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SOLUBILITY DATA SERIES

Editor-in-Chief A. S. KERTES

Volume 15

ALCOHOLS WITH WATER

Volume Editor

A. F. M. BARTON

School of Mathematical and Physical Sciences Murdoch University, Western Australia 6150

M. C. HAULAIT-PIRSON University of Leuven

A. MACZYNSKI Institute of Physical Chemistry Warsaw, Poland

Belgium

N. TSUCHIDA National Institute of Research in Inorganic Materials Ibaraki, Japan Contributors

G. T. HEFTER Murdoch University Australia

Z. MACZYNSKA Institute of Physical Chemistry Warsaw, Poland

> S. C. VALVANI Upjohn Co. Kalamazoo, Ml, USA

FU JUFU Beijing Institute of Chemical Technology China G. JANCSO Central Institute for Physics Budapest, Hungary

A. SZAFRANSKI Institute for Industrial Chemistry Warsaw, Poland

S. H. YALKOWSKY Arizona University College of Pharmacy Tucson, AZ, USA



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FOREWORD

If the knowledge is undigested or simply wrong, more is not better

How to communicate and disseminate numerical data effectively in chemical science and technology has been a problem of serious and growing concern to IUPAC, the International Union of Pure and Applied Chemistry, for the last two decades. The steadily expanding volume of numerical information, the formulation of new interdisciplinary areas in which chemistry is a partner, and the links between these and existing traditional subdisciplines in chemistry, along with an increasing number of users, have been considered as urgent aspects of the information problem in general, and of the numerical data problem in particular.

Among the several numerical data projects initiated and operated by various IUPAC commissions, the Solubility Data Project is probably one of the most ambitious ones. It is concerned with preparing a comprehensive critical compilation of data on solubilities in all physical systems, of gases, liquids and solids. Both the basic and applied branches of almost all scientific disciplines require a knowledge of solubilities as a function of solvent, temperature and pressure. Solubility data are basic to the fundamental understanding of processes relevant to agronomy, biology, chemistry, geology and oceanography, medicine and pharmacology, and metallurgy and materials science. Knowledge of solubility is very frequently of great importance to such diverse practical applications as drug dosage and drug solubility in biological fluids, anesthesiology, corrosion by dissolution of metals, properties of glasses, ceramics, concretes and coatings, phase relations in the formation of minerals and alloys, the deposits of minerals and radioactive fission products from ocean waters, the composition of ground waters, and the requirements of oxygen and other gases in life support systems.

The widespread relevance of solubility data to many branches and disciplines of science, medicine, technology and engineering, and the difficulty of recovering solubility data from the literature, lead to the proliferation of published data in an ever increasing number of scientific and technical primary sources. The sheer volume of data has overcome the capacity of the classical secondary and tertiary services to respond effectively.

While the proportion of secondary services of the review article type is generally increasing due to the rapid growth of all forms of primary literature, the review articles become more limited in scope, more specialized. The disturbing phenomenon is that in some disciplines, certainly in chemistry, authors are reluctant to treat even those limited-in-scope reviews exhaustively. There is a trend to preselect the literature, sometimes under the pretext of reducing it to manageable size. The crucial problem with such preselection - as far as numerical data are concerned - is that there is no indication as to whether the material was excluded by design or by a less than thorough literature search. We are equally concerned that most current secondary sources, critical in character as they may be, give scant attention to numerical data.

On the other hand, tertiary sources - handbooks, reference books and other tabulated and graphical compilations - as they exist today are comprehensive but, as a rule, uncritical. They usually attempt to cover whole disciplines, and thus obviously are superficial in treatment. Since they command a wide market, we believe that their service to the advancement of science is at least questionable. Additionally, the change which is taking place in the generation of new and diversified numerical data, and the rate at which this is done, is not reflected in an increased third-level service. The emergence of new tertiary literature sources does not parallel the shift that has occurred in the primary literature. Foreword

With the status of current secondary and tertiary services being as briefly stated above, the innovative approach of the *Solubility Data Project* is that its compilation and critical evaluation work involve consolidation and reprocessing services when both activities are based on intellectual and scholarly reworking of information from primary sources. It comprises compact compilation, rationalization and simplification, and the fitting of isolated numerical data into a critically evaluated general framework.

The Solubility Data Project has developed a mechanism which involves a number of innovations in exploiting the literature fully, and which contains new elements of a more imaginative approach for transfer of reliable information from primary to secondary/tertiary sources. The fundamental trend of the Solubility Data Project is toward integration of secondary and tertiary services with the objective of producing in-depth critical analysis and evaluation which are characteristic to secondary services, in a scope as broad as conventional tertiary services.

Fundamental to the philosophy of the project is the recognition that the basic element of strength is the active participation of career scientists in it. Consolidating primary data, producing a truly critically-evaluated set of numerical data, and synthesizing data in a meaningful relationship are demands considered worthy of the efforts of top scientists. Career scientists, who themselves contribute to science by their involvement in active scientific research, are the backbone of the project. The scholarly work is commissioned to recognized authorities, involving a process of careful selection in the best tradition of IUPAC. This selection in turn is the key to the quality of the output. These top experts are expected to view their specific topics dispassionately, paying equal attention to their own contributions and to those of their peers. They digest literature data into a coherent story by weeding out what is wrong from what is believed to be right. To fulfill this task, the evaluator must cover <u>all</u> relevant open literature. No reference is excluded by design and every effort is made to detect every bit of relevant primary source. Poor quality or wrong data are mentioned and explicitly In fact, it is only when the reliable data are disqualified as such. presented alongside the unreliable data that proper justice can be done. The user is bound to have incomparably more confidence in a succinct evaluative commentary and a comprehensive review with a complete bibliography to both good and poor data.

It is the standard practice that the treatment of any given solute-solvent system consists of two essential parts: I. Critical Evaluation and Recommended Values, and II. Compiled Data Sheets.

The Critical Evaluation part gives the following information:

- (i) a verbal text of evaluation which discusses the numerical solubility information appearing in the primary sources located in the literature. The evaluation text concerns primarily the quality of data after consideration of the purity of the materials and their characterization, the experimental method employed and the uncertainties in control of physical parameters, the reproducibility of the data, the agreement of the worker's results on accepted test systems with standard values, and finally, the fitting of data, with suitable statistical tests, to mathematical functions;
- (ii) a set of recommended numerical data. Whenever possible, the set of recommended data includes weighted average and standard deviations, and a set of smoothing equations derived from the experimental data endorsed by the evaluator;
- (iii) a graphical plot of recommended data.

The Compilation part consists of data sheets of the best experimental data in the primary literature. Generally speaking, such independent data sheets are given only to the best and endorsed data covering the known range of experimental parameters. Data sheets based on primary sources where the data are of a lower precision are given only when no better data are available. Experimental data with a precision poorer than considered acceptable are reproduced in the form of data sheets when they are the only known data for a particular system. Such data are considered to be still suitable for some applications, and their presence in the compilation should alert researchers to areas that need more work. The typical data sheet carries the following information:

- (i) components definition of the system their names, formulas and Chemical Abstracts registry numbers;
- (ii) reference to the primary source where the numerical information is reported. In cases when the primary source is a less common periodical or a report document, published though of limited availability, abstract references are also given;
- (iii) experimental variables;
- (iv) identification of the compiler;
- (v) experimental values as they appear in the primary source. Whenever available, the data may be given both in tabular and graphical form. If auxiliary information is available, the experimental data are converted also to SI units by the compiler.

Under the general heading of Auxiliary Information, the essential experimental details are summarized:

- (vi) experimental method used for the generation of data;
- (vii) type of apparatus and procedure employed;
- (viii) source and purity of materials;
- (ix) estimated error;
 - (x) references relevant to the generation of experimental data as cited in the primary source.

This new approach to numerical data presentation, developed during our four years of existence, has been strongly influenced by the diversity of background of those whom we are supposed to serve. We thus deemed it right to preface the evaluation/compilation sheets in each volume with a detailed discussion of the principles of the accurate determination of relevant solubility data and related thermodynamic information.

Finally, the role of education is more than corollary to the efforts we are seeking. The scientific standards advocated here are necessary to strengthen science and technology, and should be regarded as a major effort in the training and formation of the next generation of scientists and engineers. Specifically, we believe that there is going to be an impact of our project on scientific-communication practices. The quality of consolidation adopted by this program offers down-to-earth guidelines, concrete examples which are bound to make primary publication services more responsive than ever before to the needs of users. The self-regulatory message to scientists of 15 years ago to refrain from unnecessary publication has not achieved much. The literature is still, in 1984, cluttered with poor-quality articles. The Weinberg report (in 'Reader in Science Information', ed. J. Sherrod and A. Hodina, Microcard Editions Books, Indian Head, Inc., 1973, p. 292) states that 'admonition to authors to restrain themselves from premature, unnecessary publication can have little effect unless the climate of the entire technical and scholarly community encourages restraint ... ' We think that projects of this kind translate the climate into operational terms by exerting pressure on authors to avoid submitting low-grade material. The type of our output, we hope, will encourage attention to quality as authors will increasingly realize that their work will not be suited for permanent retrievability unless it meets the standards adopted in this project. It should help to dispel confusion in the minds of many authors of what represents a permanently useful bit of information of an archival value, and what does not.

If we succeed in that aim, even partially, we have then done our share in protecting the scientific community from unwanted and irrelevant, wrong numerical information.

A. S. Kertes

PREFACE

This volume is concerned with binary systems containing only water and a monohydroxy alcohol. Occasionally multicomponent systems are mentioned (for example Ringer solution, a salt solution isotonic with blood plasma) but these systems are not treated exhaustively or critically. Because the critical evaluations have been prepared by different authors, style and content vary considerably, and the editor has made no attempt to modify them for uniformity.

Amongst binary water-organic systems, 1-butanol exhibits a particularly high value for the amount of water which can be accommodated in the organic-rich phase at equilibrium. Given the number of carbon atoms in 1-butanol, this alcohol and water have a surprisingly high mutual solubility. Indeed, when 1-butanol and water are saturated with one another, "they are about as much alike as two separate phases can be" (ref 1). As the carbon chain length is shortened to 1-propanol there is complete miscibility, except between -11° C and -2° C and no reports have been found indicating gaps for ethanol and methanol with water at any temperature or pressure. Lengthening the alcohol carbon chain sharply decreases the mutual solubility of alcohol and water. The 1-butanol/water system shows low sensitivity to changes in solute character for partition equilibria, but the sensitivity to the solute nature increases with increasing chain length until it reaches a maximum at 1-octanol, and then levels out. Thus 1-octanol is often chosen as a reference point in studies of partition of solutes between water and organic liquids.

It may not be appreciated that although the proportion of alcohol in the aqueous phase falls off rapidly as the alcohol chain length increases, the proportion of water in the alcohol-rich phase remains relatively high, even for long-chain alcohols. For example, an alcohol/water mole ratio of 3 is observed for 1-dodecanol, compared with 1 for 1-butand (ref 2).

The water-solubility of homologous series of alcohols (as well as of other classes of organic liquid) is observed to decrease in geometric progression as the carbon number increases in arithmetic progression, with the ratio of water solubility of one member to that of the next being of the order of four (ref 3,4). Both experimentally (ref 5-8) and theoretically (ref 9) there is evidence for an approximately linear relationship between the logarithm of alcohol solubility in the aqueous phase and the carbon number of the alcohol (Figure 1).

For the lower alcohols, which have a substantial solubility in water and which have been studied in some detail, these correlations are probably of limited practical value. However, in the case of higher alcohols having lower solubilities, requiring novel and more difficult methods of determination and having been less studied, it is possible that the precision of prediction by this type of equation exceeds that currently available for experimental results.

Thus for the straight-chain alcohols with n carbon atoms, the following expressions have been obtained:

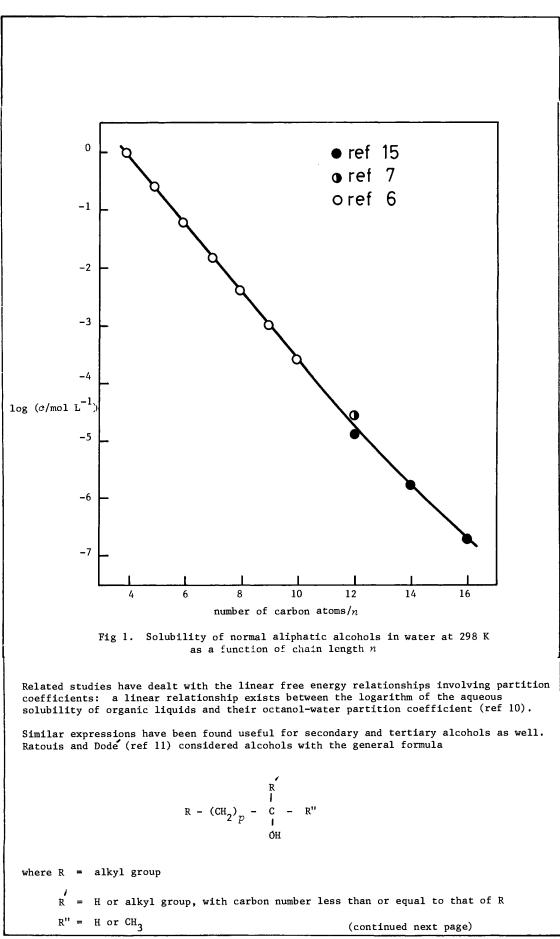
 $25^{\circ}C : \log (c/mol L^{-1}) = -0.58n + 2.3 (n = 4 \text{ to } 16, \text{ ref } 8)$ $25^{\circ}C : \log (c/mol L^{-1}) = -0.57n + 2.14 (n = 6 \text{ to } 16, \text{ ref } 7)$ $25^{\circ}C : \ln (c/mol L^{-1}) = -1.39n + 5.53 (n = 4 \text{ to } 10, \text{ ref } 6)$ $or \log (c/g(1)/100g \text{ sln}) = -0.60n + 2.40 (n = 4 \text{ to } 10)$ $20^{\circ}C \log (c/g(1)/100g \text{ sln}) = -0.56n + 3.2 (n = 4 \text{ to } 10, \text{ ref } 5)$ 4

Maczynski (ref 14) has combined the data of ref 6 and ref 7 in a second order polynomial correlation:

$$\log (c/mol L^{-1}) = 2.722 - 0.6988n + 0.006418n^2$$
 (n = 4 to 16)

5

(continued next page)



and found for pentanols and higher alcohols

$$\log \frac{\frac{c_p}{(g(1)/100g \, \text{sln})}}{\frac{c_o}{(g(1)/100g \, \text{sln})}} = -0.531p$$

 $\frac{c_o/(g(1)/100g \text{ sln})}{c_o/(g(1)/100g \text{ sln})} = 3.4^p$

or

where c_0 is the solubility of the alcohol with P = 0. Also, there was found a general relationship between the solubilities of

$$\begin{array}{c} R \\ H - C - R \\ I \\ OH \end{array} \qquad \text{and} \qquad \begin{array}{c} R \\ CH_3 - C - R \\ I \\ OH \end{array}$$

such that the ratio of the solubilities was 1.65 for R = H, 1.49 for $R = CH_3$ and 1.30 for $R = C_2H_5$.

Alcohols, like alkylamines and alkanoic acids, commonly exhibit a temperature at which a minimum solubility in the aqueous phase is observed. Although the curves for alcohols are rather broad, the minimum of each may be regarded as a characteristic point with respect to that solute in water (ref 12). Temperature-solubility plots for water in the alcohol-rich phase are also curved, the solubility decrease with decreasing temperature becoming less steep, but a minimum is not usually reached before phase separation (ref 13). However, for 1-alkanols with carbon chain length 10 atoms and greater the direction of the temperature dependence seems to be reversed (ref 2).

In general, it should be said that the solubility data in alcohol-water systems are frustrating to the compiler, the lower alcohols having a large amount of imprecise and conflicting data, and the higher alcohols having insufficient information to provide recommended values. Of the more common alcohols, the 2-butanol system in particular requires further critical study.

This volume is the result of a careful search of the literature with the aim of finding and including all published information for the systems indicated in the title. Undoubtedly some published measurements will have been overlooked, and the editor will be pleased to have these brought to his attention.

The editor would like to express his appreciation to all compilers and evaluators, but in particular to Andrzej Maczynski who has been with the project from the beginning, and to Glenn Hefter who brought much needed encouragement recently. Assistance with translations from Lu Zhen-Ya, E. Marian and Naoyuki Tsuchida is acknowledged, and the editor wishes to thank Fu Jufu, M.-C. Haulait-Pirson, G.T. Hefter, J.W. Lorimer, D.G. Shaw, and C.L. Young for their careful reviewing of the volume.

