforms to the γ-phase on standing below the transition temperature. The direct transformation of the α- to the γ-phase is not easily observed since it is slow and occurs close to the α- to β-phase transition temperature. Values selected for these temperatures are shown in table 218. The γ-phase is crystal II.

Heats of Transition and Fusion

No direct measurements of heats of transition or fusion have been made. The heats of sublimation of the γ-phase and of the liquid, based on vapor pressure data, give a heat of fusion of the γ-phase of 17.7 ± 1 kcal mol^{-1}. However, no selection of the heat of fusion of the α-phase, crystal I, can be made.

Vapor-Liquid Equilibrium

Heat of Vaporization at the Melting Point

The vapor pressure equation of Davies and Kybett [1965a] gives a heat of vaporization of the liquid of 27.1 ± 0.5 kcal mol^{-1}. Spizzichino [1956] also reported a heat of vaporization of 27.1 kcal mol^{-1}, although this was calculated from only three vapor pressure measurements rather than from her complete set of data. The Antoine constants given in table 218 for the 58 to 120 °C range give a heat of vaporization of 31.9 kcal mol^{-1} at 58 °C. This is probably too high a value because of the influence of Spizzichino's vapor pressure data which cause too large a pressure-temperature derivative at the lower end of the range. Therefore, the ΔH_v obtained from Davies and Kybett's data was selected for table 218.

Isomeric Octadecanols

The only systematic study of the properties of any of the isomeric octadecanols is the measurements of refractive index reported by Eykman [1919]. Smoothed values of refractive index at various standard wavelengths, based on his data, are given in table 220 for two such compounds. The data are not sufficient to allow the calculation of the constants in the density or vapor pressure equations for any of the compounds in this group.

TABLE 220. Isomeric Octadecanols. Selected values. Refractive index at various temperatures and wavelengths

Symbol	Wavelength, angstroms	2-Methyl-2-heptadecanol	3-Ethyl-3-hexadecanol	
		80 °C	20 °C	80 °C
He_{red}	6687.1	1.4230	1.4513	1.4257
H_c	6562.8	1.4233	1.4516	1.4260
Na_D	5892.6	1.4254	1.4543	1.4285
Hg_e	5460.7	1.4272	1.4557	1.4299
He_{blue}	5015.7	1.4297	1.4584	1.4324
H_F	4861.3	1.4307	1.4594	1.4334
Hg_g	4358.3	1.4349	1.4638	1.4375
$H_{G'}$	4340.5	1.4350	1.4641	1.4377

Isomeric Octadecanols

Investigators	Vapor Pressures and Boiling Points		Freezing Point	Density, d g cm^{-3}		Refractive Index, n_D	
	°C	mmHg	t_m, °C	20 °C	25 °C	20 °C	25 °C
2-Octadecanol, $C_{18}H_{38}O$, mol. wt. 270.50, state at 25 °C crystal							
Pangborn and Anderson [1936]			56				
Breusch and Sokullu [1953]			52–53				
3-Octadecanol, $C_{18}H_{38}O$, mol. wt. 270.50, state at 25 °C crystal							
Pickard and Kenyon [1913]	172	2	56				
6-Methyl-1-heptadecanol, $C_{18}H_{38}O$, mol. wt. 270.50							
Cason and Winans [1950]	159–161	1.8				1.4537	
16-Methyl-1-heptadecanol, $C_{18}H_{38}O$, mol. wt. 270.50, state at 25 °C crystal							
Milburn and Truter [1954]			41.8–42.0				
2-Methyl-2-heptadecanol, $C_{18}H_{38}O$, mol. wt. 270.50, state at 25 °C crystal							
See also table 220							
Eykman [1919]			39	0.7693 (80.1°)			
3-Ethyl-3-hexadecanol, $C_{18}H_{38}O$, mol. wt. 270.50, state at 25 °C liq.							
Eykman [1919]			22.1	0.8405 (22.8°)	0.7779 (79.4°)		

Isomeric Octadecanols—Continued

Investigators	Vapor Pressures and Boiling Points		Freezing Point	Density, *d* g cm^{-3}		Refractive Index, n_D	
	°C	mmHg	t_m, °C	20 °C	25 °C	20 °C	25 °C
2,2-Dimethyl-3-hexadecanol, $C_{18}H_{38}O$, mol. wt. 270.50, state at 25 °C liq.							
Zook, McAleer, and Horwin [1946]	87–90	10^{-4}	12–14			1.4490– 1.4491	
6,10,14-Trimethyl-2-pentadecanol, $C_{18}H_{38}O$, mol. wt. 270.50							
Smith and Schweitzer [1941]	146–148	1					
2,2,6-Trimethyl-6-pentadecanol, $C_{18}H_{38}O$, mol. wt. 270.50							
Gutman and Hickinbottom [1951]	136–137	0.5				1.4480	
7-*n*-Butyl-7-tetradecanol, $C_{18}H_{38}O$, mol. wt. 270.50							
Rabjohn and Latina [1954]	157–159	1				1.4516	
3,3,7,11,11-Pentamethyl-7-tridecanol, $C_{18}H_{38}O$, mol. wt. 270.50, state at 25 °C crystal							
Gutman and Hickinbottom [1951]	126–126.5	1.8	39.5				
2-*n*-Heptyl-1-undecanol, $C_{18}H_{38}O$, mol. wt. 270.50							
Mastagli [1938]				0.8446 (15°)		1.4550 (15°)	

Nonadecanols

The stable form of 1-nonadecanol at the melting point is the α-modification. Several experimental melting points are shown in the following tables. Phillips and Mumford [1934] reported the α → β transition as 54.2 ± 0.2 °C, and Tanaka, Seto, and Hayashida [1957] obtained approximately 54 °C. All of the other physical property data for the C_{19} alcohols are listed in the following tables.

Nonadecanols

Investigators	Vapor Pressures and Boiling Points		Freezing Point	Density, *d* g cm^{-3}		Refractive Index, n_D	
	°C	mmHg	t_m, °C	20 °C	25 °C	20 °C	25 °C
1-Nonadecanol, $C_{19}H_{40}O$, mol. wt. 284.53, state at 25 °C crystal							
Levene and Taylor [1924]	166–167	0.32	62–63				
Malkin [1930]			62.0				
Phillips and Mumford [1934]			61.65				
Turkiewicz [1939]	179–184	0.2	61.5				
Cason, Wolfhagen, Tarpey, and Adams [1949]	204–217	3	59–61				
Tanaka, Seto, and Hayshida [1957]			60–62				
Selected value [1967]			[a] 61.7± 0.2				

Nonadecanols—Continued

Investigators	Vapor Pressures and Boiling Points		Freezing Point	Density, *d* g cm^{-3}		Refractive Index, n_D	
	°C	mmHg	t_m, °C	20 °C	25 °C	20 °C	20 °C
2-Nonadecanol, $C_{19}H_{40}O$, mol. wt. 284.53, state at 25 °C crystal							
Fornholz and Finkelstein [1938]			48–49				
Dreger, Keim, Miles, Shedlovsky, and Ross [1944]	166	1	48				
Breusch and Sokullu [1953]			51–51.8				
Selected value [1967]			[a] 51±1				
4-Nonadecanol, $C_{19}H_{40}O$, mol. wt. 284.53, state at 25 °C liq.							
Leroide [1921]	221–224	15	19				
10-Nonadecanol, $C_{19}H_{40}O$, mol. wt. 284.53, state at 25 °C crystal							
Komarewsky and Coley [1941]			65				
Dreger, Keim, Miles, Shedlovsky, and Ross [1944]	169	1	64–65				
2-Methyl-1-octadecanol, $C_{19}H_{40}O$, mol. wt. 284.53, state at 25 °C crystal							
Fernholz and Finkelstein [1938]			32–33				
Bailey, Polgar, Tate, and Wilkenson [1955]	163–165	0.1	48.0–48.5				
16-Methyl-1-octadecanol, $C_{19}H_{40}O$, mol. wt. 284.53, state at 25 °C crystal							
Murray and Schoenfeld [1952]			27.5–31				
Milburn and Truter [1954]			30.4–30.7				
3-Methyl-3-octadecanol, $C_{19}H_{40}O$, mol. wt. 284.53, state at 25 °C crystal							
Sorensen and Sorensen [1948]	103–105	0.001	32–32.5				
4-Methyl-4-octadecanol, $C_{19}H_{40}O$, mol. wt. 284.53, state at 25 °C crystal							
Sorensen and Sorensen [1948]			16	0.8394		1.45792	
5-Methyl-5-octadecanol, $C_{19}H_{40}O$, mol. wt. 284.53, state at 25 °C liq.							
Sorensen and Sorensen [1948]			6.5–7.0	0.83745		1.45080	
6-Methyl-6-octadecanol, $C_{19}H_{40}O$, mol. wt. 284.53, state at 25 °C liq.							
Sorensen and Sorensen [1948]			−23	0.8385		1.45103	

Nonadecanols—Continued

Investigators		Vapor Pressures and Boiling Points		Freezing Point	Density, *d* g cm^{-3}		Refractive Index, n_D	
		°C	mmHg	t_m, °C	20 °C	25 °C	20 °C	25 °C
9-Methyl-9-octadecanol, $C_{19}H_{40}O$, mol. wt. 284.53, state at 25 °C liq.								
Sorensen and Sorensen	[1948]			−23	0.8355		1.45085	
9-Ethyl-9-heptadecanol, $C_{19}H_{40}O$, mol. wt. 284.53, state at 25 °C liq.								
Birch and Robinson * pressure uncertain	[1942]	190–195	* 15	−10				
2,2-Dimethyl-3-*tert*-butyl-3-tridecanol, $C_{19}H_{40}O$, mol. wt. 284.53								
Petrov, Sokolova, and Kao	[1960]	162–163	4		0.8698		1.4674	
7-*n*-Hexyl-7-tridecanol, $C_{19}H_{40}O$, mol. wt. 284.53								
Challenger and Pantony	[1954]	193–194	20					
Meshcheryakov, Erzyutova, and Kuo	[1961]	150–153	4–5		0.8408		1.4492	
Hillman	[1962]	121–123	0.2					
Selected value	[1967]	^{c}175±5.	10					

Eicosanols

The polymorphic forms of 1-eicosanol place it in Class 5, as described in Appendix E. Thus the form stable at the melting point is the α-phase. The reported values of the melting point are summarized in the following unnumbered table. Tanaka, Seto and Hayashida [1957] reported the temperature for the c,I ($\gamma \longrightarrow \alpha$) transition as 63 °C. Davies and Kybett [1965a] measured the sublimation pressure of 1-eicosanol from 54 to 64 °C. They express the results in the form of the equation, log P(mmHg) = 29.735 − 11393/T. Presumably this refers to c,II (γ-phase). This equation corresponds to a heat of sublimation of 52.1 ± 1 kcal mol^{-1}. They also measured the vapor pressure of the liquid from 66 to 85 °C and reported log P(mmHg) = 14.253 − 6213/T. The corresponding heat of vaporization is 28.4 ± 1 kcal mol^{-1}. By difference, the heat of fusion of the γ-form is 23.7 ± 2 kcal mol^{-1}. The only other physical property data available for 1-eicosanol are some boiling point values of questionable reliability listed in the following table.