The typing of repeated drafts by Eileen Rowley and Lorelei Nottage is greatly appreciated.

A. F. M. Barton

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LIQUID-LIQUID SOLUBILITY: INTRODUCTORY INFORMATION

Allan F.M. Barton

The Solubility Data Series is made up of volumes of comprehensive and critically evaluated solubility data on chemical systems in clearly defined areas. Data of suitable precision are presented on data sheets in a uniform format, preceded for each system by a critical evaluation if more than one set of data is available. In those systems where data from different sources agree sufficiently, recommended values are proposed. In other cases, values may be described as "tentative" or "rejected".

This volume is primarily concerned with liquid-liquid systems, but related gas-liquid and solid-liquid systems are included when it is logical and convenient to do so. Solubilities at elevated and low temperatures and at elevated pressures may be included, as it is considered inappropriate to establish artificial limits on the data presented if they are considered relevant or useful.

For some systems the two components are miscible in all proportions at certain temperatures or pressures, and data on miscibility gap regions and upper and lower critical solution temperatures are included where appropriate and if available.

TERMINOLOGY

In this volume a mixture (1,2) or a solution (1,2) refers to a single liquid phase containing components 1 and 2. In a mixture no distinction is made between solvent and solute.

The *solubility* of a substance is the relative proportion of l in a mixture which is saturated with respect to component l at a specified temperature and pressure. (The term "saturated" implies the existence of equilibrium with respect to the processes of mass transfer between phases).

QUANTITIES USED AS MEASURES OF SOLUBILITY

<u>Mole fraction</u> of component 1, x_1 or x(1):

$$x_1 = n_1 / \sum_{i} \frac{m_1 / M_1}{\sum_{i} (m_i / M_i)}$$

where n_i is the amount of substance (number of moles) of component i, m_i is the mass of substance i, and M_i is its molar mass.

Mole per cent of component 1 is $100x_1$

<u>Mass fraction</u> of component 1, w_1

$$w_1 = m_1 / \sum_{i=1}^{\infty} i$$

where m_i is the mass of component i.

(continued next page)

<u>Mass per cent</u> of component 1 is $100\omega_1$, and may be described as $g(1)/100g \ sln$ which makes it clear that it is mass percent of 1 solute relative to solution and not solvent. The equivalent terms "weight fraction" and "weight per cent" are not used. The mole fraction solubility is related to the mass fraction solubility in a binary system by

$$x_1 = \frac{\frac{\omega_1 / M_1}{\omega_1 / M_1 + (1 - \omega_1) / M_2}}{\omega_1 / M_1 + (1 - \omega_1) / M_2}$$

Amount of substance concentration of component 1 in a solution of volume V,

$$c_1 = n_1 / 1$$

is expressed in units of mol L^{-1} . The terms "molarity" and "molar" and the unit symbol M are not used.

<u>Mass ratio</u> is occasionally used in a two-component solution in the form g(1)/g(2), mg(1)/g(2), etc. The term "parts per million" (ppm) is not used, but may be expressed as mg(1)/kg sln or $g(1)/10^{6}$ g sln, etc.

<u>Molality</u> of component 1 in component 2 is often used in solid-liquid systems defined as $m_1 = n_1/n_2M_2$, but is not used in liquid-liquid systems where the distinction between "solute" 1 and "solvent" 2 is inappropriate. The term molality alone is inadequate, and the units (mol kg⁻¹, mmol kg⁻¹) must be stated.

Mole fractions and mass fractions are appropriate to either the "mixture" or the "solution" point of view; the other quantities are appropriate to the solution point of view only.

ORDERING OF SYSTEMS

It is necessary to establish a method of ordering chemical compounds, to be used for the lists of saturating components which define each chemical system. This order is also used for ordering systems within volumes.

The systems are ordered first on the basis of empirical formula according to the Hill system (ref 2). The organic compounds within each Hill formula are ordered as follows:

- (i) by degree of unsaturation, then
- (ii) by order of increasing chain length in the parent hydrocarbon, then
- (iii) by order of increasing chain length of hydrocarbon branches, then
- (iv) numerically by position of unsaturation, then
- (v) numerically by position by substitution, then
- (vi) alphabetically by IUPAC name.

For example,

^с 5 ^н 8	cyclopentene 2-methyl-1,3-butadiene 1,4-pentadiene l-pentyne	
C5 ^H 10	cyclopentane 3-methyl-l-butene 2-methyl-2-butene l-pentene 2-pentene	
 c ₅ H ₁₂	2,2-dimethylpropane 2-methylbutane pentane	(continued next page)
 	•	(continued next page)

C₅H₁₂0 2,2-dimethyl-1-propanol 2-methyl-1-butanol 2-methyl-2-butanol 3-methyl-1-butanol 3-methyl-2-butanol 1-pentanol 2-pentanol 3-pentanol C₆H₁₂0 cyclohexanol 4-methyl-1-penten-3-ol

1-hexen-3-ol 4-hexen-3-ol

Deuterated $\binom{2}{H}$ compounds immediately follow the corresponding $\frac{1}{H}$ compounds.

GUIDE TO THE COMPILATIONS AND EVALUATIONS

The format used for the compilations and evaluations has been discussed in the Foreword. Additional information on the individual sections of each sheet is now provided in the following.

"Components". Each component is listed by its IUPAC name (ref 1), chemical formula according to the Hill system, and Chemical Abstracts Registry Number. Also included are the "Chemical Abstracts" name if this differs from the IUPAC name, and trivial name or names if appropriate. IUPAC and common names are cross-referenced to "Chemical Abstracts" names in the System Index.

"Original Measurements". References are expressed in "Chemical Abstracts" style, journal names being abbreviated, and if necessary transliterated, in the forms given by the "Chemical Abstracts Service Source Index" (CASSI). In the case of multiple entries (for example, translations) an asterisk indicates the publication used for the data compilation.

"Variables". Ranges of variations of temperature, pressure, etc. are indicated here.

"Prepared by". The compiler is named here.

"Experimental Values". Components are described as (1) and (2), as defined in "Components". The experimental data are presented in the units used in the original paper. Thus the temperature is expressed $t/{}^{\circ}C$ or $t/{}^{\circ}F$ as in the original, and conversion to T/K is made only in the critical evaluation. However, the author's units are expressed according to IUPAC recommendations (ref 3,4) as far as possible.

In addition, compiler-calculated values of mole fractions and/or mass per cent are included if the original data do not use these units. 1975 or 1977 atomic weights (ref 5) are used in such calculations. If densities are reported in the original paper, conversions from concentrations to mole fractions are included in the compilation sheets, but otherwise this is done in the evaluation, with the values and sources of the densities being quoted and referenced.

Details of smoothing equations (with limits) are included if they are present in the original publication and if the temperature or pressure ranges are wide enough to justify this procedure.

Errors in calculations, fitting equations, etc. are noted, and where possible corrected. Material inserted by the compiler is identified by the word "compiler" in parentheses.

The precision of the original data is preserved when derived quantities are calculated, if necessary by the inclusion of one additional significant figure. In some cases graphs have been included, either to illustrate presented data more clearly, or if this is the only information in the original. Full grids are not usually inserted as it is not intended that users should read data from the graphs.

(continued next page)

"Method". An outline of the method is presented, reference being made to sources of further detail of these are cited in the original paper. "Chemical Abstracts" abbreviations are often used in this text.

"Source and Purity of Materials". For each component, referred to as (1) and (2), the following information (in this order and in abbreviated form) is provided if it is available in the original paper:

source and specification

method of preparation

properties

degree of purity

"Estimated Error". If this information was omitted by the authors, and if the necessary data are available in the paper, the compilers have attempted to estimate errors (identifiedby "compiler" in parentheses) from the internal consistency, the type of apparatus, and other relevant information. Methods used by the compilers for reporting estimated errors are based on the papers by Ku and Eisenhart (ref 6).

"References". These are the references (usually cited in the original paper) which the compiler considers particularly useful in discussing the method and material.

"Evaluator". The information provided here is the name of the evaluator, the evaluator's affiliation, and the date of the evaluation.

"Critical Evaluation". The evaluator aims, to the best of his or her ability, to check that the compiled data are correct, to assess their reliability and quality, to estimate errors where necessary, and to recommend numerical values. The summary and critical review of all the data supplied by the compiler include the following information:

(a) Critical text. The evaluator produces a text evaluating all the published data for the particular system being discussed, reviewing their merits or shortcomings. Only published data (including theses and reports) are considered, and even some of the published data may only be referred to in this text if it is considered that inclusion of a data compilation sheet is unjustified.

(b) *Fitting equations*. If the use of a smoothing equation is justifiable, the evaluator may provide an equation representing the solubility as a function of the variables reported in the compilation sheets, stating the limits within which it should be used.

(c) Graphical summary. This may be provided in addition to tables and/or fitting equations.

(d) *Recommended values*. Data are *recommended* if the results of at least two independent experimental groups are available and are in good agreement, and if the evaluator has no doubt as to the adequacy and reliability of the experimental and computational procedures used.

Data are reported as *tentative* if only one set of measurements is available, or if the evaluator is uncertain of the reliability of some aspect of the experimental or computational method but judges that it should cause only minor error, or if the evaluator considers some aspect of the computational or experimental method undesirable but believes the data to have some value in those instances when an approximate value of the solubility is needed.

Data determined by an inadequate method or under ill-defined conditions are *rejected*, the reference being included in the evaluation together with a reason for its rejection by the evaluator.

(e) *References.* All pertinent references are listed here, including all those publications appearing in the accompanying compilation sheets and also those which have been rejected and not compiled.

(f) Units. The final recommended values are reported in SI units (ref 3). It should be noted that in most cases the rounded absolute temperature values (e.g. 298 K) actually refer to 298.15 K, etc, although very few solubilities are known with such precision that the differences are significant.

Continuation Sheets. These are used for both compilations and evaluations, and include sections listing the "Components" and also the "Original Measurement" or "Evaluator" as well as the word "continued". Compilation continuation sheets may include a section headed "Comments and/or Additional Data".

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- Rigaudy, J.; Klesney, S.P. Nomenclature of Organic Chemistry (IUPAC), ("The Blue Book"), Pergamon, Oxford, <u>1979</u>.
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- Whiffen, D.H., ed. Manual of Symbols and Terminology for Physicochemical Quantities and Units (IUPAC), ("The Green Book") Pergamon, Oxford, 1979; Pure Appl. Chem. <u>1979</u>, 51, 1.
- 4. McGlashan, M.L. *Physicochemical Quantities and Units*, 2nd ed. Royal Institute of Chemistry, London, <u>1971</u>.
- 5. IUPAC Commission on Atomic Weights, Pure Appl. Chem. 1976, 47, 75; 1979, 51, 405.
- Ku, H.H., and Eisenhart, C., in Ku, H.H., ed. Precision Measurement and Calibration, NBS Special Publication 300, Vol. 1, Washington D.C., <u>1969</u>.

COMPONENTS:	ORIGINAL MEASUREMENTS:
 (1) 1-Propanol (<i>n</i>-propyl alcohol); C₃H₈0; [71-23-8] (2) Water; H₂0; [7732-18-5] 	Rosso, J-C.; Carbonnel, L. C.R. Hebd. Seances Acad. Sci., <u>1969</u> , 269, 1432-5
VARIABLES:	PREPARED BY:
Temperature: -150 to 0°C	A.F.M. Barton
EXPERIMENTAL VALUES:	
g(1)/100g sln from -10.5 [°] C to an upper cri	extends between compositions 26.5 and 73.2 Itical miscibility temperature of -1.7° C at a fraction compositions (x_1) calculated by the stively.
A full phase diagram is presented, reveali	ing a solid pentahydrate between -52 and -134° C:
t/ ^o c g((1)/100g sln x_1 (compiler)
Eutectic -134 Peritectic -52.0 Monotectic -10.5 t_c -1.7	95.10.85385.70.64326.00.095350.00.231
AUXILI	ARY INFORMATION
METHOD/APPARATUS/PROCEDURE: Thermal analysis of crystallised mixtures from liquid nitrogen temperatures.	SOURCE AND PURITY OF MATERIALS: (1) Merck; f.pt127 ^o C. (2) not specified
	ESTIMATED ERROR: Not specified
	REFERENCES:

COMPONENTS :	···	ORIGINAL MEASUREMEN	Τς•	
		ORIGINAL MEASUREMEN	15:	
(1) 2-Propanol (isopropanol); C ₃ H ₈	, ⁰ ;	Rosso, JC.; Carbonnel, L.		
[67-63-0]		C.R. Hebd. Seances Acad. Sci. <u>1969</u> , 268,		
(2) Water; H ₂ O; [7732-18-5]		1012-5.		
VARIABLES:		PREPARED BY:		
Temperature: (-115) to 0 ⁰ C		A.F.M. Barton		
EXPERIMENTAL VALUES:		1		
The region of liquid-liquid immisci 60.0 g(1)/100g sln at -20 ⁰ C to an u 51 g(1)/100g sln. The correspondi compiler are 0.1713, 0.310 and 0.23	pper crit ng mole f	ical miscibility tempraction (x_1) composi	perature of -12 ⁰ C at	
A full phase diagram is presented,			between -37 and -100 ⁰ C	
and an entirely metastable pentahyd	rate down	to -50 ⁰ C.		
	t∕°c	g(1)/100g sln	$x_1(\text{compiler})$	
Eutectic	-100	96.30	0.886	
Metastable eutectic	-108	95.2	0.856	
Peritectic	-37	82.0	0.577	
Metastable peritectic	-50	86.7	0.662	
Monotectic	-20	40.7	0.171	
t _c	-12	51.0	0.238	
		<u>. </u>	<u> </u>	
	AUXILIARY	INFORMATION		
METHOD / APPARATUS / PROCEDURE :		SOURCE AND PURITY C	DF MATERIALS:	
Thermal analysis of crystallised mf			ning 1% water allowed for	
allowed to warm up from liquid nitr temperatures.	ogen	in compositio f.p91.5°C	n;	
		(2) not stated		
		ESTIMATED ERROR:		
		Not specified		
		REFERENCES :		

2

COMPONENTS:	EVALUATO	R:			
(1) 2-Methyl-l-propanol (<i>isobutanol</i>);	G.T. He	G.T. Hefter, School of Mathematical and			
C ₄ H ₁₀ 0; [78-83-1]	Physica	l Sciences, Murdoch	ı University,		
(2) Water; H ₂ 0; [7732-18-5]	Perth,	Western Australia.			
(2) water, 120, 17752 10 55	Novembe	er 1982.			
CRITICAL EVALUATION:					
Solubilities in the system comprising	2-methyl-1-propa	nol (1) and water	(2) have been		
reported in the following publications	5 1 1				
Reference	<i>Т</i> /К	Solubility	Method		
Alexejew (ref 1)	374-405	mutual	synthetic		
Michels (ref 2)	263-406	mutual	synthetic		
Brun (ref 3)	273	mutual	synthetic		
Janecke (ref 4)	312-406	mutual	synthetic		
Jasper (ref 5)	363	mutual	refractometric		
Alberty and Washburn (ref 6)	298	mutual	refractometric		
Booth and Everson (ref 7)	298	(1) in (2)	titration		
Donahue and Bartell (ref 8)	298	mutual	analytical		
Morachevskii <i>et al</i> . (ref 9)	293	mutual	titration		
Ratouis and Dode (ref 10)	298, 303	(1) in (2)	analytical		
Mozzhukhin et_al . (ref 11)	293, 303	mutual	titration		
Mullens (ref 12)	298	mutual	interferometric		
De Santis <i>et al</i> . (ref 13)	298	mutual	analytical		
Moriyoshi <i>et al</i> . (ref 14)	303-407	mutual	refractometric		
Lyzlova (ref 15)	293, 363	mutual	refractometric		
Fu et al. (ref 16)	363	mutual	titration		
Lutugina and Reshchetova (ref 21)	363	mutual	analytical		

Apart from four further publications (ref 17-20) which did not contain sufficient information to justify their inclusion, all original data are compiled in the data sheets immediately following this Critical Evaluation.

In the Critical Evaluation the data of Booth and Everson (7), in volume fractions, and of Mullens (ref 12), in w/v fractions have been excluded from consideration.

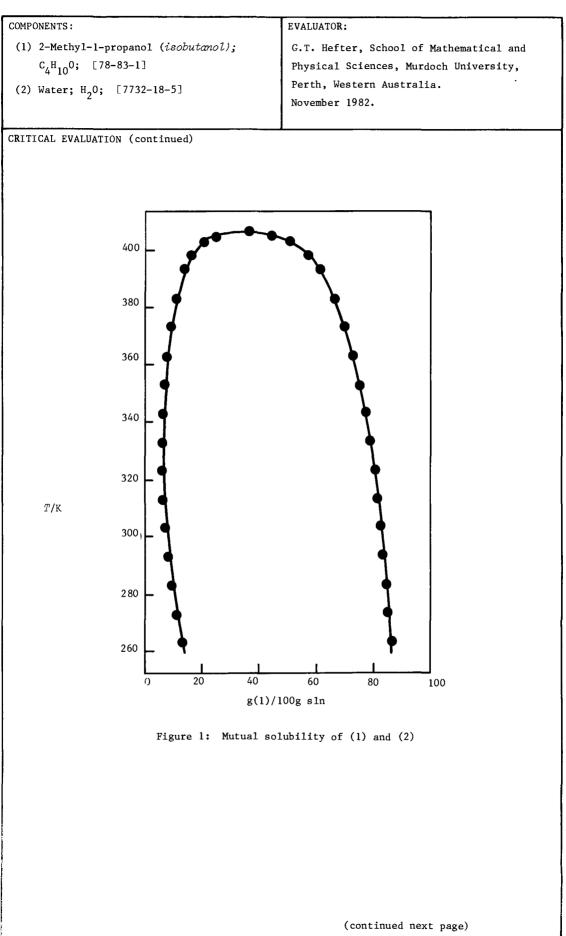
The data of Brun (ref 3), Jasper *et al.* (ref 5), Donahue and Bartell (ref 8), de Santis *et al.* (ref 13), Lutugina and Reshchetova (ref 21), and Moriyoshi *et al.* (ref 14) (alcohol-rich phase only) are in marked disagreement with all other studies and are rejected.

The following individual points in otherwise satisfactory studies are also in marked disagreement with other studies and have been rejected: in the water-rich phase, 303, 308 and 313 K (ref 14); in the alcohol-rich phase 398 and 403 K (ref 4) and 298 K (ref 9). All other reported data are included in the table below. Values obtained by the evaluator by graphical interpolation or extrapolation from the data sheets are indicated by an asterisk (*).

"Best" values have been obtained by simple averaging. The uncertainty limits (σ_n) attached to these values do not have statistical significance and should be regarded only as a convenient representation of the spread of values rather than as error limits. (continued next page)

COMPONENTS	:	EVALUATOR:	
(1) 2-Met	hyl-l-propanol (isobutanol);	G.T. Hefter, School of Mathematical and	
C4H10	0; [78-83-1]	Physical Sciences, Murdoch University,	
. 1.	; H ₂ 0; [7732-18-5]	Perth, Western Australia.	
(2) Water	, "20, [//32 10-3]	November 1982.	
CRITICAL E	VALUATION (continued)		
The lette	r (R) designates "recommended" da	ta. Data are "recommended" if two or more	
		ble (± 5% relative) agreement. All other d	ata
	ded as tentative only.	-	
J	-		
		(R) values for the solubility	
	of 2-methy1-1-propanol	(1) in water (2)	
<i>Т</i> /К		Solubility, g(1)/100g sln	
17.	Reported values	"Best" value (±σ)
		11	i'
263	13.45 [*] (ref 2)	13.5	
268	12.4 [*] (ref 2) 11.5 [*] (ref 2)	12.4	
273	11.5 (ref 2) 10.7 [*] (ref 2)	11.5	
278	10.7 (ref 2) 10.0 [*] (ref 2)	10.7	
283 288	9.3 $(ref 2)$	10.0	
288	9.3 (fef 2) 8.6 [*] (ref 2), 8.3 (ref 9), 8.	9.3 5 (mof. 11) 8 9 (mof. 15) 8 5 + 0.1 (נסי
293	8.15 [*] (ref 2), 8.02 (ref 6),		-
303	7.8 [*] (ref 2), 7.80 (ref 10),		
308	7.5 [*] (ref 2)	7.5 (101 11) 7.5	Л
318	7.0^{*} (ref 14)	7.0	
323	6.5 [*] (ref 14)	6.5	
328	6.6 [*] (ref 14)	6.6	
333	6.8 [*] (ref 14)	6.8	
338	7.0 [*] (ref 14)	7.0	
343	7.2 [*] (ref 14)	7.2	
348	7.2 [*] (ref 14)	7.2	
353	7.5 [*] (ref 2), 7.4 [*] (ref 14)	7.5 ± 0.1 (R)
358	7.9 [*] (ref 2), 7.6 [*] (ref 14)	7.8 ± 0.2 (R)
363		ref 14),8.1(ref 15),7.43(ref 16) 7.9 ± 0.3 (
368	8.8 [*] (ref 2), 8.7 [*] (ref 4), 8.		
373	9.5 [*] (ref 2), 9.4 [*] (ref 4), 9		R)
378	10.4 [*] (ref 2, 10.2 [*] (ref 4), 1		R)
383	11.4 [*] (ref 1), 11.3 [*] (ref 2),11	- · · · · · · · · · · · · · · · · · · ·	R)
388	12.2 [*] (ref 1), 12.5 [*] (ref 2), 1		<i>R</i>)
393	13.6 [*] (ref 1), 14.2 [*] (ref 2), 1	$3.3^{*}(ref 4), 15.0^{*}(ref 14)$ 14.0 ± 0.6 (<i>R</i>)
398	17.0 [*] (ref 1), 16.4 [*] (ref 2), 1		
	24.8 [*] (ref 1), 20.1 [*] (ref 2), 1	9.9^{*} (ref 4), 23.5 [*] (ref 14) 22 ± 2.	
403	24.8 (ref 1), 20.1 (ref 2), 1	9.9 (ref 4), 23.3 (ref 14) 22 ± 2 .	

COMPONENTS:	EVALUATOR:
(1) 2-Methyl-1-propanol (isobutanol);	
C ₄ H ₁₀ ⁰ ; [78-83-1]	G.T. Hefter, School of Mathematical and
	Physical Sciences, Murdoch University,
(2) Water; H ₂ 0; [7732-18-5]	Perth, Western Australia.
	November 1982.
CRITICAL EVALUATION (continued)	
Tentative and recomme	nded (R) values for the solubility
of water (2) in	2-methy1-1-propano1 (1)
T/K	Solubility, g(2)/100g sln
Reported value	es "Best" values ($\pm \sigma_n$)
263 13.7 [*] (ref 2)	13.7
268 14.3 [*] (ref 2)	14.3
273 14.7 [*] (ref 2)	14.7
278 15.0 [*] (ref 2)	15.0
283 15.5 [*] (ref 2)	15.5
288 15.9 [*] (ref 2)	15.9
293 16.2 [*] (ref 2), 16.6 [*] (ref 6), 16.4	*(ref 11), 16.6 (ref 15) 16.4 ± 0.2 (R)
298 16.7 [*] (ref 2), 17.01 (ref 6)	16.7 ± 0.1 (R)
303 17.2 [*] (ref 2), 17.5 (ref 11)	17.2
308 17.7 [*] (ref 2)	17.7
313 18.3 [*] (ref 2)	18.3
318 19.3 [*] (ref 2)	19.3
323 19.4 [*] (ref 2)	19.4
328 19.8 [*] (ref 2)	19.8
333 20.6 [*] (ref 2)	20.6
338 21.4 [*] (ref 2)	21.4
343 22.3 [*] (ref 2)	22.3
348 23.3 [*] (ref 2)	23.3
353 24.4 [*] (ref 2)	24.4
358 25.5 [*] (ref 2)	25.5
363 26.6 [*] (ref 2), 26.8 (ref 15), 26	(ref 16) 26.5 ± 0.3 (R)
368 27.8 [*] (ref 2)	27.9
373 29.4 [*] (ref 1), 29.4 [*] (ref 2)	29.4 (<i>R</i>)
378 31.2 [*] (ref 1), 31.1 (ref 2)	31.1 ± 0.1 (R)
383 34 [*] (ref 1), 33.1 [*] (ref 2)	33.5 ± 0.4
388 36 [*] (ref 1), 35.2 [*] (ref 2)	35.6 ± 0.4
393 39 [*] (ref 1), 39.4 [*] (ref 2)	39.2 ± 0.2
398 43.4 [*] (ref 1), 42.7 [*] (ref 2)	43.0 ± 0.4 (<i>R</i>)
403 52 [*] (ref 1), 49 (ref 2)	50 ± 2 (<i>R</i>)
The "best" values from the above tables are	plotted in Figure 1. As will be obvious
from the tables these values are largely the	-
Morivoshi et al. (ref 14) have also determi	ned the mutual solubility of (1) and (2) at
pressures of 200-2500 atm. (20-250 MPa).	
The upper critical solution temperature at	l atm has been reported as 396.5 K (3) and,
probably more reliably, as 407.25 K (ref 14). The corresponding critical compositions
are 37.5 (ref 3) and 36.3 (ref 14) g(1)/100	
	(continued next page)



2-10161191-	propanoi
COMPONENTS: (1) 2-Methy1-1-propanol (<i>isobutanol</i>); C ₄ H ₁₀ 0; [78-83-1] (2) Water; H ₂ 0; [7732-18-5]	EVALUATOR: G.T. Hefter, School of Mathematical and Physical Sciences, Murdoch University, Perth, Western Australia. November 1982.
CRITICAL EVALUATION (continued) References	· · · · · · · · · · · · · · · · · · ·
1. Alexejew, W. Ann. Phys. Chem. <u>1886</u> , 28	3, 305.
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 Morachevskii, A.G.; Smirnova, N.A.; Lysl <u>1965</u>, 38, 1262. 	lova, R.V. Zhur. Prikl. Khim. (Leningrad)
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 Mozzhukhin, A.S.; Serafimov, L.A.; Mitro Tekhnol. Topl. Masel <u>1966</u>, 11(4), 11. 	ppolskaja, W.A.; Rudakovskaja, T.S. <i>Khim</i> .
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17. Wratschko, F. Pharm. Presse 1929, 34, 1	143.
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21. Lutugina, N.V.; Reshchetova, L.I. <i>Vestr</i>	rik Leningr. Univ. <u>1972</u> , 16, 75.

COMPONENTS:				ORIGINAL MEASUREMENTS	:
(1) 2-Met	hyl-l-propa	anol (<i>isob</i>	utanol):	Alexejew, W.	
C ₄ H ₁₀ 0: [78-83-1]		Ann. Phys. Chem. <u>1836</u> , 28, 305–38.			
			Hint, 1190, Onlong <u>10</u>	<u></u> ,,	
(2) Wate	r; H ₂ 0; []	7732-18-5]			
VARIABLES:				PREPARED BY:	······
Temperatu	re: 101-13	2°C		A. Maczynski; Z. Ma	czynska; A. Szafranski.
EXPERIMENTA	L VALUES:				
	Mu	tual solub	ility of 2-met	hyl-1-propanol (1) and	d water (2)
t/°c		g(1)/100)g sln	$x_1^{}$ (comp	iler)
				e (2)-rich phase	
	(2)-ric	h pnase		e (2)-rich phase	
101.		-	70.3	-	0.365
103.		-	69.3	-	0.354
113	11		-	0.0315	-
123	15	.3	-	0.0420	-
125		-	56.6	-	0.240
126.		-	56.3	-	0.242
127		• 4	-	0.0552	-
129		. 39	-	0.0655	-
131.	5 32	.23	41.58	0.1036	0.1474
			AUXILIARY	INFORMATION	
METHOD /APP	ARATUS / PROCE	EDURE :		SOURCE AND PURITY OF	MATERIALS;
The synth	netic and/or	analytic	al method was	(1) not specified.	
	e latter onl ed with temp		e solubility	(2) not specified.	
aiminish	ea with temp	eracure.		(2) Not specified	
and weigh capillar reweighed mercury f and coold until the	ned, then (2 y funnel. 1, fastened thermometer	2) was add The tube to the bu and repea er (or gly ecame resp	tedly heated cerol) bath		
nomogeneo	Jub and cull			ESTIMATED ERROR:	
				Not specified	•
				REFERENCES :	

COMPONENTS:			ORIGINAL MEASUREMENTS:			
 2-Methyl-l-propanol (isobutanol); C₄H₁₀0; [78-83-1] Water; H₂0; [7732-18-5] 		Michels, A. Arch. Neerl. Sci. Exactes Nat., Ser. 3A, <u>1923</u> , 6, 127-46.				
VARIABLES:			PREPARED BY:			
Temperatu	re: (-11) to 133	°c	A. Maczynski	; G.T. Hefter		
EXPERIMENT	AL VALUES:			· · · · · · · · · · · · · · · · · · ·		
	Solubil	ity of 2-methyl-l-p	ropanol (l) i	in the water-rich	phase.	
t∕°c	g(1)/100g sln	<pre>x1 (compiler)</pre>	t∕°c	g(1)/100g sln	x ₁ (compiler)	
-10.6	13.61	0.03687	94.1	8.82	0.0230	
-8.6	13.12	0.03539	99.1	9.21	0.0241	
-3.6	12.18	0.03260	105.3	10.42	0.02748	
-2.9	12.00	0.03207	117.1	13.11	0.03536	
-2.4	11.92	0.03184	121.9	15.03	0.04121	
7.0	10.42	0.02748	126.2	17.00	0.04741	
14.9	9.21	0.0241	128.2	19.41	0.05529	
18.95	8.82	0.0230	131.8	22.93	0.06742	
21.6	8.43	0.0219	131.9	21.89	0.06375	
27.4	8.00	0.0207	132.5	29.84	0.09366	
36.3	7.48	0.0193	132.6	32.12	0.10313	
80.2	7.48	0.0193	132.9	33.88	0.11072	
87.0	8.00	0.0207	132.6	35.09	0.11610	
92.6	8.43	0.0219	132.7	37.14	0.12554	
				(continued	next page)	
	······································	AUXILIARY	INFORMATION			
METHOD/APP	ARATUS/PROCEDURE		SOURCE AND P	URITY OF MATERIAL	S:	
The synthetic method was used. A sealed glass tube, described in the paper, was used. No further details were given about the technique used.		distil b.p. r	ange 107.46-107.4 197 g cm ⁻³ .	3 [°] C,		
			ESTIMATED EF	RROR:		

COMPONENTS	MPONENTS:		ORIGINAL MEA	SUREMENTS:	
(1) 2-Met	hyl-l-propanol (i	sobutanol);	Michels, A.		
^C 4 ^H 10	; 78-83-1		Arch. Neer. Sci. Exactes Natur., Ser		tur., Ser. 3A,
(2) Hatar	; H ₂ O; [7732-18	-51	1923, 6, 12		
(2) Water	$\frac{1}{2}$; $\frac{1}{2}$; $\frac{1}{2}$				
EXPERIMENT	AL VALUES: (cont	inued)			
	Solubil	ity of 2-methy1-	l-propanol (l)	in the alcohol-r	ich phase
t∕°C	g(1)/100g sln	x ₁ (compiler)	t∕°C	g(1)/100g sln	<pre>x1 (compiler)</pre>
-14.7	86.71	0.6132	67.3	77.70	0.4585
-10.8	86.37	0.6062	76.7	75.79	0.4320
-7.9	86.03	0.5994	85.0	75.20	0.4242
-5.9	85.79	0.5946	86.9	74.17	0.4110
-2.9	85.50	0.5889	87.8	73.91	0.4077
1.0	85.28	0.5853	94.6	72.19	0.3868
7.1	84.91	0.5776	94.9	72.11	0.3858
9.4	84.57	0.5711	99.8	70.76	0.3703
12.9	84.22	0.5646	107.0	68.00	0.3405
18.2	83.91	0.5589	113.9	65.39	0.3146
23.1	83.63	0.5538	114.5	65.21	0.3129
23.9	83.44	0.5504	115.1	64.87	0.3091
26.7	83.13	0.5449	117.2	63.58	0.3044
28.5	82.91	0.5410	119.3	62.03	0.2842
29.5	82.74	0.5381	120.7	61.98	0.2837
29.9	82.59	0.5355	121.5	60.46	0.2709
33.1	82.57	0.5351	129.3	56.30	0.2384
35.7	82.32	0.5308	128.8	53.87	0.2210
36.6	82.27	0.5300	129.1	53.02	0.2152
38.7	81.72	0.5207	131.2^{a}	49.99	0.1954
39.0	81.88	0.5250	131.8	48.26	0.1848
40.7	81.82	0.5225	131.7	46.80	0.1761
41.0	81.55	0.5178	132.4	46.71	0.1756
45.6	80.66	0.5033	132.0	44.94	0.1655
53.1	80.54	0.5014	132.6	43.08	0.1553
63.8	78.82	0.4749	132.8	40.06	0.1397
68.3	77.79	0.4598	132.8	38.13	0.1302

^a Recorded as 139.2 in original, i.e. greater than U.C.S.T. Value estimated by compilers by graphical interpolation.