Physical property data on the isomeric eicosanols consists primarily of melting point values and scattered boiling points at reduced pressures. Melting points have been reported for both the racemic, *dl*, forms and the optically active *d*- and *l*-forms of 2-eicosanol. Ekyman [1919] has measured the refractive index of 2-methyl-2-nonadecanol and 3-ethyl-3-octadecanol at various wavelengths at approximately 80 °C. Smoothed values are listed in table 221. He also measured the density of the liquid at the same temperature.

Eicosanols

Investigators	Vapor Pressures and Boiling Points		Freezing Point	Density, *d* g cm^{-3}		Refractive Index, n_D	
	°C	mmHg	t_m, °C	20 °C	25 °C	20 °C	25 °C
1-Eicosanol, $C_{20}H_{42}O$, mol. wt. 298.56, state at 25 °C crystal							
Haller [1907]			71				
Wilstätter, Mayer, and Huni [1910]	243–250	8.5	63–64				
Levene, West, and Van der Scheer [1915]	210	0.3	66–67				
Levene and Taylor [1924]	178	0.4	66–67				
Adam and Dyer [1925]			65–65.5				
Jantzen and Tiedcke [1930]			65–65.2				
Backer and Strating [1940]			65.1–65.5				
Heilbron, Jones, Roberts, and Wilkinson [1941]			62				
Pajari [1943]			67–67.5				
Clark, Hicks, and Harris [1948]			66.5				
Halpern and Adams [1949]			67–69				
Tiedt and Truter [1952]			64.8–65.0				
Fujita and Yoshikawa [1953]			70–71				
Umezawa [1954]			65–66				
Tanaka, Seto, and Hayashida [1957]			63–65				
Davies and Kybett [1965]			64.9–65.3				
Selected value [1967]	^{c}251.±5.	10	^{b}66.0±1				
2-Eicosanol, $C_{20}H_{42}O$, mol. wt. 298.56, state at 25 °C crystal							
Pangborn and Anderson [1936]			62.5–63				
Ställberg-Stenhagen and Stenhagen [1944–45]			50.7(dl) 61.2(d)				
Halpern and Adams [1949]			58–59				
Church, Ward, Gibson, Meakins, and Mulley [1950]	208–212	7	58.5–59.0				
Serck-Hansen, Ställberg-Stenhagen, and Stenhagen [1953]			61.8–62.0(d) 61.5–61.8(l)				
Breusch and Sokullu [1953]			59–60				1.4312 (80°)
Selected value [1967]			59±2 (dl) 61.5±1 (d)				
4-Eicosanol, $C_{20}H_{42}O$, mol. wt. 298.56, state at 25 °C crystal							
Halpern and Adams [1949]			43–44				
Church Ward, Gibson, Meakins, and Mulley [1950]	190–192	3	55.0–55.3				
5-Eicosanol, $C_{20}H_{42}O$, mol. wt. 298.56, state at 25 °C crystal							
Wynberg and Logothetis [1956]			51–52				

Eicosanols—Continued

6-Eicosanol, $C_{20}H_{42}O$, mol. wt. 298.56, state at 25 °C crystal

Investigators		Vapor Pressures and Boiling Points		Freezing Point	Density, d g cm^{-3}		Refractive Index, n_D	
		°C	mmHg	t_m, °C	20 °C	25 °C	20 °C	25 °C
Halpern and Adams	[1949]			54–56				
Church Ward, Gibson, Meakins, and Mulley	[1950]	189	2.7	57.7–57.8				
Selected value	[1967]			[a] 57.8± 0.5				

8-Eicosanol, $C_{20}H_{42}O$, mol. wt. 298.56, state at 25 °C crystal

Investigators		Vapor Pressures and Boiling Points		Freezing Point	Density, d g cm^{-3}		Refractive Index, n_D	
		°C	mmHg	t_m, °C	20 °C	25 °C	20 °C	25 °C
Halpern and Adams	[1949]			52–54				
Church, Ward, Gibson, Meakins, and Mulley	[1950]	192	3	57.7–57.9				
Selected value	[1967]			[a] 57.8± 0.5				

10-Eicosanol, $C_{20}H_{42}O$, mol. wt. 298.56, state at 25 °C crystal

Investigators		Vapor Pressures and Boiling Points		Freezing Point	Density, d g cm^{-3}		Refractive Index, n_D	
		°C	mmHg	t_m, °C	20 °C	25 °C	20 °C	25 °C
Halpern and Adams	[1949]			65.5				
Church, Ward, Gibson, Meakins, and Mulley	[1950]	214	7	65.3–65.6				
Selected value	[1967]			[a] 65.5± 0.5				

18-Methyl-1-nonadecanol, $C_{20}H_{42}O$, mol. wt. 298.56, state at 25 °C crystal

Investigators		Vapor Pressures and Boiling Points		Freezing Point	Density, d g cm^{-3}		Refractive Index, n_D	
		°C	mmHg	t_m, °C	20 °C	25 °C	20 °C	25 °C
Morray and Schoenfeld	[1952]			50.3				
Milburn and Truter	[1954]			49.8				
Selected value	[1967]			[b] 50.0±1				

2-Methyl-2-nonadecanol, $C_{20}H_{42}O$, mol. wt. 298.56, state at 25 °C crystal

Investigators		Vapor Pressures and Boiling Points		Freezing Point	Density, d g cm^{-3}		Refractive Index, n_D	
		°C	mmHg	t_m, °C	20 °C	25 °C	20 °C	25 °C
Eykman	[1919]			46	0.7717 (79.8°)			

3-Ethyl-3-octadecanol, $C_{20}H_{42}O$, mol. wt. 298.56, state at 25 °C crystal

Investigators		Vapor Pressures and Boiling Points		Freezing Point	Density, d g cm^{-3}		Refractive Index, n_D	
		°C	mmHg	t_m, °C	20 °C	25 °C	20 °C	25 °C
Eykman	[1919]			33.5		0.7788 (80.1°)		

2,6,11,15-Tetramethyl-8-hexadecanol, $C_{20}H_{42}O$, mol. wt. 298.56

Investigators		Vapor Pressures and Boiling Points		Freezing Point	Density, d g cm^{-3}		Refractive Index, n_D	
		°C	mmHg	t_m, °C	20 °C	25 °C	20 °C	25 °C
vonBraun and Kaiser	[1923]	189–194	13		0.891			

Eicosanols—Continued

Investigators		Vapor Pressures and Boiling Points		Freezing Point	Density, *d* g cm^{-3}		Refractive Index, n_D	
		°C	mmHg	t_m, °C	20 °C	25 °C	20 °C	25 °C
2,2,4,7,10,12,12-Heptamethyl-7-tridecanol, $C_{20}H_{42}O$, mol. wt. 298.56								
Gutman	[1951]	124–126 120	0.9 0.5					
2-*n*-Octyl-1-dodecanol, $C_{20}H_{42}O$, mol. wt. 298.56								
Mastagli	[1938]	215	15		0.8456		1.4541	
vonBraun and Manz	[1934]	230	17					

Alkanols, C_{21} and Above

Tanaka, Seto, and Hayashida [1957] studied the solid phase transitions in the 1-alkanols from C_{11} to C_{29} by means of x-ray diffraction and heating and cooling curves. Tanaka, Seto, Watanabe, and Hayashida [1959] reported further observations on x-ray powder patterns and heating curves for alcohols from C_{30} to C_{37}. In all 1-alkanols containing 21 or more carbon atoms, the liquid crystallizes in the α-phase in which the molecules rotate about their long axes, as described in Appendix E. Tanaka et al. found some evidence for more than one α-phase, but the differences among these were small. Alcohols containing an odd number of carbon atoms from C_{21} to C_{29} change to the β-phase a few degrees below their melting point, and so belong to Class 2 of Appendix E. Those from C_{31} to C_{37} change to a γ-phase, which Tanaka, et al. call γ_2, to distinguish it from the γ_1-phase found in the even-numbered alcohols. In general the even-numbered alkanols form the γ_1-phase, but there is a possibility that C_{30} and C_{33} change to the β-phase. Table 222 summarizes the various melting points and transition temperatures for the alcohols of 20 or more carbon atoms. The transition temperatures were based on the observations of Tanaka, et al.

Davies and Kybett [1965a] reported the sublimation pressures of 1-docosanol from 62 to 68 °C as log P(mmHg) $= 27.066 - 10793/T$ and the vapor pressure from 71 to 86 °C as log P(mmHg) $= 13.145 - 6025/T$. These equations give a heat of sublimation of the γ-form of 49.4 ± 3 kcal mol^{-1} and a heat of vaporization of 27.6 ± 1 kcal mol^{-1}. The resulting heat of fusion of the γ-form is 21.8 ± 3 kcal mol^{-1}.

Eykman [1919] measured the refractive index of 3-ethyl-3-eicosanol and 4-*n*-proply-4-heneicosanol at several wavelengths of light. Smoothed values based on his measurements are shown in table 221. All the other physical property data for the higher alcohols are given in the following unnumbered tables. They consist mainly of melting points, scattered boiling points at reduced pressures, and a few densities and refractive indexes obtained by Eykman [1919] and Mastagli [1938].

TABLE 221. 1-Alkanols, C_{20}–C_{24}. Selected values. Refractive index at various temperatures and wavelengths

Symbol	Wavelength, angstroms	Refractive Indices, *n*			
		2-Methyl-2-nonadecanol 79.8 °C	3-Ethyl-3-octadecanol 80.1 °C	3-Ethyl-3-eicosanol 80.05 °C	4-*n*-Propyl-4-heneicosanol 36.8 °C
He_{red}	6678.2	1.4258	1.4283	1.4302	1.4480
H_C	6562.8	1.4261	1.4286	1.4305	1.4483
Na_D	5892.6	1.4282	1.4307	1.4327	1.4505
Hg_e	5460.7	1.4300	1.4325	1.4345	1.4525
He_{blue}	5015.7	1.4325	1.4350	1.4370	1.4551
H_F	4861.3	1.4335	1.4360	1.4380	1.4561
Hg_g	4358.3	1.4377	1.4402	1.4422	1.4605
$H_{G'}$	4340.5	1.4379	1.4404	1.4424	1.4607

TABLE 222. 1-Alkanols, C_{20}–C_{37}. Selected values. Melting points and transition temperatures

Number of carbon atoms	Temperatures, degrees Celsius					
	$t_m(\alpha)$	$t_m(\beta)$	$t_m(\gamma_1)$	$t_{tr}(\alpha\rightarrow\beta)$	$t_{tr}(\alpha\rightarrow\gamma_1)$	$t_{tr}(\alpha\rightarrow\gamma_2)$
20	66.0±1				63±3	
21	68.0±1			57±3		
22	70.0±0.5				64.5±1	
23	74.0±1			64±3		
24	77.0±1				68±3	
25	78.5±1			69±3		
26	79.5±0.5				74±3	
27	79.5±1			73±3		
28	83±2		82±3		75±3	
29	84±3			76±3		
30	85±3				78±3	
31	87.1±1					78±3
32	88±3		90±3		83±4	
33	90±3					85±3
34	90±3		92±3		86±3	
35	92±3					85±3
36	93±3			83±4		
37	93±3					88±3