COMPONENTS:	ORIGINAL MEASUREMENTS:
<pre>(1) 2-Methyl-1-propanol (isobutanol) C₄H₁₀0; [78-83-1]</pre>	Brun, P.
,	C.R. Hebd. Seances Acad. Sci. <u>1925</u> , 180,
(2) Water; H ₂ O; [7732-18-5]	1745-7; <u>1926</u> , <i>183</i> , 207-10
VARIABLES:	DEDADED DV.
One temperature: 0°C	PREPARED BY: A.F.M. Barton
one temperature: 0 C	K.I.M. Balton
EXPERIMENTAL VALUES:	
The mass percentage of isobutanol in the wate	
12.0 g(1)/100g sln; the corresponding mole f	raction solubility recalculated by the
compiler is $x_1 = 0.032$.	
The mass percentage of isobutanol in the alco	
82.0 g(1)/100g sln; the corresponding mole f	.faction solubility recalculated by the
compiler is $x_1 = 0.526$.	
Graphical results were reported in the 1925 p	paper for 40, 80, and 120 ⁰ C. The critical
temperature was 123.5°C, at a critical composi-	
-	
$x_1 = 0.127$).	
AUXILIARY	INFORMATION
	-
METHOD/APPARATUS/PROCEDURE: The synthetic method was used, in which the	SOURCE AND PURITY OF MATERIALS: Not specified.
turbidity temperature is determined for	
mixtures of known composition.	
	ESTIMATED ERROR:
	Not given.
	REFERENCES:
	1

COMPONENTS:		ORIGINAL 1	MEASUREMENTS:	
 2-Methyl-1-pro C₄H₁₀0; [78- Water; H₂0; 	83-1]	Jänecke, Z. Phys.	, E. Chem. <u>1933</u> , 164,	401-16.
VARIABLES:		PREPARED	BY:	
Temperature: 33-13	3 [°] C	A. Maczy A. Szafr	nski; Z. Maczynska anski	; and
EXPERIMENTAL VALUES:				
_	g(1)/100g sln		x_1 (com	piler)
t∕°c	(2)-rich phase (1)-	rich phase	(2)-rich phase	(1)-rich phase
38.9 , 38.4	-	81.7	-	0.520
90.4 , 90.4	3.0	-	0.0207	-
108.0 , 107.7	10.6	-	0.0280	-
126.4 , 126.5	-	57.8	-	0.250
126.7 , 126.7	16.3	-	0.0452	-
127.7 , 127.6	17.5	-	0.0490	-
130.6 , 130.3	20.7	-	0.0602	-
132.8 , 132.4	-	49.1	-	0.190
133.0 , 133.0	26.7	-	0.0813	-
		RY INFORMATIC		
METHOD APPARATUS / PR			D PURITY OF MATERI	ALS:
The synthetic meth	od was used.	(1) not	specified.	
	(1) and (2) were sealed d heated and cooled to and turbid points.	(2) not	specified.	
1		ESTIMATE	D ERROR:	
		Not	specified.	
		REFERENC	ES :	

COMPONENTS:	ORIGINAL MEASUREMENTS:
 (1) 2-Methyl-1-propanol (<i>isobutanol</i>); C₄H₁₀0; [78-83-1] (2) Water; H₂0; [7732-18-5] 	Jasper, J.J.; Campbell, C.J.; Marshall, D.E. J. Chem. Educ. <u>1941</u> , 18, 540-2.
VARIABLES:	PREPARED BY:
One temperature: 90 [°] C	A.F.M. Barton
EXPERIMENTAL VALUES:	
The mole fractions of 2-methyl-1-propanol (1) boiling point (89.65°C) of the binary mixture water-rich phase and $x_1 = 0.755$ in the alcoho The corresponding mass percentage solubilitie 4.0 g(1)/100g sln and 92.7 g(1)/100g sln, res	with water (2) were $x_1 = 0.010$ in the ol-rich phase. es, calculated by the compiler, are
(Actual temperatures and pressures observed w	
at 754.2 mm Hg, respectively; 1 atm = 101.32	25 kPa; 1 mm Hg(0 C) = 153.522 Pa.
AUXILIARY	INFORMATION
METHOD / APPARATUS / PROCEDURE :	SOURCE AND PURITY OF MATERIALS:
The vapor-liquid temperature-composition diagram was determined by sampling distillate and residue. Samples from distillations with both excess (2) and excess (1) were analyzed by refractive index. Ethanol was added to the samples to maintain homogen- eity during analysis, and compositions were determined from a calibration curve. The results reported were obtained while two layers remained in the distillation flask.	Not stated
	ESTIMATED ERROR:
	Not stated
	REFERENCES :

COMPONENTS :	ORIGINAL MEASUREMENTS:
(1) 2-Methyl-1-propanol (<i>isobutanol</i>),	Alberty, R.A.; Washburn, E.R. J. Phys. Chem. <u>1945</u> , 49, 4-8.
C ₄ H ₁₀ O; [78-83-1]	J. Fugs. Chem. <u>1945</u> , 48, 4-6.
(2) Water; H ₂ 0; [7732-18-5]	
VARIABLES:	DEDADED BY
Temperature: 23.3 - 26.5°C	PREPARED BY: A.F.M. Barton
	,,,,
EXPERIMENTAL VALUES:	
$t/^{O}C$ g(1))/100g sln x_1 (compiler)
Alcoh	ol-rich phase
23.33	83.12 0.545
25.00	82.99 ^{<i>a</i>} 0.543
26.14	82.93 0.542
26.51	82.85 0.540
Wate	r-rich phase
25.0	8.02 0.0208
25.0	0.02
^a By interpolation.	
AUXILIAR	(INFORMATION
METHOD/APPARATUS/PROCEDURE: For (1)-rich studies, homogeneous solutions of approximately equilibrium composition were sealed in glass tubes and cloud points $(\pm 0.07^{\circ}C)$ observed on cooling while they were rocked in a thermostat bath. For (2)-rich studies where cloud points were indistinct, the refractive indexes of several nearly saturated solutions were measured at 25.00°C with an immersion refractometer. The composition-refractive index curve was then extrapolated to the refractive index of a saturated solution.	SOURCE AND PURITY OF MATERIALS: (1) Eastman Kodak; refluxed with lime (24 h), fractionally distilled, then refluxed with Ca (4 h), refractionated; n_D^{20} 1.39615, d_4^0 0.8172, d_4^{25} 0.79811 (2) not specified ESTIMATED ERROR: Not specified REFERENCES:

COMPONENTS:	ORIGINAL MEASUREMENTS:
 (1) 2-Methyl-1-propanol (<i>isobutanol</i>); C₄H₁₀⁰; [78-83-1] (2) Water; H₂⁰; [7732-18-5] 	Booth, H.S.; Everson, H.E. Ind. Eng. Chem. <u>1948</u> , 40, 1491-3.
<pre>VARIABLES: One temperature: 25°C Sodium xylene sulfonate EXPERIMENTAL VALUES: It was reported that the solubility of 2-meth at 25°C. The corresponding figure in 40% sodium xylene > 400 mL(1)/100 mL solvent.</pre>	PREPARED BY: S.H. Yalkowsky; S.C. Valvani; A.F.M. Barton My1-1-propanol in water was 11.1 mL(1)/100mL(2) e sulfonate solution as solvent was
AUXILIARY METHOD/APPARATUS/PROCEDURE: A known volume of solvent (usually 50 mL) in a tightly stoppered calibrated Babcock tube was thermostatted. Successive measured quantities of solute were added and equilibrated until a slight excess of solute remained. The solution was centrifuged, returned to the thermostat bath for 10 mins, and the volume of excess solute measured directly. This was a modification of the method described in ref 1.	INFORMATION SOURCE AND PURITY OF MATERIALS: (1) not specified ("C.P. or highest grade commercial"). (2) distilled ESTIMATED ERROR: Solubility within 0.1 mL/100 mL. REFERENCES: 1. Hanslick, R.S. Dissertation, Columbia University, <u>1935</u> .

COMPONENTS:	ORIGINAL MEASUREMENTS:
 (1) 2-Methyl-1-propanol (<i>isobutanol</i>);	Donahue, D.J.; Bartell, F.E.
C ₄ H ₁₀ ⁰ [78-83-1] (2) Water; H₂0; [7732-18-5]	J. Phys. Chem. <u>1952</u> , 56, 480-484.
VARIABLES:	PREPARED BY:
One temperature: 25 ⁰ C	A.F.M. Barton

EXPERIMENTAL VALUES:

It was reported that at 25°C the mole fraction of water in the alcohol-rich phase (density 0.8328 g cm⁻³) was $x_2 = 0.449$ and the mole fraction of 2-methyl-l-propanol in the water-rich phase (density 0.9849 g cm⁻³) was $x_1 = 0.0195$.

The corresponding mass percentage values calculated by the compiler are 82.1 g(1)/100 sln and 7.56 g(1)/100g sln.

AUXILIARY	INFORMATION
METHOD APPARATUS / PROCEDURE: Samples of (1) with (2) were placed in glass stoppered flasks and were shaken inter- mittently for at least three days in a water- bath at 25 ± 0.1°C. The organic phase was analyzed for water by the Karl Fischer method and the aqueous phase was analyzed inter- ferometrically. The main purpose of the study was interfacial tension determination.	other appropriate treatments"
	ESTIMATED ERROR: Not stated
	REFERENCES :

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) 2-methyl-l-propanol (<i>isobutanol</i>);	Morachevskii, A.G.; Smirnova, W.A.;
$C_4 H_{10}^{0}; [73-33-1]$	Lyzlova, R.V.
(2) Water; ¹¹ 2 ⁰ ; [7732-18-5]	Zh. Prikl. Khim. (Leningrad) <u>1965</u> , 38, 1262-7.
VARIABLES:	PREPARED BY:
One temperature: 20 [°] C	A. Maczynski
EXPERIMENTAL VALUES:	
The solubility of 2-methyl-l-propanol in wate	er at 20°C was reported to be $x_1 = 0.023$.
The corresponding mass percentage calculated	by the compiler is 8.3 g(1)/100g sln.
The solubility of water in 2-methyl-1-propan	ol at 20 [°] C was reported to be $x_{2} = 0.45$.
The corresponding mass percentage calculated	
	INFORMATION
METHOD / APPARATUS / PROCEDURE :	SOURCE AND PURITY OF MATERIALS;
The titration method was used.	(1) CP reagent, source not specified; distilled; 20 +20
No details were reported in the paper.	distilled; b.p. 107.3°C, $n_{\rm D}^{20}$ 1.3953, d_4^{20} 0.8020.
	(2) not specified.
	ESTIMATED ERROR:
	Not specified.
	REFERENCES :
	1

COMPONENTS:	ORIGINAL MEASUREMENTS:	
(1) 2-Methyl-1-propanol (<i>isobutanol</i>);	Ratouis, M.; Dode M.	
С ₄ н ₁₀ 0; [78-83-1]	Bull. Soc. Chim. Fr. 1965, 3318-22.	
(2) Water; H ₂ 0; [7732-18-5]		
(2) water, n ₂ 0, [7,52 10 5]		
VARIABLES:	PREPARED BY:	
Temperature: 25-30 ⁰ C	S.C. Valvani; S.H. Yalkowsky; A.F.M. Barton	
Ringer solution also studied		
EXPERIMENTAL VALUES:		
Solubility of 2-methyl-1-propanol (1) in water (2)		
t/°C g(1))/100g sln $x_1^{(compiler)}$	
25	8.14 0.0211	
30	7.80 0.0202	
Solubility of 2-methyl-	l-propanol in Ringer solution	
t/ ^o c	g(1)/100g sln	
25	7.65	
30	7.40	
AUXILIARY	INFORMATION	
METHOD / APPARATUS / PROCEDURE :	SOURCE AND PURITY OF MATERIALS:	
In a round bottom flask, 50 mL of water and sufficient quantity of alcohol was introduced	(1) Prolabo, Paris; redistilled	
until two separate layers were formed. The	b.p. 10/.8-10/,9//54.2 mm Hg;	
flask assembly was equilibrated by agitation for at least 3 h in a constant temp. bath.	$n_{\rm D}^{25} = 1.39391$	
Equilibrium solubility was attained by first	(2) twice distilled from silica apparatus	
supersaturating at a slightly lower tempera- ture (solubility of alcohols in water is	or ion exchanged with Sagei A20.	
inversely proportional to temperature) and		
then equilibrating at the desired tempera- ture. The aqueous layer was separated after	d	
an overnight storage in a bath. The alcoho content was determined by reacting the		
aqueous solution with potassium dichromate	ESTIMATED ERROR:	
and titrating the excess dichromate with ferrous sulfate solution in the presence of	Solubility: relative error of 2 determina- tions less than 1%.	
phosphoric acid and diphenylamine barium	Temperature: ± 0.05°C.	
sulfonate as an indicator.	REFERENCES :	

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) 2-Methyl-1-propanol (<i>isobutanol</i>); C ₄ H ₁₀ ⁰ ; [78-33-1]	Mozzhukhin, A.S.; Serafimov, L.A.; Mitropolskaja, W.A.; Rudakovskaja, T.S.
(2) Water; H ₂ 0; [7732-18-5]	Khim. Tekhnol. Topl. Masel, <u>1966</u> , 11(4), 11-15.
VARIABLES:	PREPARED BY:
Temperature: 20 and 30 ⁰ C	A. Maczynski
EXPERIMENTAL VALUES:	
Mutual solubility of 2-me	thyl-1-propanol (1) and water (2)
$t/^{0}C$ g(1)/100g sln	x_1 (compiler)
	phase (2)-rich phase (1)-rich phase
20 8.5 33	
30 7.5 82	
AUXILIARY	INFORMATION
METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
The titration method was used. No details were reported in the paper.	 (1) source not specified; dried and distilled; b.p. 107.4°C, n²⁰_D 1.3858, 0.17% water. (2) not specified.
	ESTIMATED ERROR:
	Temperature: $\pm 0.1^{\circ}$ C.
	REFERENCES :

COMPONENTS: (1) 2-methyl-1-propanol (<i>isobutanol</i>); C ₄ H ₁₀ O [78-83-1] (2) water; H ₂ O; [7732-18-5]	ORIGINAL MEASUREMENTS: Mullens, J. <i>Alcoholassociaten;</i> Doctoraatsproefschrift, Leuven, 1971. Huyskens, P.; Mullens, J., Gomez, A.,Tack,J. <i>Bull. Soc. Chim. Belg.</i> <u>1975</u> , 84, 253-62.
VARIABLES:	PREPARED BY:
One temperature: 25 [°] C	M.C. Haulait-Pirson; A.F.M. Barton.

EXPERIMENTAL VALUES:

At 25° C solubility of 2-methyl-1-propanol(1) in the water-rich phase was reported as 1.029 mol(1)/L sln, and the solubility of water(2) in the alcohol-rich phase was reported as 9.438 mol(2)/L sln.

The corresponding values on a weight/volume basis are 76.27 g(l)/L sln, and 170.1 g(2)/L sln (compiler).