Alkanols, C_{21} and Above

Investigators	Vapor Pressures and Boiling Points		Freezing Point	Density, d g cm^{-3}		Refractive Index, n_D	
	°C	mmHg	t_m, °C	20 °C	25 °C	20 °C	25 °C
1-Heneicosanol, $C_{21}H_{44}O$, mol. wt. 312.58, state at 25 °C crystal							
Levene and Taylor [1924]			68–69				
Malkin [1930]			68–50				
Lukes and Dalezal [1957]			70–71				
Tanaka, Seto, and Hayshida [1957]			65–68				
Selected value [1967]			[b]68.±1.				
18-Methyl-1-eicosanol, $C_{21}H_{44}O$, mol. wt. 312.58, state at 25 °C crystal							
Milburn and Truter [1954]			39.8–40.2				
1-Docosanol, $C_{22}H_{26}O$, mol. wt. 326.61, state at 25 °C crystal							
Levene, West, and van der Scheer [1915]			73–74				
Willstätter and Halt [1919]			71.–71.5				
Levene and Taylor [1924]	180	0.22	70.5–71.5				
Malkin [1930]			72.0				
Jantzen and Tiedcke [1930]			70.8				
Bleyberg and Ulrich [1931]			70.0–70.5				
Sauer and Adkins [1937]			69				
Clark, Hicks, and Harris [1948]			70.5				
Hoffman and Smyth [1949]			69.6				
Meakins and Mulley [1951]			70.5				
Umezawa [1954]			70–71				
Bergman, Cregiton, and Stokes [1956]			70–71.5				
Tanaka, Seto, and Hayashida [1957]			67–72				
Davies and Kybett [1965a]			68.9–69.6				
Selected value [1967]			[b]70.0±0.5				

Alkanols, C_{21} and Above—Continued

Investigators		Vapor Pressures and Boiling Points		Freezing Point	Density, d g cm^{-3}		Refractive Index, n_D	
		°C	mmHg	t_m, °C	20 °C	25 °C	20 °C	25 °C
20-Methyl-1-heneicosanol, $C_{22}H_{46}O$, mol. wt. 326.61, state at 25 °C crystal								
Murray and Schoenfeld	[1952]			57.1				
Milburn and Truter	[1954]			56.8–57.2				
Selected value	[1967]			[b] 57.0±0.5				
11-Methyl-11-heneicosanol, $C_{22}H_{46}O$, mol. wt. 326.61, state at 25 °C liq.								
Birch and Robinson	[1942]	225–230	12	21				
3-Ethyl-3-eicosanol, $C_{22}H_{46}O$, mol. wt. 326.61, state at 25 °C crystal								
Eykman	[1919]			42.5		0.78231 (80°)		
8-*n*-Heptyl-8-pentadecanol, $C_{22}H_{46}O$, mol. wt. 326.61								
Moyer and Marvel	[1931]	195–200	6					
Challenger and Pantony	[1954]	165–166	0.4					
2-*n*-Nonyl-1-tridecanol, $C_{22}H_{46}O$, mol. wt. 326.61								
Mastagli	[1938]	235	15		0.8476 (17.5°)		1.4582 (17°)	
2,2,10,10-Tetramethyl-6-(4,4-dimethyl-*n*-pentyl)-6-undecanol, $C_{22}H_{46}O$, mol. wt. 321.61, state at 25 °C crystal								
Gutman and Hickinbottom	[1951]	140.5	0.8	48				
1-Tricosanol, $C_{23}H_{48}O$, mol. wt. 340.64, state at 25 °C crystal								
Levene and Taylor	[1924]	191–193	0.7	73.5–74.5				
Lukes and Dolezal	[1957]			73–74.5				
Taneka, Seto, and Hayashida	[1957]			69–73				
Selected value	[1967]			[b] 74.0±1.				
20-Methyl-1-docosanol, $C_{23}H_{48}O$, mol. wt. 340.64, state at 25 °C crystal								
Murray and Schoenfeld	[1952]			48.5				
Milburn and Truter	[1954]			48.5–48.7				
Selected value	[1967]			[b] 48.6±0.5				

Alkanols, $C_{21}$and Above—Continued

Investigators		Vapor Pressures and Boiling Points		Freezing Point	Density, *d* g cm^{-3}		Refractive Index, n_D	
		°C	mmHg	t_m, °C	20 °C	25 °C	20 °C	25 °C
2-*n*-Nonyl-2-tetradecanol, $C_{23}H_{48}O$, mol. wt. 340.64								
Polgar and Robinson	[1943]	200–204	0.2					
3-*n*-Decyl-1-tridecanol, $C_{23}H_{48}O$, mol. wt. 340.64								
Polgar and Robinson	[1945]	163–165	0.15				1.4612	
1-Tetracosanol, $C_{24}H_{50}O$, mol. wt. 354.67, state at 25 °C crystal								
Levene and Taylor	[1924]	210–210.5	0.40	76.5–77.5				
Malkin	[1930]			76.5–77				
Bleyberg and Ulrich	[1931]			75.2–75.5				
Lukes and Dolezal	[1957]			75–76				
Tanaka, Seto, Watanabe, and Hayashida	[1959]			74–75				
Selected value	[1967]			^{b}77.0±1.				
2-Tetracosanol, $C_{24}H_{50}O$, mol. wt. 354.67, state at 25 °C crystal								
Serck-Hansen and Klaus	[1955]			70.9–71.1, dl, c, I 62.7–62.9, dl, c, III 71.8–72.0, d, c, I 70.8–71.0, d, c, II 62.8–63.0, d, c, III 71.6–71.8, l, c, I 70.8–71.0, l, c, II 62.9–63.1, l, c, III				
Wynberg and Logothetis	[1956]			73.3–73.8				
6-Tetracosanol, $C_{24}H_{50}O$, mol. wt. 354.67, state at 25 °C crystal								
Fritz-Brini and Berschandy	[1951]			76				
Kirrmann and Gerger-Berschandy	[1955]			65				
22-Methyl-1-tricosanol, $C_{24}H_{50}O$, mol. wt. 354.67, state at 25 °C crystal								
Murray and Schoenfeld	[1952]			62.4				
Milburn and Truter	[1954]			62–62.4				
Selected value	[1967]			^{b}62.4±0.3				

Alkanols, C_{21} and Above—Continued

Investigators		Vapor Pressures and Boiling Points		Freezing Point	Density, d g cm^{-3}		Refractive Index, n_D	
		°C	mmHg	t_m, °C	20 °C	25 °C	20 °C	25 °C
4-n-Propyl-4-heneicosanol, $C_{24}H_{50}O$, mol. wt. 354.67, state at 25 °C crystal								
Eykman	[1919]			36.2		0.8258 (36.8°)		
2-Methyl-4-isobutyl-4-nonadecanol, $C_{24}H_{50}O$, mol. wt. 354.67								
Petrov, Melekhin, and Nefedov	[1955]	196	2		0.8413		1.4545	
2-n-Decyl-1-tetradecanol, $C_{24}H_{50}O$, mol. wt. 354.67								
Mastagli	[1938]				0.8489		1.4590	
1-Pentacosanol, $C_{25}H_{52}O$, mol. wt. 368.69, state at 25 °C crystal								
Levene and Taylor	[1924]	214-216	0.36	78.5–79.5				
Malkin	[1930]			78.5				
Tanaka, Seto, and Hayashida	[1957]			76–77				
Selected value	[1967]			[b] 78.5±1.				
22-Methyl-1-tetradecanol, $C_{25}H_{52}O$, mol. wt. 368.69, state at 25 °C crystal								
Murray and Schoenfeld	[1952]			54.6				
Milburn and Truter	[1954]			54–54.5				
Selected value	[1967]			[b] 54.6± 0.3				
9-n-Octyl-9-heptadecanol, $C_{25}H_{52}O$, mol. wt. 368.89, state at 25 °C crystal								
Challenger and Pantony	[1954]	186–190	0.08–0.1					
		110–120	0.02					
1-Hexacosanol, $C_{26}H_{54}O$, mol. wt. 382.72, state at 25 °C crystal								
Levene, West, and van der Scheer	[1915]			79				
Bleyberg and Ulrich	[1931]			79.3–79.6				
Trapeznikov	[1945]			79.4				
Meakins and Mulley	[1951]			79.8				
Lukes and Dalezal	[1957]			78–79.5				
Tanaka, Seto, Watanabe, and Hayashida	[1959]			77–79				
Selected value	[1967]			[b] 79.5± 0.5				

Alkanols, C_{21} and Above—Continued

Investigators		Vapor Pressures and Boiling Points		Freezing Point	Density, d g cm^{-3}		Refractive Index, n_D	
		°C	mmHg	t_m, °C	20 °C	25 °C	20 °C	25 °C
24-Methyl-1-pentacosanol, $C_{26}H_{54}O$, mol. wt. 382.72, state at 25 °C crystal								
Murray and Schoenfeld	[1952]			67.2				
Milburn and Truter	[1954]			67–67.2				
Selected value	[1967]			^{b}67.2±0.3				
1-Heptacosanol, $C_{27}H_{56}O$, mol. wt. 396.75, state at 25 °C crystal								
Gascard	[1921]			79.5–80				
Tanaka, Seto, and Hayashida	[1957]			78–80				
Selected value	[1967]			^{b}79.5±1.				
24-Methyl-1-hexacosanol, $C_{27}H_{56}O$, mol. wt. 396.75, state at 25 °C crystal								
Murray and Schoenfeld	[1952]			61.0				
Milburn and Truter	[1954]			50.8				
Selected value	[1967]			^{b}60.9±0.3				
1-Octacosanol, $C_{28}H_{58}O$, mol. wt. 410.77, state at 25 °C crystal								
Bleyberg and Ulrich	[1931]			82.9–83.1				
Tanaka, Seto, Watanabe, and Hayashida	[1959]			80				
Selected value	[1967]			^{a}83.±2.				
10-*n*-Nonyl-10-nonadecanol, $C_{28}H_{50}O$, mol. wt. 410.77, state at 25 °C crystal								
Challenger and Pantony	[1954]	209–210	0.6					
2,2,4,10,12,12-Hexamethyl-7-(3,5,5-trimethyl-*n*-hexyl)-7-tridecanol, $C_{28}H_{58}O$, mol. wt. 410.77								
Gutman and Hickinbottom	[1951]	176–178	0.8				1.4558–1.4459	
1-Nonacosanol, $C_{29}H_{60}O$, mol. wt. 424.80, state at 25 °C crystal								
Sosa	[1950]			84				
Ställberg, Ställberg-Stenhägen, and Stenhägen	[1952]			84.5–84.7				
Tanaka, Seto, and Hayashida	[1957]			80–82				
Tanaka, Seto, Watanabe, and Hayashida	[1959]			73–80				
Selected value	[1967]			^{b}84.±1.				