AUXILIARY	INFORMATION
ROLLDING	THEOREMITON

METHOD /APPARATUS / PROCEDURE :	SOURCE AND PURITY OF MATERIALS:
The partition of the two components was made using a cell described in ref 1. The Rayleigh Interference Refractometer M154 was used for the determination of the concen- trations. Standard solutions covering the whole range of concentration investigated were used for the calibration.	<pre>(1) Merck product (p.a.) (2) distilled.</pre>
	ESTIMATED ERROR:
	Soly ± 0.001 mol(1)/L sln.
	REFERENCES:
	 Meeussen, E.; Huyskens, P. J. Chim. Phys. <u>1966</u>, 63, 845

CONTOURNIES -	
COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) 2-Methyl-1-propanol (isobutanol); C ₄ H ₁₀ 0; [78-83-1]	De Santis, R.; Marrelli, L.; Muscetta, P.N.
(2) Water; H ₂ 0; [7732-18-5]	Chem. Eng. J., <u>1976</u> , 11, 207–14.
VARIABLES:	PREPARED BY:
One temperature: 25 [°] C	A. Maczynski
EXPERIMENTAL VALUES:	<u></u>
The solubility of 2-methyl-propanol in the way $9.4 \text{ g(1)}/100 \text{ g sln.}$	ater-rich phase at 25° C was reported to be
The corresponding mole fraction, x_1 , calculat	ed by the compiler is 0.025.
The solubility of water in the alcohol-rich p	phase at 25 ⁰ C was reported to be
17.3 g(2)/100g sln.	
The corresponding mole fraction, x_2 , calculated and the corresponding mole fraction, x_2 , calculated and the correspondence of	ed by the compiler is 0.463.
AUXILIARY	INFORMATION
METHOD / APPARATUS / PROCEDURE :	SOURCE AND PURITY OF MATERIALS:
The determinations were carried out using	 Merck, analytical purity; fractionated before use.
separator funnel with a thermostatic jacket. The extracter was loaded with (1) and (2)	
and after an extended period of mixing and quantitiative gravity separation, samples were withdrawn from the aqueous phase. The concentration of (1) in (2) was determined by colorimetric analysis (double-beam Lange colorimeter) of the cerium complex. The concentration of (2) in (1) was derived from a material balance based upon starting quantities and compositions. Each of the	(2) doubly distilled
determinations was carried out several times.	ESTIMATED ERROR:
	Temp. ± 0.1 ⁰ C.
	REFERENCES:

COMPONENTS	S:		ORIGI	NAL MEASUREMENTS:	
<pre>(1) 2-Methyl-1-propanol (isobutanol); C₄H₁₀0; [78-83-1]</pre>			Moriyoshi, T.; Aoki, Y.; Kamiyama, H. J. Chem. Thermodyn. 1977, 9, 495-502.		
(2) Wate:	r; H ₂ 0; [7	7732–18–5]			
VARIABLES	:		PREPA	RED BY:	
Temperat Pressure	ure: 303 : 1-2	-407 K 500 atm (0.1~250 MPa)	A.F.	M.Barton; G.T. Hefter	
EXPERIMEN	TAL VALUE	S: Mutual solubility of	2-meth	yl-l-proponol (1) and	water (2)
7/K	p/atm	g(1)/100g sln		$x_1 (comp$	oiler)
		(2)-rich phase (1)-ric	ch phas	e (2)-rich phase	(1)-rich phase
302.95	1	8.4	31.8	0.0218	0.522
302.95	500	011	30.6	0.0249	0.503
302.95	952		79.4	0.0272	0.484
302.95	1524	2000	77.3	0.0286	0.453
302.95	1633		76.8	0.0295	0.446
302.95	1837		75.9	0.0303	0.434
302.95	1973	11.7	75.0	0.0312	0.422
302.95	2245		73.9	0.0333	0.408
302,95	2449	12.7	73.5	0.0342	0.403
312.85	1	7.6	82.0	0.0196	0.526
312.85	503	8.7	80.6	0.0226	0.503
312.85	680	9.0	80.0	0.0235	0.493
312.85	1000	9.4	79.4	0.0246	0.484
312.85	1571	10.3	77.6	0.0272	0.457
312.85	1728	10.6	77.0	0.0280	0.449
				(0	continued next page)
		AUXILIAR	Y INFOR	MATION	
METHOD /AE	PARATUS / F	PROCEDURE :	SOUR	CE AND PURITY OF MATE	RIALS:
The meth	nod, descri	bed in ref 1, was that use		"best grade reagent"	
		er studies. Both compon- in a cut-off glass syringe		dried by refluxing	over freshly ignited
of about	: 20 cm ³ c	apacity used as a sample		calcium oxide, dist: n^{25} 1.3939. d^{25}	0.7983 g cm^{-3}
		s placed in a stainless essel mechanically shaken i	n	n 1.5959, a	0.7905 g cm
an oil t	hermostat	bath (± 0.05K). After east 6h and then standing		deionized, distille	d from alkaline
		the desired temperature	(2)	KMNO, and then redi	stilled;
-		umple of the upper layer Subsequently the pressure		n^{25} 1.3327	
vessel v	was moved,	the contents allowed to			
settle,	and the 1	ower layer sampled. samples was made by refract	- ESTI	MATED ERROR:	
ive index, methanol being added by weight		ten	temp. ± 0.05K		
to produ	uce homoge	eneity.		ubility ± 0.21 g(1)/ pe of error not spec	
			RFFF	RENCES :	
					china S.
			1.	Moriyoshi, T.; Kane Aihara, K.; Yabumot <i>Thermodyn</i> . <u>1975</u> , 7,	o, K. J. Chem.

(1) 2-METHYI-1-propanal (<i>isobutanol)</i> ; C ₁ (<i>j</i>) (<i>i</i> / <i>n</i> - <i>a</i>)-1) Nortyoshi, T.; Aoki, Y.; Kaniyama, B. J. Chem. Thermodyn. <u>1977</u> , <i>9</i> , 495-502. (2) Water; B ₂ 0; [7732-18-5] Nortyoshi, T.; Aoki, Y.; Kaniyama, B. J. Chem. Thermodyn. <u>1977</u> , <i>9</i> , 495-502. TK p/atm g(1)/100g aln r_1 (compiler) C2)-rich phase (1)-rich phase (2)-rich phase (1)-rich phase 312.85 2041 11.6 75.9 0.0309 0.434 312.85 2449 12.0 74.5 0.0312 0.422 312.85 2449 12.0 74.5 0.0321 0.415 322.75 1 6.5 81.5 0.0207 0.430 322.75 1561 8.0 77.0 0.0235 0.449 322.75 1565 9.0 77.0 0.0235 0.441 322.75 163 10.6 73.3 0.0266 0.430 322.75 163 10.6 73.3 0.0277 0.412 322.75 281 11.1 71.1 0.0235 0.442 322.65 100 8.2 79.4 0.02	COMPONENT	S:		ORIGINA	L MEASUREMENTS:		
Lange (1/8-83-1) J. Chem. Thermodyn. 1977, 9, 495-502. (2) Water; H_20 ; [7732-18-5] LATPERIMENTAL VALUES (continued) T/K g/atm g(1)/100g sln x_1 (compiler) (2)-rich phase (1)-rich phase (2)-rich phase (1)-rich phase 312.85 2041 11.6 75.9 0.0309 0.434 312.85 2041 11.6 75.9 0.0309 0.434 312.85 2041 1.6 7.5 0.0309 0.434 322.75 164 0.0207 0.4457 322.75 254 8.0 7.0 0.0235 0.449 322.75 164 1.0 0.077.0 0.0235 0.4427 322.75 2.64 0.637 0.4427							
$ \begin{array}{ c c c c c c c c c c c c c c c c c c c$	$C_{\lambda}H_{10}O;$ [78-83-1]						
EXPERIMENTAL VALUES (cont funce) T/K p/atm g(1)/100 1 a_1 (control phase (1)-rich phase (2)-rich phase (1)-rich phase (1)-rich phase (1)-rich phase (1)-rich phase 312.85 2001 11.7 75.0 0.0309 0.434 312.85 2449 12.0 74.5 0.0321 0.415 322.75 1 6.5 81.5 0.0204 0.437 322.75 952 8.0 78.5 0.0207 0.437 322.75 952 8.0 78.5 0.027 0.457 322.75 1840 10.1 7.6 0.0225 0.412 322.75 1840 10.1 7.1 0.0255 0.412 322.75 2163 10.6 73.3 0.0260 0.400 322.75 1840 10.1 7.1 0.0275 0.412 322.75 1843 9.9 7.5 0.0260 0.400 322.65 137 9.0 7.5 <td colspan="3"></td> <td>J. Che</td> <td>m. Thermodyn. <u>1977</u></td> <td>2, 9, 495-502.</td>				J. Che	m. Thermodyn. <u>1977</u>	2, 9, 495-502.	
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352.3517.477.00.01910.449352.355008.875.30.02290.426352.35100010.173.60.02660.404352.35124510.472.80.02750.394352.35143211.671.70.03090.381352.35190513.069.20.03500.353352.35220013.766.60.03710.327352.35235414.564.10.03960.303352.35253017.455.60.04870.233357.35161012.569.00.03360.351357.35183613.567.40.03640.344357.35197314.066.90.03800.329357.35231315.361.80.04200.282357.35240016.259.40.04490.262357.35245016.757.50.04650.248362.2517.774.70.01990.418							
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352.35235414.564.10.03960.303352.35253017.455.60.04870.233357.35150012.069.50.03210.357357.35161012.569.00.03360.351357.35183613.567.40.03640.334357.35197314.066.90.03800.329357.35223114.763.60.04020.298357.35231315.361.80.04200.282357.35240016.259.40.04490.262357.35245016.757.50.04650.248362.2517.774.70.01990.418							
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357.35240016.259.40.04490.262357.35245016.757.50.04650.248362.2517.774.70.01990.418							
357.35245016.757.50.04650.248362.2517.774.70.01990.418							
362.25 1 7.7 74.7 0.0199 0.418							
557715 2000 2012 5570 010445 01204	367.15	2000	16.2	59.6	0.0449	0.264	
(continued next page)					(cor		

COMPONENTS			ORIGIN	AL MEASUREMENTS	
(1) 2-Methyl-l-propanol (isobutanol);		, Moriy	Moriyoshi, T.; Aoki, Y.; Kamiyama, H.		
^с 4 ^н 10	0; [78-8	3-1]		iem. Thermodyn. 1977	0 405 502
			<i>ø</i> . сл	iem. 1ne1moagn. <u>191</u>	, 9, 495-502.
(2) Water	; H ₂ 0; [7732-18-5]			
EXPERIMEN	TAL VALU	ES (continued)			
<i>Т</i> /к	p / atm	g(1)/100g	g sln	x_1 (com	piler)
		(2)-rich phase	(1)-rich phase	e (2)-rich phase	(1)-rich phase
367.15	2007	16.3	59.2	0.0452	0.261
367.15	2200	21.3	46.0	0.0617	0,172
367.15	2320	26.8	39.5	0.0817	0.1370
370.15	1560	13.2	65.8	0.0356	0.319
370.15	1578	13.4	64.6	0.0361	0.307
370.15	1810	15.2	59.9	0.0471	0.267
370.15	1986	20.2	54.0	0.0579	0.222
370.15	2109	26.8	45.9	0.0817	0.171
372.15	1	9.9	71.7	0.0260	0.381
372.15	667	10.8	67.7	0.0286	0.338
372.15	1000	11.4	66.4	0.0303	0.325
372.15	1500	14.2	62.8	0.0386	0.291
372.15	1769	18.9	56.8	0.0536	0.242
372.15	1878	22.9	52.2	0.0673	0.210
372.15	1980	30.8	43.4	0.0976	0.156
372.15	2000	39.5	-	0.1370	-
377.15	1330	15.8	61.1	0.0436	0.276
377.15	1568	23.2	53.6	0.0684	0.218
377.15	1710	34.0	44.0	0.1113	0.160
382.05	1	11.1	67.7	0.0295	0,338
382.05	500	11.6	64.3	0.0309	0.305
382.05	677	11.7	64.1	0.0312	0.303
382.05	1219	16.8	61.3	0.0468	0.277
382.05	1374	22.5	55.2	0.0659	0,231
382.05	1487	32.5	45.9	0.1048	0.171
386.95	262	12.7	-	0.0342	-
386.95	500	13.8	61.3	0.0374	0.277
386.95	1000	19.4	54.7	0.0552	0.227
386.95	1080	22.2	51.5	0.0649	0.205
386.95	1184	29.9	43.4	0.0915	0.156
391.85	1	14.5	62.3	0.0396	0.287
391.85	340	16.0	59.9	0.0443	0.267
391.85	500	16.8	58.2	0.0468	0.253
391.85	670	19.0	56.6	0.0539	0.239
391.85	870	22.9	51.3	0.0673	0,204
391.85	982	33.5	42.2	0.1091	0.151
396.85	1	17.5	58.7	0.0490	0.257
396.85	500	20.6	54.5	0.0593	0.226
396.85	680	23.6	50.2	0.0699	0.197
396.85	719	27.7	45.5	0.0852 (con	0.169 tinued next page)

<pre>COMPONENTS: (1) 2-Methyl-1-propanol (isobutanol); C₄H₁₀0; [78-83-1] (2) Water; H₂0; [7732-18-5]</pre>		ORIGIN	ORIGINAL MEASUREMENTS: Moriyoshi, T.; Aoki, Y.; Kamiyama, H. J. Chem. Thermodyn. <u>1977</u> , 9, 495-502.		
		-			
EXPERIME	ENTAL VALU	ES (continued)			
		g(1)/10	Og sln	$x_1^{(comp}$	iler)
<i>т</i> /к	p/atm	(2)-rich phase	(1)-rich phase	(2)-rich phase	(1)-rich phase
396.85	816	30.6	40.7	0.0968	0.143
398.75	1	19.9	56.3	0.0570	0.238
398.75	350	23.2	51.8	0.0684	0.207
398.75	500	32.9	42.4	0.1065	0.152
401.75	1	21.8	52.4	0.0635	0.211
401.75	201	25.9	48.9	0.0783	0.189
401.75	298	29.7	44.4	0.0932	0,162
403.75	1	24.3	48.9	0.0724	0.189
405.75	1	28.6	44.4	0,0888	0,162
407.25	1	35.4	38.1	0.118	0.130

Properties of the critical solutions

$p_{\rm c}^{\rm /atm}$	T_{c} (UCST)/K	<i>x</i> 1c
1	407.25	0.123
300	402.75	0.124
346	401.75	0.127
560	398.75	0.128
700	398.15	0.128
829	396.85	0.124
993	391.85	0.128
1000	392.25	0.128
1208	386.95	0.127
1500	382.75	0.132
1512	382.05	0.131
1726	377.15	0.131
2000	372.35	0.131
2004	372.15	0.130
2156	370.15	0.129
2394	367.15	
2400	366.15	0.132

 $(dT_c/dp) \approx -(0.017 \pm 0.002)$ K atm⁻¹ $(dx_c/dT) = -(0.0002 \pm 0.00001)$ K⁻¹ 1 atm = 101.325 kPa

COMPONENTS:		ORIGINAL MEASUREMENTS:
(1) 2-Methyl-1-p:	ropanol (<i>isobutanol</i>);	Lyzlova, R.V.
с ₄ н ₁₀ 0; [78-		Zh. Prikl. Khim. (Leningrad) 1979, 52,
(2) Water; H ₂ 0;		545-50; J. App. Chem. USSR <u>1979</u> , 52, 509-14
(2) water, n ₂ °,		
VARIABLES:	0	PREPARED BY:
Temperature: 20	and 90°C	A.F.M. Barton
		<u> </u>
EXPERIMENTAL VALU	ES:	
	Mutual solubility of	2-methyl-l-propanol (1) and water (2)
Temperature	x_1	g(1)/100g sln (compiler)
t∕°c	Alcohol-rich phase Water-r	ich phase Alcohol-rich phase Water-rich pha
20	0.55 0	9.023 83.4 8.9
90		0.021 73.2 8.1
	· · · · · · · · · · · · · · · · · · ·	
	AUXILIARY	INFORMATION
METHOD / APPARATUS /	PROCEDURE :	SOURCE AND PURITY OF MATERIALS:
The applution m	ethod was used, samples	(1) CP grade
being withdrawn	from coexisting liquid phases	dried over freshly ignited K ₂ CO ₂ ;
	or analysis by refractometry. tometer measured the refract-	
ure index correc	t to 0.00002. The study	$n_{\rm D}^{20} = 1.39574; d_4^{20} = 0.8020 \text{ g cm}^{-3};$
	th phase equilibria in the -butanol/2-methyl-1-	b.p 107.8°C
propanol/water,	and only a few experiments	
systems.	l solubilities in the binary	(2) not specified
1		ESTIMATED ERROR:
		Not specified for binary systems; error below ± 1.5% for alcohol ratios in
		ternary systems.
1		REFERENCES :
1		

COMPONENTS:	ORIGINAL MEASUREMENTS:
<pre>(1) 2-Methyl-1-propanol (isobutanol); C₄H₁₀0; [78-83-1] (2) Water; H₂0; [7732-18-5]</pre>	Fu, C.F.; King, C.L.; Chang, Y.F.; Xeu, C.X. Hua Kung Hsueh Pao <u>1980</u> (3), 281-92.
VARIABLES:	PREPARED BY:
One temperature: 89.8 [°] C	C.F. Fu.

The proportion of 2-methyl-1-propanol(1) in the water-rich phase at equilibrium at 89.8° C was reported to be 7.43 g(1)/100g sln. The corresponding mole fraction solubility, x_1 , is 0.0191.