Alkanols, C_{21} and Above—Continued

Investigators	Vapor Pressures and Boiling Points		Freezing Point	Density, *d* g cm^{-3}		Refractive Index, n_D	
	°C	mmHg	t_m, °C	20 °C	25 °C	20 °C	20 °C
26-Methyl-1-octacosanol, $C_{29}H_{60}O$, mol. wt. 424.80, state at 25 °C crystal							
Milburn and Truter [1954]			65–65.3				
6-Pentyl-6-tetracosanol, $C_{29}H_{60}O$, mol. wt. 424.80, state at 25 °C crystal							
Fritz-Brini and Berschandy [1951]			34				
1-Triacontanol, $C_{30}H_{62}O$, mol. wt. 438.83, state at 25 °C crystal							
Sosa [1950]			86				
Tanaka, Seto, Watanabe, and Hayashida [1959]			82–85				
Selected value [1967]			[b] 85.±3.				
1-Hentriacontanol, $C_{31}H_{64}O$, mol. wt. 452.86, state at 25 °C crystal							
Ställberg, Ställberg-Stenhägen, and Stenhägen [1952]			87.1–87.2				
Tanaka, Seto, Watanabe, and Hayashida [1959]			85–86				
Selected value [1967]			[a] 87.1±0.5				
16-Hentriacontanol, $C_{31}H_{64}O$, mol. wt. 452.86, state at 25 °C crystal							
Boelhouwer, Nederbragt, and Verberg [1950]	277–278	4			0.797 (90°)		
28-Methyl-1-triacontanol, $C_{31}H_{64}O$, mol. wt. 452.86, state at 25 °C crystal							
Milburn and Truter [1954]			69.0–69.3				
11-*n*-Decyl-11-heneicosanol, $C_{31}H_{64}O$, mol. wt. 452.86							
Challenger and Pantony [1954]	255–256	0.3					
1-Dotriacontanol, $C_{32}H_{66}O$, mol. wt. 466.88							
Sosa [1950]			89				
Tanaka, Seto, Watanabe, and Hayashida [1959]			88				
Selected value [1967]			[b] 89.±2				

Alkanols, C_{21} and Above—Continued

Investigators	Vapor Pressures and Boiling Points		Freezing Point	Density, *d* g cm^{-3}		Refractive Index, n_D	
	°C	*mmHg*	t_m, °C	20 °C	25 °C	20 °C	25 °C
1-Tritriacontanol, $C_{33}H_{68}O$, mol. wt. 480.91, state at 25 °C crystal							
Tanaka, Seto, Watanabe, and Hayashida [1959]			87–89				
17-Tritriacontanol, $C_{33}H_{68}O$, mol. wt. 480.91, state at 25 °C crystal							
Fritz-Brini and Berschandy [1951]			86				
Kirrmann and Geiger-Berschandy [1955]			86				
1-Tetratriacontanol, $C_{34}H_{70}O$, mol. wt. 494.94, state at 25 °C crystal							
Tanaka, Seto, Watanabe, and Hayashida [1959]			90				
12-Undecyl-12-tricosanol, $C_{34}H_{70}O$, mol. wt. 494.94							
Challenger and Pantanoy [1954]	242–243	0.6					
1-Pentatriacontanol, $C_{35}H_{72}O$, mol. wt. 508.96, state at 25 °C crystal							
Tanaka, Seto, Watanabe, and Hayashida [1959]			89–90				
18-Pentatriacontanol, $C_{35}H_{72}O$, mol. wt. 508.96, state at 25 °C crystal							
Komarewsky and Coley [1941]			89.5–90.0				
1-Hexatriacontanol, $C_{36}H_{74}O$, mol. wt. 522.99, state at 25 °C crystal							
Tanaka, Seto, Watanabe, and Hayashida [1959]			89–91				
1-Heptatriacontanol, $C_{37}H_{76}O$, mol. wt. 537.02, state at 25 °C crystal							
Tanaka, Seto, Watanabe, and Hayashida [1959]			90–92				
13-Dodecyl-13-pentacosanol, $C_{37}H_{76}O$, mol. wt. 537.02, state at 25 °C crystal							
Challenger and Pantony [1954]	245–251	0.6					

Alkanols, C_{21} and Above—Continued

Investigators		Vapor Pressures and Boiling Points		Freezing Point	Density, *d* g cm^{-3}		Refractive Index, n_D	
		°C	mmHg	t_m, °C	20 °C	25 °C	20 °C	25 °C
1-Hentetracontanol, $C_{41}H_{84}O$, mol. wt. 593.13, state at 25 °C crystal								
Ställberg, Ställberg-Stenhägen, and Stenhägen	[1952]			97.3–97.6				
17-Hexadecyl-17-tritriacontanol, $C_{49}H_{100}O$, mol. wt. 705.34, state at 25 °C crystal								
Fritz-Brini and Berschandy	[1951]			60				
1-Pentacontanol, $C_{50}H_{102}O$, mol. wt. 719.37, state at 25 °C crystal								
Ställberg, Ställberg-Stenhägen, and Stenhägen	[1952]			104.5– 104.7				

IV. Bibliography

The following bibliography has been obtained from a thorough search of the world's scientific literature published through 1967, and a partial search for 1968. It contains citations for numerical values of the common physical and thermodynamic properties of pure monohydroxy aliphatic alcohols in the solid, liquid, and gaseous states.

Each literature citation lists the last name(s) of the author(s), the abbreviated name of the periodical, the volume number, the beginning page number, and the year of publication. Appropriate identification of other sources of information, such as books, dissertation, or reports, are also given. Journal abbreviations listed in "1961 Chemical Abstracts List of Periodicals," American Chemical Society, Washington, D.C., 1962, and in later supplements, have been used. The citations are arranged alphabetically according to the name of the first author and are numbered serially.

Whenever more than one citation is given to the same author or group of authors in the same year, the letters a, b, c, . . . , are placed after the date to distinguish among the different citations.

References to the citations in the bibliography are made in two ways. In the text and tables of numerical data the names of the author(s) and the year of publication are given. In the indexes to specific compounds the serial numbers are given. These indexes are given for the more common alcohols and will be found at the end of each section for the corresponding alcohol. A complete identification of citations to properties of the other alcohols is given in the unnumbered tables of reported data.

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* Serial numbers listed here are consistent with those in the Indices to the Properties of the various compounds, even though they are not all consecutive or unique.

V. Appendices

Appendix A. Intermolecular Association in Alcohols

In general the interaction between molecules leads to attraction at large distances, repulsion at small distances, and a balance of forces at some intermediate distance. Attraction between neutral molecules is produced by dispersion forces (the average effect of induced dipole interactions), interactions between permanent electric dipoles in the molecules, and the formation of hydrogen bonds. If the attractive forces are sufficiently large, the minimum potential energy of interaction will be more negative than the average thermal energy. The equilibrium state of the system will then contain an appreciable fraction of dimers, or higher polymers.

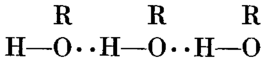
The attraction between hydrocarbon molecules results almost entirely from the relatively weak dispersion forces. In alcohols, the hydroxyl group brings into play the much larger dipole forces and hydrogen bond formation. Thus alcohols illustrate the effect of large intermolecular attractions on the properties of matter in the solid, liquid, and gaseous phases and in both pure states and mixtures. Numerous investigations from this viewpoint have been made during the past half-century and are still part of much current research. These studies include not only the classical methods but also include the use of new experimental tools. Specific problems which have been considered are the identification and characterization of the polymeric species which exist, the determination of the relative amounts present at equilibrium under various conditions, the molecular structure and properties of the polymerization reactions.

Intermolecular forces are responsible for the deviation of properties of gases and solutions from the ideal laws. The effect of a given intermolecular potential on the properties of bulk matter can be calculated using the familiar principles of statistical mechanics. The second virial coefficient reflects the interaction of pairs of molecules, the third virial coefficient reflects the interaction of triplets of molecules, etc. When the interaction energy is small these methods are very successful. When the interaction energy is large, and especially when strong orientation forces are present, a model which pictures the system as an equilibrium mixture of monomers, dimers, and perhaps higher polymers, usually gives a better interpretation of the physical properties. A gas consisting of such an equilibrium mixture may also be described in terms of the virial equation. Woolley]1953] has calculated the relations of the virial coefficients to the equilibrium constants for the polymerization reactions. However, the distinction between nonspecific intermolecular attraction and the formation of recognizable polymeric species is not a sharp one. Questions of this type frequently arise in the interpretation of properties of gases, pure liquids, and solutions.

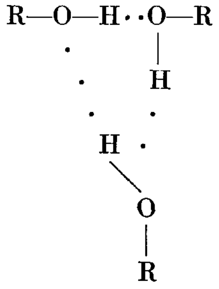
In alcohols, dipole interactions and hydrogen bond formation generate intermolecular interaction energies in the order of 2 to 6 kcal mol^{-1}. This cuts across the region of uncertainty between simple intermolecular attraction and formation of polymers. These distinctions are easier to visualize for the gas phase than for the condensed phases, so theorectical interpretations of properties of the gas phase should be more successful than those of the liquid phase. Pressure-volume-temperature studies of alcohols in the gas phase have shown large deviations from ideal behavior. A few studies of gas phase heat capacity have also been made. There are many serious experimental difficulties involved in measuring these properties with sufficient accuracy over a range of temperature and pressure wide enough to distinguish between various proposed models of the gas state. Available data have been summarized in the sections on the individual alcohols. Other thermodynamic properties such as the Joule-Thompson coefficient and the velocity of sound would also provide information on intermolecular forces but these are scarce. Accurate studies of transport properties such as viscosity and thermal conductivity are also scarce. Thermodynamic properties reflect average molecular properties and are not highly sensitive to details of intermolecular interactions. Weltner and Pitzer [1951] concluded that the P-V-T and heat capacity data for gaseous methanol available at that time were best explained by an equilibrium mixture of monomers, dimers, and tetramers. Following their lead, similar interpreations were applied to several other alcohols during the next few years. However, it has become evident in recent years that this model does not adequately account for the data accumulated at this time.

Alcohols have long been considered as highly associated in the liquid state. It is generally much easier to measure properties of liquids that of gases. Thus, there is a wealth of experimental data on liquid alcohols. Data related to association include density, heat capacity, viscosity, dielectric properties, as well as infrared and nuclear magnetic resonance spectra. The distinction between intermolecular interactions and polymer formation is even more tenuous for liquids than for gases. The lack of an adequate theory of association in liquids results in a wide divergence in models derived from different types of properties, and even among models proposed by different investigators derived from the same properties.

A complete description of intermolecular association in alcohols should include not only the degree of polymerization and the equilibrium concentrations but also the nature of the polymeric species. For example two forms of the trimer, the linear and the cyclic, might be considered.



$$\mathrm{H{-}\overset{R}{O}\cdots H{-}\overset{R}{O}\cdots H{-}\overset{R}{O}}$$



Although the geometry of the cyclic form is less favorable for hydrogen bond formation than is the linear form, it cannot be dismissed entirely since it contains three hydrogen bonds while the linear form contains only two hydrogen bonds. It may be that both linear and cyclic forms are present in alcohols. Complications of this type may account for some of the difficulties in interpreting the observed properties.

Many of the major studies of association in alcohols published during the past twenty years are listed in the following outline. A brief statement of the major conclusions is also given for each one.

Summary of Literature Concerning Self-Association of Alcohols

Authors	State	Method	Compounds Studied	Conclusions
[1] Hoffmann (1943)	CCl_4 solution	Infrared spectra	methanol, ethanol, 1-propanol, 2-propanol, 2-methyl-2-propanol	Trimer, and tetramer only, no dimer.
[2] Lambert, Roberts, Rowlinson and Wilkinson [1949]	gas	PVT measurement	methanol	Monomers and dimers only.
[3] Mecke [1950]	CCl_4 solution	Infrared spectra	methanol	Trimer (probably cyclic) and higher chain polymers present, no dimer.
[4] Smith and Creitz [1951]	CCl_4 solution	Infrared spectra	2-methyl-2-propanol, 3-pentanol, 2,4-dimethyl-3-ethyl-3-pentanol, 1-dodecanol	Monomer, dimer (probably chain), and higher polymers present; ring type dimer may also be present.
[5] Coggeshall and Saier [1951]	CCl_4 solution	Infrared spectra	1-propanol, 1-butanol, 2-methyl-2-propanol, benzyl alcohol	Monomer, dimer and higher polymers present.
[6] Weltner and Pitzer [1951]	gas	heat capacity	methanol	Monomer, dimer, and tetramer most probably; mixture of monomer, trimer, tetramer and pentamer possible—tetramer is probably cyclic.
[7] Foz Gazulla, Banda and Masia [1952]	gas	thermal conductivity	methanol, ethanol, 1-propanol, 2-propanol, 1-butanol, 2-butanol, 2-methyl-2-propanol	Monomers and dimers present; valuesI0 K_2 given.
[8] Barrow [1952]	gas	heat capacity and *PVT*	ethanol	Monomer, dimer, trimer, and tetramer, with $K_3=3/2K_2^2$.
[9] Harris, Haycock and Alder [1953]	pure liquid	dielect. const. at *T&P*	1-butanol	Inf. chains held together by H-bonds, with free rotation.
			2-methyl-2-butanol	Short chains only, 2–4 molec., in range 27–50 °C.
[10] Kretschmer and Wiebe [1954]	gas	*PVT* meas.	methanol, ethanol, 2-propanol	Monomers, dimers, trimers, with $K_3=3/2K_2^2$ and tetramers.
[11] Stavely and Taylor [1956]	benzene solution	viscosity	1-alkanols, C_1–C_6, 1-octanol, 1-decanol	No dimers, lowest polymer is the trimer.
[12] Rathman, Curtis, McGreer and Smyth [1956]	pure liquid	dielect. const., microwave absorpt.	2-methyl-2-propanol, 1-alkanols, C_8, C_{10}, C_{12}, C_{14}, C_{16}, C_{18}	Quasi-crystalline H-bonded structure.
[13] Cohen and Reid [1956]	CCl_4 and $CHCl_3$ solutions	NMR	methanol, ethanol	Cyclic trimers and tetramers assumed.
[14] Ens and Murray [1957]	CCl_4 solution	Infrared spectra	methanol, ethanol, 2-methyl-1-propanol, 2-methyl-2-butanol, 2-octanol	Assuming equil. between monomer and one polymer, gets avg. deg. of assoc. between 3 and 4, 0.1–6M–cyclic polymer most likely.
[15] Becker [1957]	CCl_4 solution	Infrared spectra	methanol, ethanol, 2-methyl-2-butanol	Monomer and cyclic dimer.
[16] Liddel and Becker [1957]	CCl_4 solution	Infrared spectra	methanol, ethanol, 2-methyl-2-propanol	Monomer and cyclic dimer predominate at low conc.; higher polymers and poss. linear dimer at high conc..
[17] Van Thiel, Becker and Pimentel [1957]	solid N_2 matrix at 20 K	Infrared spectra	methanol	Monomer, cyclic dimer and trimer, and higher linear polymers.
[18] Saunders and Hyne [1958] [1959]	CCl solution	NMR	methanol	Monomer and cyclic tetramer only.
			ethanol (data of Becker)	Monomer and trimer or tetramer.
			2-methyl-2-propanol	Monomer and cyclic trimer only.
[19] Coburn and Grunwald [1958]	CCl_4 solution	Infrared spectra	ethanol	Monomers, dimer, trimer, tetramer, and higher polymers. $K_3=3/2K_2^2$ assumed; dimer and trimer are linear; tetramer and higher mainly linear.
[20] Inskeep, Kelliher, McMahon and Somers [1958]	gas	Infrared spectra	methanol	Monomer, dimer, and tetramer only; no trimer; tetramer is cyclic.
[21] Becker, Liddel and Shoolery [1958]	CCl_4 solution	NMR	ethanol	Mainly monomer and dimer at low conc.; higher cyclic polymers at high conc
[22] Huyskens, Huyskens-Zeegers and Capart [1959]	CCl_4 and benzene solutions	NMR	1-butanol, 2-methyl-2-butanol	Both cyclic and chain polymers present in CCl_4; much less associated in benzene.
[23] Becker [1959]	CCl_4 solution	NMR	ethanol	Mainly dimer and monomer at low conc.; trimers may predominate above 0.1M.
[24] Davis, Pitzer and Rao [1960]	CCl_4 solution	NMR	methanol, ethanol, 2-propanol, 2-methyl-2-propanol	Presence of dimers definitely established; higher polymers also present.

Summary of Literature Concerning Self-Association of Alcohols—Continued

Authors	State	Method	Compounds Studied	Conclusions
[25] Cracco and Huyskens [1960]	gas	*PVT* meas.	1-butanol	Monomers and dimers.
[26] Inskeep, Dickson and Olson [1960]	gas	Infrared spectra	methanol-*d* (CH_3OD)	Monomers, dimers, and tetramers only; no trimers.
[27] Mathews and McKetta [1961]	gas	Heat capacity and *PVT* data of Foz Gazulla et al.	1-propanol	Monomers, dimers, and tetramers only.
[28] Fishman [1961]	pure liq. and solns. in solv. up to T_c	Infrared spectra	ethanol	Absorp. due to bound O–H shows no evidence of distinct polymers.
[29] Hammaker [1961]	CCl_4 solution	Infrared spectra	*methanol, 2-methyl-2-propanol*	*Monomer, cyclic dimer, and higher* polymers present.
[30] Cox [1961]	gas	*PVT* meas.	1-propanol, 2-propanol, 1-butanol, 2-butanol, 2-methyl-1-propanol, 2-methyl-2-propanol	Monomers and dimers from dipole interaction as in Stockmayer potential; virial coeff. above 2nd not needed.
[31] Berman and McKetta [1962]	gas	heat capacity	2-butanol	Monomers, dimers, and tetramers only.
[32] Piekara [1962]	benzene and hexane solutions	dielect. saturation	1-pentanol, 1-butanol, 1-hexanol	Various polymers present in two states—normal and excited—differing in position of H atom between the 2 O atoms; chain type assumed.
[33] Fruwert, Petzold and Geiseler [1963]	solns. in CCl_4, $CHCl_3$ benzene and chlorobenzene	Infrared spectra	1-propanol	Equil. among monomer, dimer, trimer, and tetramer; conc. not much influenced by solvent.
[34] Beynon and McKetta [1963]	gas	heat capacity	2-methyl-2-propanol	Monomers, dimers, and tetramers only.
[35] Hales, Cox and Lees [1963]	gas	heat capacity	2-propanol	Monomers, dimers, and tetramers only.
[36] Thomas [1963]	pure liquid	ΔH_V, viscosity and vap. press.	C_1–C_6 alkanols	Primarily ring type polymers, with max. deg. of assoc. at low temp. about 2 for st. chain alcohols, increasing to about 4–5 for branched chain isomers—at any given temp. one part. polymer predominates.
[37] Blanks and Prausnitz [1963]	CCl_4 solution	Infrared spectra	2-propanol	Monomers, dimers (probably cyclic) and higher polymers.
[38] Everett and Munn(s) [1963]	gas	refractive index	methanol	Too complex to analyze
[39] Dunken and Fritzsche [1964]	CCl_4 solution 20–55 °C	Infrared spectra	2-propanol, 2-methyl-2-propanol, 2-methyl-2-butanol	Generalized assoc. with monomers, dimers, trimers, tetramers, etc. present; determination of indiv. constants very difficult.
[40] Dannhauser and Bahe [1964]	pure liquid T_c	Dielect. const.	methanol, ethanol, 1-propanol, 2-propanol, 1-butanol, 2-methyl-1-propanol, 2-butanol, 2-methyl-2-propanol	Monomer and a series of chain type polymers up to high degree of association.
[41] Bamelis, Huyskens and Meeussen [1965]	CCl_4 solution and other solvents	viscosity	all C_1–C_4 alkanols except 2-propanol, 1-alkanols, C_5–C_8	Cyclic polymers predominate at low conc., chain polymers increase at high conc.; stability of cyclic polymers increase in order 1-but., 2-but., 2-me.-2-prop.
[42] Counsell, Hales and Martin [1965]	gas	heat capacity	1-butanol	Monomers, dimers, and tetramers only.
[43] Durocher and Sandorfy [1965]	dil. CCl_4 solution	Infrared spectra	methanol, ethanol, 2-propanol, 2-methyl-2-propanol	Monomers, dimers, and higher poly mers

Appendix B. The Representations of Density and Vapor Pressure as Functions of Temperature

The density of a liquid can be represented as a function of temperature by the equation,

$$d = A - Bt - \frac{C}{E - t}$$

where d is the density in grams per cubic centimeter, t is the temperature in degrees Celsius, and A, B, C, and E are constant parameters characteristic of a particular compound. The equation has been discussed by A. W. Francis, *Ind. Eng. Chem.* **49**, 1779 (1947) and *Chem. Eng. Sci.* **10**, 37 (1959). He found that, by adjusting the values of the parameters, the experimental densities of a wide variety of organic compounds could be expressed by the function over a wide range of temperatures. He assumed the constant C to be an integer in the range from 5 to 30. He also found that when the temperatures extended to near the critical temperature the best fit was obtained when E was about 34 °C above the critical temperature.

The vapor pressures of pure compounds can be represented by the Antoine equation,

$$\log P = A - \frac{B}{C + t}$$

where P is the vapor pressure in mmHg, t is the temperature in °C, and A, B, and C are characteristic parameters. This equation has been discussed by G. W. Thomson, *Chem. Revs.* **38**, 1 (1946) and extensive tables of Antoine constants may be found in "Selected Values of Properties of Chemical Compounds," Thermodynamics Research Center Data Project, and "Selected Values of Properties of Hydrocarbons and Related Compounds," American Petroleum Institute Research Project 44, Thermodynamics Research Center, Texas, A&M University, College Station, Texas (loose-leaf data sheets extant, 1968). When C is 273.15, the Antoine equation gives the Clausius-Clayperon equation, which represents the vapor pressure of a compound whose vapor behaves as an ideal gas and which has a constant heat of vaporization. Experience has shown that when C is adjusted to give the best fit, the Antoine equation accurately represents experimental vapor pressures in the pressure range of 10 to 1500 mmHg.

When experimental values of density or vapor pressure are available for a particular alcohol over a range of temperature, the selected values of these properties are calculated from the Francis or Antoine equations, respectively, in the appropriate tables in the report. Thus the selected values are tabulated as smooth functions of temperature over the range of temperature covered by the experimental measurements. The values of the constant parameters in these equations are also listed for each compound. These may be used to calculate the corresponding properties at intermediate temperatures.

The parameters in the two equations were adjusted to give the "best" fit to a selected set of experimental values for each compound according to the "least squares" criterion. This is characterized by a minimum value of the sum,

$$S = \sum w_i \, [x(t_i) - y_i]^2$$

where y_i is the ith observed value of a property (density or vapor pressure), $x(t_i)$ is the corresponding property calculated at the experimental temperature, t_i, and w_i is a weighting factor. For any given set of experimental data the sum, S, is a function of the parameters A, B, C, and E, or A, B, and C. Both the Francis and the Antoine equations involve nonlinear functions of the parameters. Therefore the standard procedure for calculating the parameters applicable to linear functions cannot be directly applied to these equations. In some cases the parameters were evaluated by means of a nonlinear least-squares fitting procedure. Such calculations were carried out on a digital computer programmed to follow a modified Newton-Raphson procedure described by Strand, Kohl, and Bonham, *J. Chem. Phys.* **39**, 1307 (1963). However, the specific calculation procedure used for any given situation depends on the nature of the experimental data available for that compound.