The proportion of water(2) in the alcohol-rich phase at equilibrium at 89.8° C was reported to be 25.96 g(2)/100g sln. The corresponding mole fraction solubility, x_2 , is 0.5905.

AUXILIARY	INFORMATION
METHOD/APPARATUS/PROCEDURE: The turbidimetric method was used. Homogeneous solutions were prepared and boiled at 760 mm Hg in a specially designed flask attached to a condenser of negligible hold-up compared with the volume of liquid solution. The solution was stirred by a magnetic stirrer and titrated with (1) or (2). The end point of titration was judged both by cloudiness and constancy of boiling temperature.	<pre>SOURCE AND PURITY OF MATERIALS: (Some information not in the published paper has been supplied by the compiler). (1) Riedel-DE HAEN AG reagent for chromatography; used as received; b.p. 107.8°C (760 mm Hg) n¹⁵ 1.3976, d¹⁵ 0.8055. (2) distilled. ESTIMATED ERROR: (supplied by compiler) Temperature: ± 0.02°C Solubility: 0.4% REFERENCES:</pre>

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) 2-Methyl-1-propanol (<i>isobutanol</i>)	Lutugina, N.V., Reshchetova, L.I.
$C_{4}H_{10}O;$ [78-83-1]	Vestnik Leningr. Univ. 1972, 16, 75-81
4-10-, 21-10-13	<u> </u>
(2) Water; H ₂ 0; [7732-18-5]	
VARIABLES:	PREPARED BY:
One temperature: 89.9 [°] C	C.F. Fu and G.T. Hefter
one competatule: 09:90	
EXPERIMENTAL VALUES:	
	1
The solubility of 2-methyl-l-propanol (1) in to be 0.059 mole fraction.	the water-rich phase at 69.9 C was reported
The solubility of 2-methyl-l-proponal in the	alcohol-rich phase at 89.9 ⁰ C was reported
to be 0.677 mole fraction.	
The corresponding mass solubilities calculate	d by the compilers are 20.3 g(l)/100g sln
and 89.6 g(1)/100g sln.	
AUXILIARY	INFORMATION
METHOD / APPARATUS / PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
Vapour-liquid-liquid equilibrium still described in ref l was used for liquid-	<pre>(1) Source not specified; distilled over a column of 20</pre>
liquid equilibrium determination at boiling	theoretical plates (according to
point. Immediately after cutting off heating and stopping of violent boiling,	$C_{6H_6} - CC\ell_4$;
samples were taken from both layers for	b.p. 108-0 ^o C (760 mm Hg), $n_{\rm D}^{20}$ 1.3960 $d_{\rm L}^{20}$ 0.8020
analysis. Analytical method was described in detail.	a ₄ 0.8020
	(2) distilled
1	ESTIMATED ERROR:
	Not specified
	REFERENCES :
	1. Morachevski, A.G., Smirnova, N.A.
	2h. Prinkl. Khim. 1963, 36, 2391.

COMPONENTS :	EVALUATOR:
(1) 2-Methyl-2-propanol (tert-butyl alcohol,	A.F.M. Barton, School of Mathematical and
tert-butanol); C ₄ H ₁₀ 0; [75-65-0]	Physical Sciences, Murdoch University,
(2) Water; H ₂ O; [7732-18-5]	Perth, Western Australia July 1983.

CRITICAL EVALUATION:

In the two studies (ref 1,2) reported, no region of liquid-liquid immiscibility has been observed at atmospheric pressure over the temperature range 193 K to 298 K, and at 298 K in the pressure range 0.1 - 142 MPa.

References:

- 1. Rosso, J.-C.; Carbonnel, L. C.R. Hebd. Seances Acad. Sci., Ser. C. 1968, 267, 4.
- 2. Nakagawa, M.; Inubushi, H.; Moriyoshi, T. J. Chem. Thermodyn. 1981, 13, 171.

COMPONENTS:	<u> </u>		ORIGINAL MEASUREMEN	TS:
<pre>(1) 2-Methyl-2-propanol; (tert-butanol, tert-butyl alcohol); C₄H₁₀0; [75-65-0]</pre>		Rosso, JC.; Carbonnel, L. C.R. Hebd. Seances Acad. Sci., <u>1968</u> , 267, 4-6.		
(2) Water; H ₂ (D; [7732-18-5]			
VARIABLES: Temperature: (-80) - 25 ⁰ C		PREPARED BY:		
		A.F.M. Barton		
EXPERIMENTAL V	ALUES:			
	liquid-liquid immiscibi olid dihydrate between			phase diagram is presented, te from –6 to 0.7 ⁰ C.
		t/ ^o c	g(1)/100g sln	<i>x</i> ₁
	Eutectic	- 8.2	16.60	0.0462
	Metastable eutectic	- 9.6	18	0.051
	Peritectic	- 6.0	21.20	0.0613
	Congruent melting of dihydrate	0.7	67.36	0.334
	Eutectic	- 3.3	89.10	0.665
	Melting point	25.5	100.0	1.000
	A	UXILIARY	INFORMATION	
	NS/PROCEDURE: ysis of crystallized mi arm up from -80 ⁰ C.	xtures	SOURCE AND PURITY ((1) Prolabo R.P. three succes ations; m.p. 25.5 ±	; sive fractional crystalliz-
			m.p. 23.3 ±	0.2 C
			ESTIMATED ERROR:	
			REFERENCES:	

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) 2-Methyl-2-propanol (tert-butyl alcohol,	Nakagawa, M.; Inubushi, H.; Moriyoshi, T.
tert-butanol); C4H100; [75-65-0]	J. Chem. Thermodyn. <u>1981</u> , 13, 171-8
(2) Water; H ₂ O; [7732-18-5]	
L	
VARIABLES:	PREPARED BY:
One temperature: 298.15 K	G.T. Hefter
Pressure: 0.1-142 MPa	
EXPERIMENTAL VALUES:	A
No region of liquid-liquid immiscibility was	observed over the entire pressure range
in solutions containing up to $35 g(1)/100g sl$	In. Isothermal compressibilities and
partial molar volumes of the components are g	given.
	,
	INFORMATION
METHOD /APPARATUS / PROCEDURE :	SOURCE AND PURITY OF MATERIALS: (ref 1)
Compressibility studies	(1) "best grade"; refluxed with freshly ignited calcium
	oxide and twice fractionally distilled;
	density and refractive index agreed
	with literature to within 0.00015 g cm ⁻³
	and 0.0002 respectively.
	(2) de-ionized, distilled from alkaline
	permanganate and redistilled.
	ESTIMATED ERROR:
	Temperature: control to ± 0.003 K
1	Pressure: ± 0.05%
	REFERENCES :
	1. Moriyoshi, T.; Morishita, T.; Inubushi,
	H. J. Chem. Thermodyn. <u>1977</u> , 9, 577

Four-carbon Alcohols

COMPONENTS :	EVALUATOR:			
(1) 1-Butanol (<i>n</i> -butyl alcohol); C ₄ H ₁₀ 0;	,0; G.T. Hefter, School of Mathematical and			
[71-36-3]	Physical Sciences, Murdoch University,			
		Perth, Western Australia.		
(2) Water; H ₂ 0; [7732-18-5]		ber 1982.		
	ito ven	1902 ·		
CRITICAL EVALUATION:	ł			
Solubilities in the system comprising 1-1	butanol (1)	and water (2) have	been reported	
in the following publications:				
Reference	T/K	Solubility	Method	
Reilly and Ralph (ref 1)	293	(1) in (2)	titration	
Fuhner (ref 2)	273-383	(1) in (2)	synthetic	
Drouillon (ref 3)	293-393	(1) in (2)	synthetic	
Hill and Malisoff (ref 4)	278-398	mutual	volumetric	
Jones (ref 5)	255-398	mutual	synthetic	
Mueller <i>et al</i> . (ref 6)	273-378	mutual	densimetric	
Stockhardt and Hull (ref 7)	298	(1) in (2)	gravimetric	
Butler <i>et al.</i> (ref 8)	292-304	mutual	turbidimetric	
Berkengeim (ref 9)	255-313	(2) in (1)	analytical	
Reber et al. (ref 10)	364-397	mutual	synthetic	
Othmer et al. (ref 11)	299,323	(1) in (2)	synthetic	
Booth and Everson (ref 12)	298	(1) in (2)	titration	
Hansen $et al.$ (ref 13)	298	(1) in (2)	interferometric	
Donahue et al. (ref 14)	298	mutual	analytical	
Erichsen (ref 15)	273-293	(1) in (2)	synthetic	
Erichsen (ref 16)	273-398	mutual	synthetic	
McCants <i>et al.</i> (ref 17)	311	mutual	titration	
Jones and McCants (ref 18)	311	mutual	titration	
Skrzec and Murphy (ref 19)	300	mutual	titration	
	303	(1) in (2)	turbidimetric	
Hayashi and Sasaki (ref 20)		.,		
Kakovskii (ref 21)	298	(1) in (2)	not stated	
Rao and Rao (ref 22)	300	mutual	turbidimetric	
Kinoshita et al. (ref 23)	298	(1) in (2)	surface tension	
Venkataratnam and Rao (ref 24)	303	mutual	turbidimetric	
Petriris and Geankopolis (ref 25)	298	mutual	titration	
Ababi and Popa (ref 26)	298	mutual	turbidimetric	
Smirnova and Morachevskii (ref 27)	293	mutual	densimetric	
Ratouis and Dode (ref 28)	298,303	(1) in (2)	analytical	
Meussen and Huyskens (ref 29)	298	(1) in (2)	interferometric	
Lesteva <i>et al</i> . (ref 30)	293,348	mutual	titration	
Hanssens (ref 31)	298	(1) in (2)	interferometric	
Mullens (ref 32)	298	mutual	interferometric	
Vochten and Petre (ref 33)	288	(1) in (2)	surface tension	
Korenman <i>et al</i> . (ref 34)	298	mutual	analytical	
Prochazka <i>et al</i> . (ref 35)	396-398	mutual	turbidimetric	
De Santis <i>et al</i> . (ref 36)	298	mutual	analytical	
De Santis <i>et al</i> . (ref 37)	293-313	(1) in (2)	analytical	
Lavrova and Lesteva (ref 38)	313-333	mutual	titration	
Aoki and Moriyoshi (ref 39)	303-398	mutual	refractometric	
		(continued next page	ge)	

1-Butanol

COMPONENTS:		EVALUATOR:		
(1) 1-Butanol (n-butyl alcohol); C ₄ H ₁₀ 0;		G.T. Hefter, School of Mathematical and		
[71-36-3]		Physic	al Sciences, Murdoch	University,
(2) Water; H ₂ 0; [7732-18-5]	Perth, Western Australia. November 1982.			
CRITICAL EVALUATION (continued)				
Reference	T	/K	Solubility	Method
Lyzlova (ref 40)	293,3	363	mutual	analytical
Singh and Haque (ref 41)	30	3	mutual	titration
Fu et al. (ref 42)	366		mutual	turbidimetric
Tokunaga et al. (ref 43)	288-3	308	(2) in (1)	analytical
Nishino and Nakamura (ref 44)	275-1	360	mutual	turbidimetric
Lutugina and Reshchetova (ref 47)	360	6	mutual	analytical

Apart from one other publication (ref 45), which did not contain sufficient information to justify its inclusion, all the original data are given in the data sheets following this Critical Evaluation. Solubilities in the system comprising 1-butanol-d, C_4H_9D0 , and water- d_2 , D_20 , (ref 46) are also included.

In the Critical Evaluation the data of Booth and Everson (ref 12), in volume fractions, and the data in ref 1, 7, 21, 23, 31-34, in weight/volume fractions, are excluded from further consideration as density information was not given in the original references. The data of Nishino and Nakamura (ref 44) were also excluded as only a graphical presentation was given.

The data of Drouillon (ref 3), Jones (ref 5) (water-rich phase data only), Berkengeim (9), Othmer *et al*. (ref 11), Donahue and Bartell (ref 14) (alcohol-rich phase data only) Venkataratnam and Rao (ref 24), Meeussen and Huyskens (ref 29), Lesteva *et al*. (ref 30), Lyzlova (ref 40) and Singh and Haque (ref 41), disagree markedly from all other studies and are rejected.

The following individual points in otherwise satisfactory studies are also in marked disagreement with other studies and have been rejected: in the water-rich phase 303 K (ref 16), 323 and 333 K (ref 39), in the alcohol-rich phase 353 K (ref 4). All other data are included in the tables below.

Values obtained by the Evaluator by graphical interpolation or extrapolation from the data sheets are indicated by an asterisk (*). "Best" values have been obtained by simple averaging. The uncertainty limits (σ_n) attached to these "best" values do not have statistical significance and should be regarded only as a convenient representation of the spread of the values and not as error limits. The letter (*R*) designates "recommended" data. Data are "recommended" if two or more apparently reliable studies are in reasonable ($\pm 5\%$ relative) agreement. All other data are regarded as tentative only.

		EVALUATOR:	NTS:	COMPONENTS :
and	l of Mathematical a	G.T. Hefter, School o	Butanol (<i>n-butyl alcohol);</i> C ₄ H ₁₀ O;	(1) 1-Butanol (
ty,	Murdoch University	Physical Sciences, Mu	+ 15	[71-36-3]
	tralia.	Perth, Western Austra	ter; H ₂ 0; [7732-18-5]	(2) Water: H 0:
		November 1982.		(2) water, "2",
			EVALUATION (continued)	CRITICAL EVALUAT
	he solubi <u>lity</u>	ded (R) values for the	Tentative and recommen	
		(1) in water (2)		
	.00g sln	Solubility g(l)/100g		T/K
es (±σ_)	"Best" values		Reported values	
	10.4 ± 0	28 (ref 16)	10.45 (ref 2), 10.32 (ref 15), 10	273 10.4
0.1 ()	9.6	.20 (121 10)	9.55 (ref 4)	
0.1 (R)		(ref 15). 8.83 (ref 16)	9.00 (ref 2), 8.91 (ref 4), 8.68	
v	8.2	(101 10),	8.21 (ref 4)	
		ef 8). 7.56(ref 15),	7.90 (ref 2), 7.81(ref 4), 7.72(r	
0.2 (R)	36) 7.8 ± 0	.63(ref 16), 7.8(ref 36		275
0.1 (R)	.4(ref 35) 7.4 ± (f 13), 7.3(ref 14), 26), 7.34(ref 27),7.4(7.35(ref 4), 7.31(ref 8), 7.41(re 7.4(ref 23), 7.2(ref	298 7.35
0.1 (R)		f 15), 7.01(ref 20), f 27), 7.1(ref 37), 7.0	7.10(ref 2), 7.08(ref 4), 7.06(re 6.99(re	303 7.10
	6.8		6.83 (ref 4)	308 6.83
0.1 (R)	, 6.6(ref 38) 6.6 ± 0		6.55 (ref 2), 6.60(ref 4), 6.72(r	313 6.55
0.2	.38(ref 16) 6.4 ± 0	11), 6.55(ref 15),6.38	6.35(ref 2), 6.46(ref 4), 6.1(ref	323 6.35
0.1 (R)	5(ref 38) 6.5 ± 0	6),6.52(ref 15),6.45(r	6.35(ref 2), 6.52(ref 4),6.52(ref	333 6.35
0.1 (R)	9) 6.7 ± 0	(ref 15), 6.7 [*] (ref 39)	6.55 (ref 2), 6.73 (ref 4), 6.67	343 6.55
0.1 (R)			6.8 (ref 6), 6.9 [*] (ref 39)	
0.1 (R)	.1 [*] (ref 39) 7.0 ± 0		7.00(ref 2), 6.89(ref 4), 6.90(re	
0.1 (R)			7.2 [*] (ref 4), 7.5 [*] (ref 35), 7.2 [*] (r	
0.2 (R)	(ref 35), (ref 39) 7.7 ± 0	7.5 (re	7.80(ref 2), 7.6 [*] (ref 4),7.8(ref	
0.1 (R)		ef 39)	8.3 [*] (ref 4), 8.4 [*] (ref 35), 8.2 [*] (r	368 8.3*
0.1 (R)	39) 9.1 ± (f 10), 8.82(ref 15), (ref 35), 9.2 (ref 39)	9.05(ref 2), 9.2 [*] (ref 4), 9.1 [*] (re 9.1	373 9.05
0.2 (R)		ef 10), 9.9 [*] (ref 35), 10.2 [°] (ref 39	10.3 [*] (ref 4), 9.8(ref 6), 10.0 [*] (r	378 10.3
0.2 (R)	15), 39) 11.1 ± ((ref 10), 11.05(ref 15) 1 (ref 35), 11.0(ref 39	10.90(ref 2), 11.5 [*] (ref 4), 11.3 [*] 11.	383 10.9
0.2 (R)			12.8 [*] (ref 4), 13.2 [*] (ref 10), 13.1	388 12.8
	39) 11.1 ± 0	1 (ref 35), 11.0(ref 39		

CONTRAVEN			
COMPONEN	ns: Butanol (<i>n-butyl alcohol);</i> C ₄ H ₁₀ 0;	EVALUATOR: G.T. Hefter, School of Mathem	matical and
1	[-36-3]	Physical Sciences, Murdoch U	
		Perth, Western Australia.	liverbicy,
(2) Wat	cer; H ₂ 0; [7732-18-5]	November 1982.	
		November 1982.	
CRITICAL	. EVALUATION (continued)		
		nded (R) values for the solubi	lity
	of water (2)	in 1-butanol (1)	
Τ/К		Solubility g(2)/100g s	
	Reported values	ויי	Best values (± σ_n)
258	19.0 (ref 5)		19.0
268	19.18 (ref 5)		19.2
273	19.4 (ref 5), 18.95 (ref 15)		19.7 ± 0.3 (R)
278	19.62 (ref 4)		19.6
283	19.67 (ref 4), 19.5 (ref 15)		19.6 ± 0.1 (_R)
288	19.86 (ref 4), 19.9 (ref 43)		19.9
293	20.07(ref 4),19.8(ref 5),20.08(ref 8),20.0(ref 15),20.1(ref 27), 20.0(ref 37),20.1(ref 43)	20.0 ± 0.1 (R)
298	20.07(ref 4),20.36(ref 8), 20.7 [*] (ref	25),19.9 [*] (ref 26), 20.49 [*] (ref 36),20.4(ref 43)	20.3 ± 0.3 (R)
303	20.62(ref 4),20.68 [*] (ref 8),20.63(ref	15),20.6 (ref 37)	20.6 ± 0.1 (R)
308	21.06 (ref 4), 21.1 (ref 43)		21.1 (<i>R</i>)
313	21.41(ref 4),21.4(ref 5),21.40(ref 1	5),21.4(ref 37),21.5(ref 38)	21.4 ± 0.1 (R)
323	22.42 (ref 4), 22.41 (ref 15), 22.4*	(ref 39)	22.4 (<i>R</i>)
328	23.2 [*] (ref 39)		23.2
333	23.62(ref 4),23.8(ref 5),23.71(ref 1	5),23.69(ref 38),23.9 [*] (ref 39)	23.7 ± 0.1 (R)
338	24.5 [*] (ref 39)		24.5
343	25.21 (ref 4), 25.43 (ref 15), 25.1*	(ref 39)	25.2 ± 0.1 (R)
348	26.3 (ref 6), 26.4 (ref 39)		26.3 ± 0.1 (R)
353	27.3 (ref 5), 27.60 (ref 15), 27.7 [*] (27.5 ± 0.2 (R)
358	28.3 [*] (ref 4), 29.1 [*] (ref 35), 29.1 [*] (r		28.8 ± 0.4 (R)
363	30.1 [*] (ref 4),30.2(ref 6),30.7 [*] (ref 1	0),30.10(ref 15),30.2 [*] (ref 35) 30.5 (ref 39)	30.3 ± 0.2 (R)
368	32.0 [*] (ref 4), 32.3 [*] (ref 10), 31.9 [*] (ref		32.0 ± 0.2 (<i>R</i>)
373	33.9 [*] (ref 4), 33.6(ref 5), 34.2 [*] (ref		0110 012 ()
1		34.0 (ref 35)	33.8 ± 0.3 (R)
378	35.8 [*] (ref 4), 35.7 (ref 6), 36.6 [*] (ref		36.1 ± 0.4 (R)
383		39.4 (ref 35),38.3*(ref 39)	38.6 ± 0.5 (R)
388	42 [*] (ref 4), 42.9 [*] (ref 10), 43.0 [*] (ref		42.5 ± 0.5 (R)
393	47 [*] (ref 4), 47.5(ref 5), 48.5 [*] (ref 1)	0), 46.65(ref 15), 48.5 [*] (ref 35),46.3 (ref 39)	47.4 ± 0.9 (R)

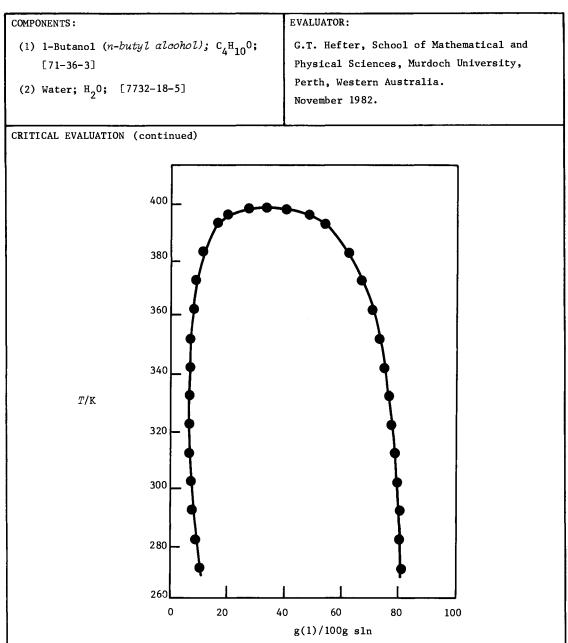


Figure 1. Mutual solubility of (1) and (2)

The "best" values from the above tables are plotted in Figure 1. The "best" values are in general in excellent agreement with the single most extensive determination (ref 4). Aoki and Moriyoshi (ref 39) have also determined mutual solubilities of (1) and (2) and the upper critical solution temperature at pressures of 200-2500 atm (20 - 250 MPa).

Excluding those data (ref 3,5) already rejected, the upper critical solution temperature has been reported as 397.55 (ref 10), 397.85 (ref 39), 398.30 (ref 4), and 398.5 K (ref 15). The corresponding critical solution compositions have been reported as 32.96 g(1)/100g sln (ref 10), $x_1 = 0.110$ (ref 39) and 32.5 g(1)/100g sln (ref 4).

1	-8	lut	an	ol
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COMPON	IENTS :	EVALUATOR:		
[1-Butanol (<i>n-butyl alcohol);</i> C ₄ H ₁₀ 0; [71-36-3] Water; H ₂ 0: [7732-18-5]	G.T. Hefter, School of Mathematical and Physical Sciences, Murdoch University, Perth, Western Australia. November 1982.		
CRITIC	CAL EVALUATION			
Refe	rences			
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0000	NICHIMO -			
	DNENTS:	EVALUATOR:		
(1)	1-Butanol (<i>n</i> -butyl alcohol); C_4H_{10} ;	G.T. Hefter, School of Mathematical and		
	[71-36-3]	Physical Sciences, Murdoch University,		
(2)	Water; H ₂ 0: [7732-18-5]	Perth, Western Australia.		
	2	November 1982.		
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20	Alli V. Manimali T. I. Cham. Theorem	a - b = a - 10 10 1173		
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43.	• • • • • • •	hama Kogyo Koto Semmon Gakko Kiyo, Rikogaku		
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COMPONENTS:	ORIGINAL MEASUREMENTS:
<pre>(1) 1-Butanol; C₄H₁₀0; [71-36-3] (2) Water; H₂0; [7732-18-5]</pre>	Reilly, J.; Ralph, E.W. Sci. Proc. Roy. Dublin Soc. <u>1919</u> , 15, 597-608
VARIABLES: One temperature: 20 [°] C	PREPARED BY: S.H. Yalkowsky; S.C. Valvani, A.F.M. Barton

The proportion of 1-butanol in the water-rich phase at 20° C was reported to be 79 g(1)/L sln.

The corresponding amount of substance concentration calculated by the compiler is 1.07 mol(1)/L sln.

AUXILIARY	INFORMATION
METHOD/APPARATUS/PROCEDURE: The behavior of three component 1-butanol/ water/acetone systems was investigated. A mixture containing a slight excess of n-butanol over saturation was taken in a long-necked 50 mL flask fitted with a buret having a long-delivery tube reaching almost to the level of the liquid. The flask was immersed in a thermostat bath (20 ± 0.005°C) and acetone run in drop by drop with frequent shaking until the cloudy mixture just became clear on standing. From the increased weight the relative proportions of the components	
	ESTIMATED ERROR: Not stated
	REFERENCES:

COMPONENTS:		ORIGINAL MEASUREMENTS:
(1) 1-Butanol; C ₄ H ₁₀ 0; [71	-36-3]	Fühner, H.
(2) Water; H ₂ 0; [7732-18-5		Ber. Dtsch. Chem. Ges. <u>1924</u> , 57, 510-5.
VARIABLES:		PREPARED BY:
Temperature: 0-110 ⁰ C		A. Maczynski; Z. Maczynska; Z. Szafranski
EXPERIMENTAL VALUES:		
So	lubility of 1-1	outanol (1) in water (2)
t/°c	g(1)100g slr	x_1 (compiler)
0	10.45	0.0275
10	9.00	0.0235
20	7.90	0.0204
30	7.10	0.0182
40	6.55	0.0167
50	6.35	0.0162
60	6.35	0.0162
70	6.55	0.0167
80	7.00	0.0180
90	7.80	0.0201
100	9.05	0.0236
110	10,90	0.0289
	AUXILIARY	INFORMATION
METHOD / APPARATUS / PROCEDURE :		SOURCE AND PURITY OF MATERIALS:
Rothmund's synthetic method (r used. Small amounts of (1) and (2) w		<pre>(1) source not specified; specially purified but no details provided.</pre>
a glass tube and heated with s oil bath to complete dissoluti solution was cooled until a mi appeared and this temperature as the equilibrium temperature	shaking in an Lon. The Llky turbidity was adopted	(2) not specified.
		ESTIMATED ERROR:
		Not specified.
		REFERENCES:
		1. Rothmund, V. Z. Phys. Chem. <u>1898</u> , 26, 433.

COMPONENTS:			ORIGINAL MEASUREMENTS:		
(1) 1-Butanol; C ₄ H ₁₀ 0; [71-36-3]		Drouillon, F.			
• =-		J. Chim. Phys. <u>1925</u> , 22, 149-68.			
(2) Water; H ₂ 0; [7732-18-5]		<i>b</i> . <i>Onum</i> . <i>Ingb</i> . <u>1725</u> , <i>ab</i> ,	117 001		
	2				
VARIABLES			PREPARED BY:		
Temperat	ture: 20-120 ⁰ C		S.C. Valvani; S.H. Yalkov	wsky; A.F.M. Barton	
EXPERIMEN	VTAL VALUES:			2)	
	Mutua	l solubility of	1-butanol (1) and water (2)	
t/°c	g(1)/100g	sln	$x_1(\text{compine})$	ler)	
	Alcohol-rich phase	Water-rich pha	ase Alcohol-rich phase	Water-rich phase	
20.0 ^a	81.6	6.6	0.519	0.169	
20.0		6.5	-	0.0166	
23.0	81.9	-	0.524	_	
23.5	-	6.5	_	0.0166	
32.5	_	6.2	-	0.0158	
38.5	_	6.0	-	0.0153	
40.0 ^a	80.3	6.0	0.498	0.0153	
45.0	-	5.7	-	0.0145	
54.5	78.9	-	0.476	-	
57.0	-	5.5	_	0.0140	
60.0 ^a	78.2	5.5	0.466	0.0140	
60.5	78.2	-	0.466	-	
67.0	-	5.7	-	0.0145	
71.0	-	6.0	_	0.0153	
72.0	76.3	_	0.439	-	
· · · · · · · · · · · · · · · · · · ·			(contin	ued next page)	
		AUXILIARY	INFORMATION		
ME THOD /A	PPARATUS/PROCEDURE:		SOURCE AND PURITY OF MATE	RIALS:	
The beh	avior of three-compone	nt 1-butano1/	Not stated.		
	thanol system was inve s of known composition				
	tubes to complete solu				
	er, then cooled slowly loudiness appeared.				
	xtures, where a closed urs, observations were				
	and cooling.	made on both			
			ESTIMATED ERROR:		
		Solubility: about 2%			
		Temperature: ± 0.5 [°] C			
		REFERENCES :			

41

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) 1-Butanol; C ₄ H ₁₀ 0; [71-36-3]	Drouillon, F.
(2) Water; H ₂ O; [7732-18-5]	J. Chim. Phys. <u>1925</u> , 22, 149–68.

EXPERIMENTAL VALUES (continued)

t/°c	g(1)/100g sln		$x_1(\text{compiler})$		
	Alcohol-rich phase	Water-rich phase	Alcohol-rich phase	Water-rich phase	
76.0	-	6.2	-	0.0158	
80.0 ^a	74.6	6.4	0.417	0.0164	
81.5	-	6.5	-	0.0166	
88.0	72.4	-	0.390	-	
90.5	-	6.5	-	0.0166	
94.0	-	7.2	-	0.0185	
97.0	69.9	-	0.361	-	
100.0 ^a	68.8	7.5	0.349	0.0196	
102.0	-	7.6	-	0.0196	
105.5	-	8.4	-	0.0218	
107.5	66.3	-	0.324	-	
119.5	57.8	11.5	0.250	0.0306	
120.0 ^a	57.3	11.8	0.246	0.0315	
124.5	53.2	-	0.216	-	
125.0	50.8	-	0.200	-	
126.5	-	16.4	-	0.0455	
127.0	45.8	-	0.171	-	
128.0	-	18.6	-	0.0526	
128.5	39.6	-	0.137	-	
 129.0	34.0	22.5	0.111	0.0659	
129.5	30.1	28.0	0.095	0.0864	

^a interpolated

The critical point was reported as 129.5°C, at 25 g(1)/100g sln ($x_1 \approx 0.086$)

COMPONE	ENTS:			ORIGI	NAL MEASUREMEN	ITS:	
(1) 1-	-Butanol; C ₄ H ₁₀ O	; [71-36-3]		Hill, A.E.; Malisoff, W.M.			
	4 10			J. Am. Chem. Soc. 1926, 48, 918-27.			
(2) Wa	ater; H ₂ 0; [7732	-18-5]		0. 11		<u></u> ,,,	
				ļ			
VARIABLES:			PREPARED BY:				
Tempei	rature: 5-125°C]		A.F.1	1. Barton		
FXPFRT	MENTAL VALUES:	<u> </u>					
DA DAL		Mutual Solub:	ility of 1-b	utanol	(1) and water	(2)	
t∕°c	Alco	hol -ri ch pha	SA		Wat	er-rich phas	e
07 0		x_{1}		-3			density/g cm ⁻³
	g(1)/100g sln	(compiler)	density/g (em j	g(1)/100g sin		
5.0	80.38	0.499	0.8598		9.55	0.0250	0.9883
10.0	80.33	0.498	0.8567		8.91	0.0232	0.9877
15.0	80.14	0.495	0.8533		8.21	0.0213	0.9881
20.0	79.93	0.492	0.8484		7.81	0.0202	0.9873
25.0	79.73	0.489	0.8450		7.35	0.0189	0.9865
30.0	79.38	0.484	0.8424		7.08	0.0182	0.9851
35.0	78.94	0.477	0.8397		6.83	0.0175	0.9835
40.0	78.59	0.472	0.8345		6.60	0.0169	0.9841
50.0	77.58	0.457	0.8307		6.46	0.0165	0.9799
60.0	76.38	0.440	0.8253		6.52	0.0166	0.9766
70.0	74.79	0.419	0.8200		6.73	0.0172	0.9721
80.0	73.53	0.403	0.8159		6.89	0.0177	0.9675
92.0 97.9	69.24 -	0.354	-		8.74	0.0227	-
106.1	63.88	0.300	_		-	-	-
						(continue	ed next page)
			AUXILIARY	INFOR	MATION		
METHOD	APPARATUS/PROC	EDURE:		SOUR	CE AND PURITY	OF MATERIALS	:
The v	olumetric method	d previously	described	(1)	Eastman Koda	k Co.;	
	 was used, by wo phases which 	-		f	refluxed wit repeatedly f	<i>c</i>	
	nents are combin				still head;		with J-bdib
	en 5 ⁰ C and 40 [°] C				b.p. 117.70-	117.80°C.	
metho	d, with total vo	olumes of 40	0 mL and a	(2)	not stated		
	of 3:1; those 50 mL and a volu			}			
The r	emainder of the	results are	by the				
Alexe	jeff plethostat:	ic method (r	ef 2).				
				ESTI	MATED ERROR:		
				Not	stated		
				REFE	RENCES :		
				1.	Hill, A.E.	J. Am. Chom	. Soc. 1923,
					<i>45</i> , 1143.	S. INIL OILEIN	<u>1723</u> ,
				2.	Alexejeff, W	. Wied. Ann	. <u>1886</u> , <i>28</i> , 305
L				1			

COMPONENTS:			OR	ORIGINAL MEASUREMENTS;			
(1) 1-Butanol; C ₄ H ₁₀ 0; [71-36-3]) F	Hill, A.E.; Malisoff, W.M.			
(2) Water; H ₂ 0; [7732-18-5]				J. Am. Chem. Soc. <u>1926</u> , 48, 918-27.			
EXPERI	MENTAL VALUES	(continued)					
.0			bility of l-buta				
t∕°C	Alc	ohol-rich pha	se	Water-rich phase			
	g(1)/100g s1m	(compiler)	density/g cm^{-3}	g(1)/100g sln	x ₁ (compiler)	density/g cm ⁻³	
114.5	-	-	-	12.73	0.0343	-	
116.9	-	-	-	13.46	0.0364	-	
100 0	10.05						
122.3	49.85	0.195	-	-	-	-	
122.3		0.195	-	- 19.73	- 0.0564	-	
	-	-	- -		- 0.0564 	-	
123.3	42.02	-	- - -		- 0.0564 - 0.0835		
123.3 124.33	42.02	-		19.73 -	- 0.0835		

The two-liquid system was found to range from the quadruple point (-2.95°C) to 125.15°C, the consolute solution is 32.5 g(1)/100g sln ($x_1 = 0.1048$).