The principal purpose in carrying out these calculations in this report is to obtain equations which represent the corresponding properties as accurately as possible, considering the experimental uncertainties and discrepancies, within the experimental range of temperature. In general, the following procedure was followed. A set of data, judged to be the most accurate and reliable, was selected from the literature values. Weighting factors, which reflect the relative accuracy of the data points, were then assigned. A preliminary calculation of the parameters was made and the differences between observed and calculated values was examined. If some systematic relation between the deviations and temperature could be seen, an attempt was made to determine the reason for the systematic relation and steps taken to remove it by further calculations. In some cases it was necessary to separate the data into two different regions of temperature and to evaluate the parameters separately for these two regions. If some of the deviations were excessively large the data were screened further and the calculations were repeated for the remaining data. Although the parameters were, in general, not forced through preconceived values, the choice of data used in the calculation did exert some effect on the parameters.

Ideally, if the least-squares fitting procedure were applied to a series of closely spaced exact values of the density or vapor pressure, the parameters in the Francis or Antoine equation would represent definite properties of the particular compound and of the range of temperature covered by the data. As for any bulk properties of a pure compound, these would depend ultimately on the properties of the molecules which make up the compound. Although it has not yet been possible to calculate either these parameters or the densities and vapor pressures themselves, in terms of any fundamental statistical theory, there have been attempts to develop empirical correlations among these parameters and molecular structures. Since the parameters given in this report reflect only the original experimental data, they do not contain any distortions introduced by extraneous correlations. Therefore, they may be used to develop or test such empirical correlations without fear of complications due to such "artificial" adjustments.

However, calculation of the Francis and Antoine constants for most of the compounds treated in this report was far from ideal. Thus the values of these constants must be interpreted with caution. Even with data of high accuracy, the effects of variations in temperature range, distribution of points within the range, and choice of weighting factors can introduce large changes in the values of the parameters obtained with a least-squares regression. In both equations the constants can be changed considerably without necessarily affecting the calculated values of density or vapor pressure very much. Therefore, minor variations in the data resulting from experimental errors may be highly magnified when expressed in terms of the parameters. Only those parameters which are obtained from accurate data well distributed over a wide temperature range should be used in molecular structural correlations or in calculating data outside the experimental temperatures.

Density is nearly a linear function of temperature within the temperature range considered for most of the liquid alcohols in this report. Thus most of the temperature variation is given by the term Bt in the Francis equation. The last term accounts for the slight curvature in this function. Specifically the curvature is determined primarily by the constant E. When fitting the equation to densities up near the critical temperature, Francis found that the best value of E was a little larger than the critical temperature. However, in most of the cases treated here the densities extended only up to within 100 to 200 °C of the critical temperature. For this range the best value of E appeared to be somewhat larger, say 100 °C or more above the critical temperature. In fact when the sum of the squares of the deviations, S, was minimized with respect to A, B, and C, it was found that, for this range of temperatures, S is only slightly dependent on E. This means that S has only a very shallow minimum with respect to E. As a result E is not well determined by the data in most cases. If the random scatter in the data masks the curvature, then the constant E cannot be calculated at all from the data. It was found that in most of the cases in which the Francis constants were obtained from a direct nonlinear least squares procedure, the value of the constant E was highly erratic. It was often quite large—in the range of 1000 to 10,000 or even higher. Close examination of these cases showed that S not only had a shallow minimum with respect to E but also had more than one minimum. Thus the calculation converges on different values, when starting from different initial values. Since it is obvious that such large values of E cannot represent the density data up to temperatures near the critical point, most of these results were discarded. For, although the equations did represent the data within the experimental range with a minimum error, they would be useless for purposes of extrapolation.

The following procedure was followed to evaluate the Francis constants for most of the compounds. A fixed value of E was chosen and the constants A, B, and C which minimized S were calculated from the standard linear least squares technique. This was repeated for a series of values of E in the range of about 450 to 800, and the one which gave the smallest sum of squared deviations was chosen. Since a variation of 50 or 100 in E had only a small effect in most cases, only multiples of 50 or 100 were considered. If the minimum was not found below 800, E was set at 800. The densities calculated from constants obtained in this way did not differ significantly from those obtained from the direct nonlinear procedure, but did give more reasonable densities when extrapolated above the experimental range.

Since the last term (involving C and E) in the Francis equation was determined by the curvature as expressed by the last one or two significant figures in the experimental densities, it was found that the values of C and E were very sensitive to the effects of truncation errors in the calculations. Therefore, in order to avoid carrying a large number of significant figures in the calculations, the densities were first expressed in terms of a linear function of temperature. The constants A, B, C, and E were then calculated from the differences between experimental densities and the linear function. These were then converted back into the constants in the equation for the original densities. In cases where the range of temperature was too small to indicate any curvature at all, the densities were expressed as a linear function only.

The situation for the calculation of vapor pressures by means of the Antoine equation is similar, in the sense that $\log P$ is nearly a linear function of $1/T$, where T is the absolute temperature. Therefore, the curvature in the $\log P$ versus $1/T$ function is represented by the difference between C and 273.15. Thus the constant C is well determined only if the vapor pressure data are sufficiently accurate and distributed evenly over a wide temperature range. In many cases, reasonably accurate values of boiling points in the vicinity of one atmosphere and at low pressures in the vicinity of 10 mmHg were available. However, these were not sufficient to determine C. Data for at least three widely spaced temperatures are required. It was found for those alcohols with good vapor pressure data, that C was always less than 273.15, and that C became smaller on the average as the molecular weight of the alcohol became larger. For alcohols containing 10 or more carbon atoms C appeared to be near, or even less than, 100.

The Antoine constants were calculated by means of one of three general procedures. The following procedure was followed for those compounds which have the most accurate and complete data. As shown in Appendix C the slope of the vapor pressure curve with temperature is related to the heat of vaporization. In terms of the Antoine constants B and C, the heat of vaporization,

ΔH_v, is given by

$$\Delta H_v = \frac{2.303\ TP\Delta VB}{(C+t)^2}$$

where $\Delta V = V(\text{gas}) - V(\text{liquid})$. Therefore, when justified by the data, the measured values of both vapor pressure and calorimetric heats of vaporization were used to determine the Antoine constants. This was accomplished by minimizing the sum,

$$S = \sum f\,(P_c - P_0)^2 + \sum \frac{w}{\Delta V^2}\,(\Delta H_c - \Delta H_0)^2\,.$$

The summation is carried over all of the observed values of the vapor pressure, P_0, and heat of vaporization, ΔH_0. The corresponding calculated values are P_c and ΔH_c. The weighting function f, for the vapor pressure, was calculated as $w/P^{1/2}$, where w represents the estimated reliability of the data and $1/P^{1/2}$ is a scaling factor introduced to cancel the effects of the large variation in the magnitude of the vapor pressure. The factor, w, for the heat of vaporization represents the accuracy of the measurement, and also adjusts the relative importance of the vapor pressure and heat of vaporization in the sum S. The factor $1/\Delta V^2$ converts the heat of vaporization into units of pressure. The volume of the gas phase was calculated using values of the second virial coefficients which are discussed in the corresponding sections in the report for each compound. Values of the second virial coefficients are highly uncertain at low temperatures, but since vapor pressures at low temperatures are also low, the effect of nonideality is quite small. Estimates were introduced where there were no experimental values of the second virial coefficients. The entire calculation was made on a digital computer following the nonlinear least-squares procedure. The Antoine constants for all the alcohols in the range C_1 through C_6, as well as 1- and 2-heptanol were calculated in this way and reported in the numbered tables of Selected Values for these compounds. Experimental heats of vaporization were included in all the compounds in the range from C_1 through C_6, except for 1-pentanol and 2,2-dimethyl-1-propanol.

The following procedure was followed for compounds in which the data were not sufficiently extensive to justify the nonlinear least-squares technique. The Antoine equation can be converted into the form,

$$t \log P = (AC - B) + At - C \log P\,.$$

In this equation the variable $t \log P$ can be considered to be a function of the independent variables t and $\log P$. The parameters are then $(AC - B)$, A and $-C$. The equation is linear in the parameters which therefore can be evaluated by the usual procedure for such functions. After these parameters are obtained, the original constants, A, B, and C, can be easily calculated. This procedure has been discussed by Willingham, Taylor, Pignocco and Rossini, *J. Res. Nat. Bur. Stand.* (*U.S.*), 35, 219 (1945). It usually gives better results than the nonlinear calculation when the data are scarce or not very consistent. Antoine constants of compounds obtained in this way are also reported in the numbered tables, and the vapor pressure has been calculated at intervals of 5 degrees throughout the experimental rage.

Antoine constants are also reported for compounds for which the data are not suitable to establish even approximately the constant C. These were obtained by making C either 125 or 273, and then adjusting A and B to obtain the best fit. The constants were selected to correspond to the value of C which gives the minimum sum of the squared deviations between observed and calculated values of $\log P$. Usually in such cases there is no physically significant difference between the two values of C. Vapor pressures calculated from Antoine constants obtained in this way are listed only at 10 degree intervals. The constants obtained by this third procedure make possible rough interpolations of boiling points between experimental values, but otherwise very little physical significance should be attached to them.

Appendix C. Some Thermodynamic Formulae Used in the Calculations

1. General Relations

Heat capacity at constant pressure,

$$C_p = \left(\frac{\partial H}{\partial T}\right)_P \qquad (1)$$

$$\frac{C_p}{T} = \left(\frac{\partial S}{\partial T}\right)_P \qquad (2)$$

$$S = -\left(\frac{\partial G}{\partial T}\right)_P \qquad (3)$$

$$V = \left(\frac{\partial G}{\partial P}\right)_T \qquad (4)$$

Third law entropy of a solid

$$S^0(c, T) = \int_0^T \frac{C_p(c)}{T}\,dT \qquad (5)$$

Third law entropy of a liquid

$$S^0(l, T) = \int_0^{T_m} \frac{C_p(c)}{T}\,dT + \frac{\Delta Hm}{T_m} + \int_{T_m}^{T} \frac{C_p(l)}{T}\,dT \qquad (6)$$

Third law entropy of an ideal gas

$$S^0(g, T) = S^0(l, T) + \frac{\Delta H_v}{T} + R \ln P_e + (S^0 - S^r) \qquad (7)$$

where P_e is the equilibrium vapor pressure at temperature T in atmospheres, and S^r is the entropy of the real gas at P_e.

For any change from an initial to a final state, at constant temperature,

$$\Delta H = \Delta E + \Delta(PV) \qquad (8)$$

$$\Delta G = \Delta H - T\Delta S \qquad (9)$$

For a change from an initial temperature, T_1, to a final temperature, T_2

$$H(T_2)-H(T_1)=\int_{T_1}^{T_2} C_p\,dT \tag{10}$$

$$S(T_2)-S(T_1)=\int_{T_1}^{T_2} \frac{C_p}{T}\,dT \tag{11}$$

2. Virial Equations of State

The Leiden expansion is

$$Z=1+\frac{B_v}{V}+\frac{C_v}{V^2}+\frac{D_v}{V^3}+\ldots. \tag{12}$$

where the compressibility coefficient, Z, is defined as

$$Z=\frac{PV}{RT}\,. \tag{13}$$

The Berlin expansion is

$$Z=1+B_pP+C_pP^2+D_pP^3+\ldots. \tag{14}$$

This may also be written as

$$Z=1+\frac{B_p'}{RT}P+\frac{C_p'P^2}{RT}+\frac{D_p'P^3}{RT}+\ldots \tag{15}$$

$$V=\frac{RT}{P}+B_p'+C_p'P+D_p'P^2+\ldots. \tag{16}$$

The three types of virial coefficients used in these equations are related by

$$B_p'=B_pRT=B_v \tag{17}$$

$$C_p'=C_pRT=\frac{C_v-B_v^2}{RT} \tag{18}$$

$$D_p'=D_pRT=\frac{D_v-3B_vC_v+2B_v^3}{(RT)^2}\,. \tag{19}$$

3. Differences Between Properties of a Real and Ideal Gas

$$H^0-H^r=\int_0^P\left[V-T\left(\frac{\partial V}{\partial T}\right)_P\right]dP \tag{20}$$

$$C_p^0-C_p^r=T\int_0^P\left(\frac{\partial^2 V}{\partial T^2}\right)_P dP \tag{21}$$

$$S^0-S^r=R\ln\frac{P^*}{P}+\int_{P^*}^P\left(\frac{\partial V}{\partial T}\right)_P dP\,. \tag{22}$$

The substitution of (16) into eqs (20)–(22) gives

$$H^0-H^r=\left[T\frac{dB_p'}{dT}-B_p'\right]P+\left[T\frac{dC_p'}{dT}-C_p'\right]\frac{P^2}{2}+T\left[\frac{dD_p'}{dT}-D_p'\right]\frac{P^3}{3}+\ldots \tag{23}$$

$$S^0-S^r=-\frac{dB_p'}{dT}P-\frac{dC_p'}{dT}\frac{P^2}{2}-\frac{dD_p'}{dT}\frac{P^3}{3}-\ldots \tag{24}$$

$$C^0{}_p-C_p{}^r=-T\frac{d^2B_p'}{dT^2}P-T\frac{d^2C_p'}{dT^2}\frac{P^2}{2}-T\frac{d^2D_p'}{dT^2}\frac{P^3}{3}-\ldots. \tag{25}$$

4. Thermodynamic Formulae for Phase Equilibria

In formulae (26) through (33) and (36), the quantities ΔX (where $X = H, C_p, S, V$, or G) represent the change in the property when 1 mol of substance is transferred from one phase to another phase in equilibrium with it.

$$\Delta G=0 \tag{26}$$

$$\Delta S=\frac{\Delta H}{T} \tag{27}$$

$$\Delta H=T\Delta V\left(\frac{dP}{dT}\right)_e \tag{28}$$

dP/dT_e is the temperature derivative of the equilibrium pressure in the presence of the two phases.

$$\Delta C_p=\left(\frac{\partial\Delta H}{\partial T}\right)_p \tag{29}$$

$\left(\frac{d\Delta H}{dT}\right)_e$ is the temperature derivative of ΔH under conditions of equilibrium temperature and pressure.

$$\left(\frac{d\Delta H}{dT}\right)_e=\left(\frac{\partial\Delta H}{\partial T}\right)_P+\left(\frac{\partial\Delta H}{\partial P}\right)_T\left(\frac{dT}{dP}\right)_e \tag{30}$$

$$\left(\frac{d\Delta H}{dT}\right)_e=\Delta C_p+\left[\Delta V-T\left(\frac{\partial\Delta V}{\partial T}\right)_P\right]\left(\frac{dP}{dT}\right)_e \tag{31}$$

$$\left(\frac{d\Delta H}{dT}\right)_e=\Delta C_p+\left[\frac{1}{T}-\left(\frac{\partial\ln\Delta V}{\partial T}\right)_P\right]\Delta H\,. \tag{32}$$

The temperature derivative of the heat of vaporization, $d\Delta H/dT$ given in the summary sheets and in the text of this report is the same as $(d\Delta H/dT)_e$ which appears in eqs (30)–(32). For condensed phases (solid-solid and solid-liquid equilibria), the equation

$$\left(\frac{d\Delta H}{dT}\right)_e=\Delta C_p+\Delta S \tag{33}$$

is a good approximation.

The Antoine vapor pressure equation is,

$$\log P_e=A-\frac{B}{C+t} \tag{34}$$

where P_e is the equilibrium vapor pressure and t, the temperature in degrees Celsius. The temperature derivative of P_e is then given by,

$$\left(\frac{dP}{dT}\right)_e=\frac{2.30258\,BP_e}{(C+t)^2}\,. \tag{35}$$

Combination of eqs (16), (28), and (35) gives an equation for calculating the heat of vaporization from vapor pressure data.

$$\Delta H_v = \left(RT - V_l P_e + B_p' P_e + C_p' P_e^2\right) \frac{2.30258\ BT}{(C+t)^2} \qquad (36)$$

V_l is the volume of the liquid in equilibrium with the vapor.

5. Thermodynamic Formulae for Chemical Reactions

For the combustion of a compound, $C_aH_bO_c$, $\Delta X_c{}^0$ ($X = H, E, S$, or G) refers to the reaction

$$C_aH_bO_c\ (c,\ l,\ \text{or}\ g) + (a + \frac{1}{4}b - \frac{1}{2}c)\ O_2(g) \rightarrow aCO_2(g) + \frac{1}{2}\,bH_2O(l)$$

and $\Delta X_f{}^0$ refers to the reaction,

$$aC(\text{graphite}) + \tfrac{1}{2}\,bH_2(g) + \tfrac{1}{2}\,CO_2(g) \longrightarrow C_aH_bO_c\ (c,\ l,\ \text{or}\ g)$$

$$\Delta H_c{}^0 = \Delta E_c{}^0 + \Delta n\ RT \qquad (37)$$

where Δn is the change in number of moles of gas on combustion. If the compound is a solid or liquid, $\Delta n = c - \frac{1}{2}b$

$$\Delta H_f{}^0 = -\Delta H_c{}^0 - 94.051a - 34.1575b \qquad (38)$$

$$\Delta H_f{}^0(g) = \Delta H_f{}^0(l) + \Delta H_v + (H^0 - H^r) \qquad (39)$$

$$\Delta S_f{}^0 = S^0 - 1.372a - 15.604b - 24.498c \qquad (40)$$

$$\Delta H_f{}^0(T) = \Delta H_f{}^0(0) + T\Delta\,\frac{(H^0 - H_0{}^0)}{T} \qquad (41)$$

$$\Delta G_f{}^0(T) = \Delta H_f{}^0(0) + T\Delta\,\frac{(G^0 - H_0{}^0)}{T} \qquad (42)$$

$$\Delta G^0 = -RT \ln K. \qquad (43)$$

Appendix D. Thermodynamic Functions of Elements

T K	Carbon, c(graphite)		Hydrogen $H_2(g)$		Oxygen $O_2(g)$	
	$H^0 - H_0{}^0$	$\frac{-(G^0 - H_0{}^0)}{T}$	$H^0 - H_0{}^0$	$\frac{-(G^0 - H_0{}^0)}{T}$	$H^0 - H_0{}^0$	$\frac{-(G^0 - H_0{}^0)}{T}$
273.15	202.8	0.469	1852.0	23.826	1899.4	41.436
298.15	251.2	.530	2023.8	24.420	2074.6	42.038
300	255.0	.536	2036.6	24.462	2087.6	42.082
400	502	.837	2731.0	26.422	2797.6	44.104
500	821	1.157	3429.4	27.948	3528.8	45.672
600	1198	1.488	4129.4	29.200	4285.6	46.964
700	1622	1.821	4831.6	30.264	5061.8	48.072
800	2082	2.150	5537.0	31.186	5859.4	49.044
900	2569	2.472	6248.0	32.002	6673.4	49.912
1000	3074	2.79	6966.0	32.732	7501.0	50.968

$H^0 - H_0{}^0$ in units of cal mol^{-1}, $\frac{-(G^0 - H_0{}^0)}{T}$ in units of cal deg^{-1} mol^{-1}

References

at 298.15 K, Wagman, Evans, Halow, Parker, Bailey, and Schumm, National Bureau of Standards Technical Note 270-1 (1965)

at other temperatures

carbon: National Bureau of Standards Report 6928 (1960), Table B-39 by Wm. Evans

hydrogen and oxygen: Hilsenrath, Beckett, Benedict, Fano, Hoge, Masi, Nutall, Touloukian, and Woolley, "Thermal Properties of Gases, National Bureau of Standards Circular 564 (1955)

Appendix E. Melting Points and Polymorphism in the Higher Alcohols

It has been found that the melting points of several types of homologous series of alkane derivatives show a strong alternation between compounds containing odd and even numbers of carbon atoms in the chain. This phenomenon has been related to the packing of the straight chain alkyl groups in the crystalline phase. Examples of such series are the alkanes, alkenes, alkyl halides, mono- and dicarboxylic acids, and esters. The effect of the alternation can frequently be seen up to 20 carbon atoms.

The effect of the alternation in the n-1-alkanols can be readily seen in a plot of melting point versus number of carbon atoms from 2 to about 12. The compounds with an odd number of carbon atoms melt at a lower temperature than those with an even number of carbon atoms.

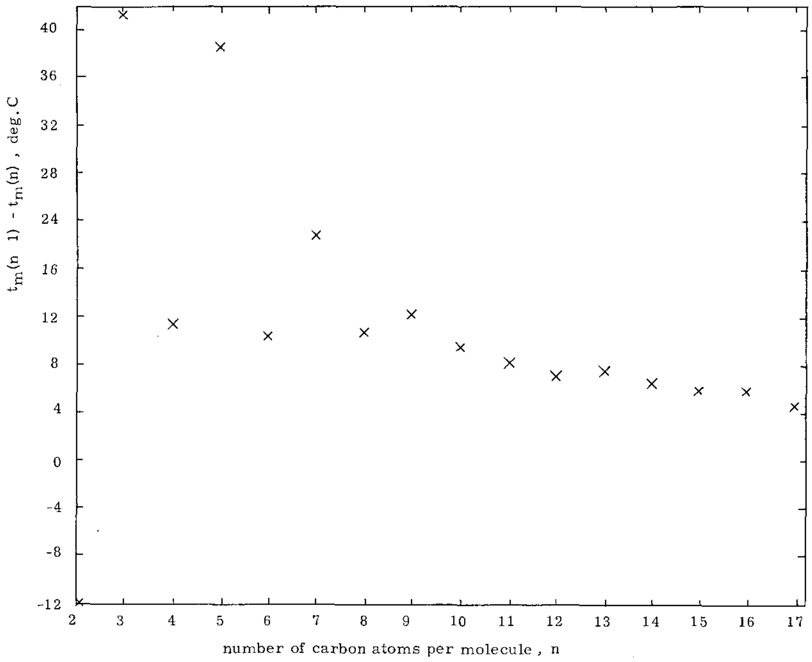


FIGURE 3. Differences in the melting points of successive members the homologous series of n-1-alkanols.

The difference becomes less at the number of carbon atoms increases. This alternation is shown in a more pronounced fashion in figure 3 in which the difference between the melting points of successive members of the n-1-alkanol series is plotted againsts n, the number of carbon atoms in the molecule. An obvious difference exists between odd and even values of n, at least up to $n = 9$, and some possible difference can be seen up to about $n = 14$. In contrast to several other homologous series however, the alternation does not noticeably exist above about 14 carbon atoms.

Condensed phasee quilibria in the higher alcohols are complicated by the presence of complex polymorphism in these compounds. Extensive studies of these phenomena have been made by Malkin [1930], Meyer and Reid [1933], Hoffman and Smyth [1949], Phillips and Mumford [1933] and [1934], Kolp and Lutton [1951], Tanaka, Seto and Hayashida [1957], Tanaka, Seto, Watanabe, and Hayashida [1959], and Davies and Kybett [1965]. The literature contains numerous discrepancies, not only of the transition temperatures, but also of the existence and identification of crystalline phases. Differences in symbols used by different authors to identify the phases have also contributed to the confusion.

The most thorough x-ray diffraction analyses of the crystalline forms of the alcohols above C_{10} have been made by Tanaka, et al., and their notation is adopted here. Their measurements of transition temperatures and melting points, however, are only approximate. In many cases their measurement is the only one available, especially for the higher members of the series.

At least four major types of crystalline forms have been recognized in the n-1-alkanols containing ten or more carbon atoms. In all cases the hydrocarbon chains are aligned parallel in the crystal lattice and they are packed in a head-to-head manner. A qualitative description of the various types of crystalline phases is given below. Additional quantitative details may be found in the papers by Tanaka et al.

α-phase: The long axes of the molecules are perpendicular to the layer planes. The molecules rotate, or twist, about their long axis. The crystals are nearly transparent and are either metastable or have only a short range of stability below the melting point. Tanaka et al. have found evidence of several different but closely related modifications of this form.

β-phase: The long axes of the molecules are perpendicular to the layer planes, as in the α-form, but the side packing is paraffin-like.

γ-phase. The molecules are tilted to an angle of about 60 °C to the layer planes. The side packing is also paraffin-like. This form is found only in the even-numbered alcohols of C_{14} and above.

γ_2-phase. The molecules are also tilted as in the γ_1-phase, although the diffraction pattern is significantly different from the γ_1-phase. It has not been analyzed in detail. This form is present only in the odd numbered alcohols of C_{31} and above.

The relationships among these various crystalline forms, and of these forms with the liquid, are complex, and not yet completely understood for all of the various alcohols. However, on the basis of the experimental data at present, they seem to fall into five classes, according to the existence of the types of solid phases and to the relative magnitudes of the transition temperatures and melting points. Using symbols such as $t(\alpha, \beta)$ to stand for the transition temperature for the α- and β-phases, and $t(\alpha, L)$ as the melting temperature of the α-phase, the relationships in these five classes is shown below.

class 1. $t(\beta, L) > t(\alpha, L)$
class 2. $t(\alpha, L) > t(\beta, L) > t(\alpha, \beta)$
class 3. $t(\alpha, L) > t(\gamma, L) > t(\beta, L) > t(\alpha, \gamma) > t(\alpha, \beta)$
class 4. $t(\gamma, L) > t(\alpha, L) > t(\beta, L) > t(\alpha, \beta)$
class 5. $t(\alpha, L) > t(\gamma, L) > t(\alpha, \gamma)$.

The symbol γ represents either the γ_1 of the γ_2-phase, whichever is appropriate for that alcohol.

These relationships can be most easily understood in terms of the schematic graphs of the Gibbs energy versus temperature shown in figure 4. At any given temperature the phase which has the lowest value of the Gibbs energy is the stable one, and the others are metastable. Points of intersection are the transition temperatures between the corresponding phases.

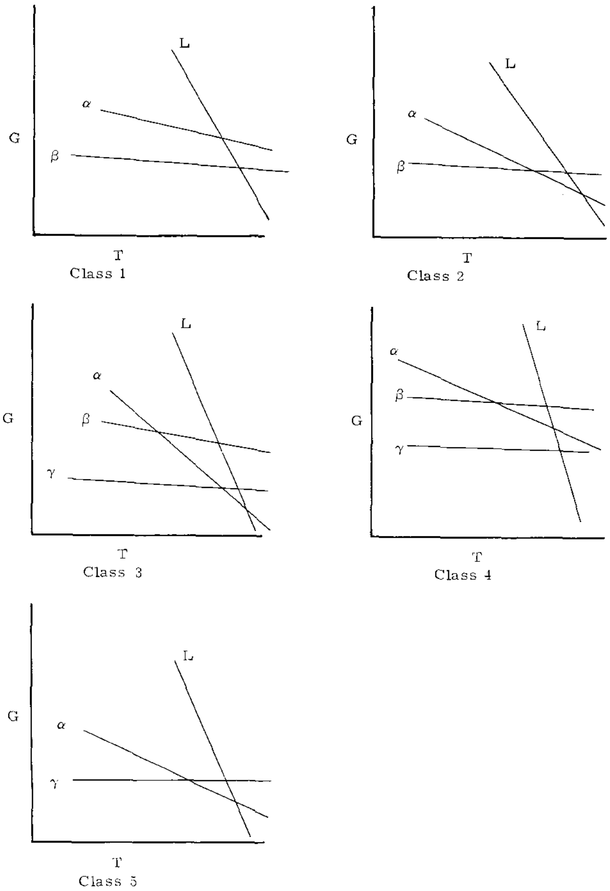


FIGURE 4. Schematic graphs of Gibbs energy versus temperature.
L—liquid phase
α, β, γ—solid phases

Although not all of the theoretically possible transitions have been observed, the following assignments are at least consistent with most of the observations reported in the literature. All the odd-numbered alcohols from C_{11} to C_{29} are in Class 2. The even-numbered alcohols are in the classes shown below.

n	Class
12	1
14	4
16	3
18	3

All the remaining even-numbered alcohols are in Class 5. It may be that 1-Dodecanol is in Class 2 rather than Class 1. Alcohols containing an odd number of carbon atoms from C_{31} to C_{37} are in Class 5, and form the γ_2-phase at the transition temperature.

Appendix F. Enthalpies of Formation of the 1-Alkanols

A large amount of very accurate data for several classes of hydrocarbons shows that the heats of formation of compounds in a homologous series represented by $R\text{-}(CH_2)_v\text{-}CH_3$ are linear functions of n, for n greater than two, in both the gas and liquid phases. Similar assumptions are usually made for homologous series of other kinds of organic compounds, although the experimental evidence is less extensive. However, the analogy with other classes of compounds, as well as theoretical predictions, indicates that the heats of formation of the 1-alkanols in the gas phase would correspond to a constant—CH_2—increment to within at least a few tenths of a kcal mol^{-1}. If the heats of vaporization also follow a linear dependence on the number of carbon atoms, then the heats of formation in the liquid phase would also show the constant—CH_2—increment. However, this prediction is less certain for liquids than it is for gases.

Nearly all experimental data on the enthalpies of formation of the alcohols above ethanol refer to the liquid state. The enthalpies of formation in the gas state must be calculated by adding the heat of vaporization to the heat of formation of the liquid. Reliable data exist for the heats of vaporization at 25 °C of 1-alkanols up to 1-hexanol. From $n = 3$ to $n = 6$ these data fit the equation $\Delta H_v = 7.94 + 1.14\,n$ kcal mol^{-1} well within the estimated uncertainties. Therefore, it is very probable that the heats of formation of the 1-alkanols in the liquid phase are a linear function of n, at least within this range. Above 1-hexanol the uncertainties in the experimental heats of vaporization become larger, and the scatter from a straight line also becomes larger. Whether this scatter is real or is due to experimental errors cannot be definitely established at this time.

Except in a few cases where the experimental data are missing or obviously in error the selections made in this review are based on the observations reported for each individual compound. Theoretical expectations or correlations are not usually considered, so as to avoid biasing the selected values. There are two significant sources of experimental values of the heats of combustion and heats of formation of alkanols from 1-pentanol through 1-decanol. These are Verkade and Coops [1927] and Chao and Rossini [1965]. Verkade and Coops purified their samples by repeated fractional distillation until they obtained constant values for the heats of combustion. Although they did not report any other information which would be very helpful in establishing the purity, it seems likely that they burned high purity samples. Chao and Rossini obtained their samples from the Petroleum Research Laboratory at Carnegie Institute of Technology. However, they did not attempt to further purify the samples or to apply any additional tests for purity. Water is the most probable impurity in a these materials. Verkade and Coops based their calculations on the mass of the sample, and the presence of water would cause their heats of combustion to be low (more positive) by a corresponding amount. Chao and Rossini based their calculations on the mass of carbon dioxide produced by the combustion. Their results would not be affected by the presence of water, except for the trivial effect of heat of mixing. The principal sources of uncertainty in the data of Verkade and Coops are the limitations in the instruments and calorimetric techniques available in 1927, and the lack of sufficient information to accurately convert their values to the modern standard state and energy unit. Uncertainties in the data of Chao and Rossini arise because of possible impurities other than water in the samples, and because of possible errors in determining the mass of carbon dioxide.

A least square calculation of the enthalpies of formation of liquid 1-alkanols from $n = 4$ to $n = 10$ based on the data of Verkade and Coops gives the equation $\Delta H_f^\circ(\text{liq}) = -54.17 - 6.109\,n$ kcal mol^{-1} with a root mean-square deviation of 0.21 kcal mol^{-1}. These deviations appear somewhat systematic and the cubic equation, $\Delta H_f^\circ(\text{liq}) = -46.37 - 10.088\,n + 0.6213\,n^2 - 0.03097\,n^3$ gives a root mean square deviation of only 0.08 kcal mol^{-1} for the same data.

The enthalpies of formation of the same series ot 1-alkanols obtained by Chao and Rossini fit the equation $\Delta H_f^\circ(\text{liq}) = -54.07 - 6.057\,n$ kcal mol^{-1} with a root mean square deviations appear to be random and no significant improvement can be obtained by going to equations of higher order in n. The two linear equations agree closely although the data of Chao and Rossini scatter much more from the straight line than do those of Verkade and Coops. The combination of the equation for the heats of vaporization of 1-alkanols from C_3 to C_6 with the linear equations for heats of formation of the liquids gives a —CH_2— increment for the heat of formation in the gas phase of 4.97 kcal mol^{-1} from the data of Verkade and Coops and of 4.92 kcal mol^{-1} from the data of Chao and Rossini. These are very close to the corresponding —CH_2— increment of 4.93 kcal mol^{-1} which has been established for the normal alkanes in the gas phase.

The heats of combustion of Verkade and Coops and of Chao and Rossini are relatively close for 1-hexanol, 1-octanol, and 1-decanol. The values of Chao and Rossini were selected for these compounds. The values reported by Chao and Rossini for 1-pentanol, 1-heptanol, and 1-nonanol show large differences from the values of Verkade and Coops, and also scatter from the linear function by 1.0 to 1.2 kcal mol^{-1}. Since these large deviations from the straight line seem to be unlikely, the selected values were obtained by adjusting the values of Chao and Rossini back toward the straight line by about one kcal mol^{-1}. The resulting values are close to those of Verkade and Coops. The estimated uncertainties attached to the selected values reflect the various discrepancies found in the experimental data.

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