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) 1-Butanol; C ₄ H ₁₀ 0; [71-36-3]	Jones, D.C.
(2) Water; H ₂ 0; [7732-18-5]	J. Chem. Soc. <u>1929</u> , 799-813.
VARIABLES:	PREPARED BY:
Temperature: -15 [°] C - 125 [°] C	S.H. Yalkowsky; S.C. Valvani; A.F.M. Barton

	Mutual solubility of 1-butanol (1) and water (2)				
t/°c	Alcohol-r	ich phase	Water-rich	phase	
	g(1)/100g sln	x_1 (compiler)	g(1)/100g sln	x_1 (compiler)	
-18.01^{d}	-	-	12.72	0.0342	
-15.0^{2}	81.0	0.509	12.0	0.0321	
-5.0^{k}	80.82	0.506	-	-	
- 3.11	-	-	9.79	0.0257	
0.0 ²	80.6	0.503	9.1	0.0238	
13.0	80.46	0.500	-	-	
19.3 ^b	81.0	0.509	-	-	
20.0 ²	80.2	0.496	6.4	0.0164	
29.82 ^k	79.51	0.486	-	-	
40.0 ^{<i>a</i>}	-	-	6.03	0.0154	
40.0 ²	78.6	0.472	6.0	0.0153	
58.50^{d}	76.27	0.439	-	-	
60.0 ²	76.2	0.437	6.0	0.0153	
65.0 ^a	-	_	6.03	0.0154	
80.0 ²	72.7	0.393	6.4 (continued ne	0.0164 xt page)	
	A	JXILIARY INFORMATION		1-0-7	
METHOD/APPARATUS	/PROCEDURE:	SOURCE AND	PURITY OF MATERIALS	:	

METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
The synthetic method described by Jones and Betts (ref 2) was used. Well-steamed Pyrex glass gave consistent results identical with those in quartz glass tubes (soda glass did not give reproducible results). The thermometer was tested at the National Physical Laboratory.	 prepared as in ref 1; dried with calcium oxide, fraction- ated (the several fractions giving identical C.S.T.'s with a hydrochloric acid soln); d^{14.4} = 0.81417, n²⁰_D = 1.39711. conductivity water from Bousfield still freshly boiled.
	ESTIMATED ERROR:
	Temperature: given in footnote to experimental values; most accurate to 0.02°C.
	REFERENCES:
	1. Orton, K.J.P.; Jones, D.C. J. Chem.
	Soc. <u>1919</u> , 115, 1194.
	2. Jones, D.C.; Betts, H.F. J. Chem.
	Soc. <u>1928</u> , 1179.

COMPONENTS :		ORIGINAL N	IEASUREMENTS :	
(1) l-Butanol;	C ₄ H ₁₀ 0; [71-36-3]	Jones, D.		
			Soc. <u>1929</u> , 799-81	3.
(2) Water; H ₂ (J; [//32-18-5]		,	
EXPERIMENTAL VAL	LUES (continued)	<u> </u>	<u></u>	
	····· (
	Mutual :	solubility of 1-buta	anol (1) and water	(2)
t∕°C	Alcohol-r:	ich phase	Water-rich	n phase
	g(1)/100g sln	<pre>x (compiler)</pre>	g(1)/100g sln	<pre>x (compiler)</pre>
81.0 ^b	_		6.47	0.0166
100.0 ^Z	66.4	0.325	8.2	0.0213
106.05 ^d	63.44	0.326	-	-
107.72 [°]	_	_	9.79	0.0257
110.0 ^Z	61.5	0.279	10.2	0.0269
115.00 ^d	57.8	0.250		_
117.40^d	-	-	12.72	0.0342
120.0 ^Z	52.5	0.212	14.7	0.0402
120.30 ^e	_	_	15.15	0.0416
122.45^d	_	_	17.51	0.0490
122.60 ^d	48.01	0.183	-	-
123.0 ^Z	46.8	0.176	19.0	0.0539
123.75 ^d	44.03	0.160	-	-
123.75 124.05 ^{<i>d</i>, <i>j</i>}	41.30	0.146		-
124.66 ^{<i>d</i>, <i>f</i>}	38.05	0.130		_
124.00 124.72 ^{<i>d</i>,<i>e</i>}	33.79	0.110	_	_
124.73 ^{<i>d</i>,g}	30.39	0.0960		-
124.74 ^{<i>d</i>} , <i>h</i>	32.49	0.105	_	
124.74 ^{<i>d</i>} , <i>f</i>	28.16	0.0870		_
124.74 ^d	27.88	0.0858	_	-
124.75 ^{<i>d</i>} , <i>i</i>	32.85	0.106	_	_
124.75 ^Z	32.4	0.1043	32.4	0.1043
a	K; slightly cloudy b	etween these temper		
Accuracy ±2 b Accuracy ±2		between these temper	atures.	
	erature, 107.72 ⁰ C; fa	$111 mg 107 60^{0} c$		
	-			
those list	accurate to 0.02 K; s of accuracy.	rising and falling	temperatures ident	ical within
	ter 3 months.			
f Slight original	fcal opalescences; s	triations -1 · · ·		
^g Lower layer	very large	LIIALIONS AIMOST Ab	sent.	
h Foual volum	es; clearest critica	1 phonemone		
i Upper lave	es; clearest critica greater than lower;	sucrete or or other	1.1.	
j Dotorminati	Breater than lower;	quartz experimenta	⊥ tube.	c .
heating to	ons made at intervals	up to 8 days; no	cnange observed ev	en after
		(hotmos	6-114	
Interpolate	1 K; difference of 1 H	verween rising and	Ialling temperatu:	res.
interpolate	u.			

			I-bu	lanoi			4
COMPONEI	NTS:			ORIGI	NAL MEASUREME	ENTS:	
(1) 1-	Butanol; C,H,	LO ^{0; [71-36-3]}		Muel	Mueller, A.J.; Pugsley, L.I.; Ferguson, J.B.		
(2) Water; H ₂ 0; [7732-18-5]			J. I	Phys. Chem. <u>1</u>	<u>931</u> , <i>35</i> , 1314	-27.	
VARIABL	PC .			DDDD			
				PREPA	ARED BY:		
Temperature: 0-105 [°] C			S.H	. Yalkowsky;	S.C. Valvani	; A.F.M. Barton	
EXPERIM	ENTAL VALUES:						
		Mutual so	olubility of	1-but	anol (1) and	water (2)	
t∕°c	Alco	ohol-rich phase	e		W	ater-rich pha	ise
	g(1)100g slu	x ₁ n (compiler)	density/g c	m ⁻³	g(1)100g sln	x ₁ (compiler)	density/g cm ⁻³
0 ^{<i>a</i>}	80.38	0.499			9.55	0.0251	
15 ^{<i>a</i>}	80.2	0.496	0.853		8.30	0.0216	0.988
30 ^{<i>a</i>}	79.4	0.484	0.842		7.08	0.0182	0.985
45 ^{<i>a</i>}	78.2	0.466	0.833		6.50	0.0166	0.982
60 ^{<i>a</i>}	76.4	0.440	0.825		6.52	0.0167	0.977
75	73.7	0.406			6.8	0.0174	
90	69.8	0.360			7.8	0.0202	
105	64.3	0.305			9.8	0.0257	
	-	interpolated f		nd des	cribed by the	e authors as	being in good
			AUXILIARY	INFOR	RMATION		
METHOD	/APPARATUS/PR	OCEDURE:		SOUR	CE AND PURITY	OF MATERIAL	S:
These data are from a study of the ternary l butanol/methanol/water system. Values for the binary system were determined by extra- polation of ternary binodal curves to zero methanol, giving results largely in agree- ment with those of ref 1.			(1)	b.p. 117.6 ⁰	etone Co. (19 th lime, dist C, d_4^{20} 0.80	illed;	
At 0° C the amount of one component necessary to give rise to heterogeneity was found by weighing. Between 15°C and 60°C a sample was held in a calibrated Pyrex tube and the volume of the final homogeneous solution			7				
obtained from cathetometer readings. The densities of these solutions were calculated from the volumes and weights. The volumes of the two phases present in the sample selected for the detn of a tie line were found in a similar manner. The tie lines			Ter ±0. Sol ±0.	MATED ERROR: nperature: ±0 ,2°C (100°C); Lubility ±0.3 .5 wt% above	±0.3°C (12) wt% below 6	D_C).	
two p At 75	hases being s	lirectly detern separated and v samples were se ation.	veighed.	1	ERENCES: H111, A.E.; J. Am. Chem.	Malisoff, W. . <i>Soc</i> . <u>1926</u> , -	

COMPONENTS:	ORIGINAL MEASUREMENTS:
	Stockhardt, J.S.; Hull, C.M.
(1) i-Butanol; C ₄ H ₁₀ 0; [71-36-3]	Ind. Eng. Chem. 1931, 23, 1438-1440
(2) Water; H ₂ 0; [7732-18-5]	114. Ling. origin. <u>1991</u> , 20, 1130 1110
VARIABLES:	PREPARED BY:
One temperature: 25 ⁰ C	S.H. Yalkowsky; S.C. Valvani; A.F.M. Barton
EXPERIMENTAL VALUES:	
The proportion of 1-butanol in the water-rich	
7.45 g(1)/100 cm ⁻³ sln corresponding to 1.01	mol (1)/L sln.
AUXILIARY	INFORMATION
METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
The method of ref 1 was used, except that the	
determinations were wholly gravimetric.	column at 4:1 reflux:
	b.p. 117.3-117.5°C, d_4^{20} 0.8097
	ESTIMATED ERROR:
	Not stated
	REFERENCES :
	1. Hill, A.E.; Malisoff, W.M. J. Am. Chem. Soc. <u>1926</u> , 48, 918.
1	L

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) 1-Butanol; C ₄ H ₁₀ O; [71-36-3]	Butler, J.A.V.; Thomson, D.W.; Maclennan W.H.
(2) Water; H ₂ 0; [7732-18-5]	J. Chem. Soc. <u>1933</u> , 674–86.
VARIABLES:	PREPARED BY:
Temperature: 18-31 ⁰ C	S.H. Yalkowsky; S.C. Valvani; A.F.M. Barton
EXPERIMENTAL VALUES:	

Mutual solubility of 1-butanol(1) and water(2)				
t∕°C	Alcohol-ri	ch phase	Water-ric	ch phase
	(1)/100g sln	$x_1(\text{compiler})$	g(1)/100g sln	x ₁ (compiler)
18.45	80.01	0.493	-	-
22.60	-	-	7.497	0.0193
23.40	79.73	0.489	-	-
23.70	-	-	7.407	0.0191
24.85	-	-	7.318	0.0188
25.00	79.64	0.488	7.31	0.0188
26.40	-	_	7.202	0.0185
27.45	79.50	0.486	-	-
28.06	-	-	7.090	0.0182
29.18	-	-	7.016	0.0180
30.83	79.28	0.482	~	-
METHOD/APPARATUS/PROCEDURE: The method of ref 1 was used. Solutions of suitable composition by weight were placed in a soda-glass flask fitted with a thermo- meter. The flask was constantly shaken in a slowly-heated water bath, and the temper- ature of onset of cloudiness was noted. Disappearance of cloudiness was also studied. The determinations were repeated in Pyrex- glass flasks, but no difference was observed.			fractionated; the whole dis 775.3 mm Hg; middle fracti used d_4^{25} 0. (2) not stated.	0 for a week, refluxed 8 h,
			ESTIMATED ERROR:	
			Temperature: repe 0.05	ated observations within 0°C
			REFERENCES:	
				<pre>'.; Pickford, P.; J. Chem. Soc. <u>1911</u>, 99,</pre>

COMPONENTS :	ORIGINAL MEASUREMENTS:	
(1) l-Butanol; C ₄ H ₁₀ 0; [71-36-3]	Berkengeim, T.I.	
(2) Water; H ₂ O; [7732-18-5]	Zavod. Lab. <u>1941</u> , 10, 952–4.	
2		
VARIABLES:	PREPARED BY:	
Temperature: (-18)-40 [°] C	A. Maczynski	
EXPERIMENTAL VALUES:		
	f water (2) in 1-butanol (1)	
t/ ^o C g(2)/10	Og sln ω_2 (compiler)	
-18 2.8	0 0.106	
- 7 12.5	0.370	
20 23.1	0.553	
40 26.4	0.596	
AUXILIARY INFORMATION		
METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:	
The analytical method was used.	 CP reagent, source not specified; used as received; 	
The solubility of (2) in (1) was determine by the Karl Fischer reagent method.	ned b.p. range 116.5-117 [°] C.	
	(2) not specified.	
	ESTIMATED ERROR:	
	Not specified.	
	REFERENCES:	
L		

COMPONENTS:			ORIGINAL MEASUREMENTS:	
(1) 1-Butanol; C ₄ H ₁₀ 0; [71-36-3] (2) Water; H ₂ 0; [7732-18-5]		Reber, L.A.; McNabb, W.M.; Lucasse, W.A.		
		J. Phys. Chem. <u>1942</u> , 46, 500–15.		
VARIABLES:			PREPARED BY:	
Temperature	: 91-125 [°] C		A.F.M. Barton	
Added sodiu	m salts			
EXPERIMENTAL	VALUES:			
	Muta	ual solubil:	ity of 1-butanol (1) and water (2)	
	Alcohol-	rich phase	Water-rich phase	
t∕°c	g(1)/100g sln	x_1 (comp	iler) g(1)/100g sln x_1 (com	npiler)
91.15	69.01	0.3513		-
98.35	-	-	8.89 0.0	0232
99.45	66.07	0.3213		-
103.50	64.22	0.3038		-
104.35	-	-	9.86 0.0	0259

AUXILIARY INFORMATION

12.30

15.03

16.99

21.12

-

-

-

0.2690

0.2440

0.2107

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0.1885

0.1625

110.90

112.95

115.15

118.25

119.40

120.75

121.60

123.20

123.60

60.21

_

57.03

52.33

_

48.86

44.39

_

METHOD /APPARATUS / PROCEDURE : SOURCE AND PURITY OF MATERIALS: The "synthetic" method was used. (1) Eastman Kodak Co. "best grade" 5 mL purified according to ref 1 ampoules were boiled with hydrochloric acid, (refluxed with lime 4 h, Mg and iodine washed, steamed and dried. (1) was added by hypodermic syringe, (2) by microburet, weighed, and sealed. The ampoules were for 4 h, distilled in 15 bulb Snyder column); ^{column}); b.p. 117.55 $\pm 0.05^{\circ}$ C (corrected). $n_{\rm D}^{25}$ 1.3974, d_4^{25} 0.8058, rotated in an oil bath, the temperature by NBS-tested thermometer being read to ±0.05°C. In mixtures with 50-80% water, negative iodoform test. temperatures of appearance and disappearance of a second phase were essentially the same. (2) distilled water, redistilled from Beyond these limits the clouding temperature was 0.1-0.5°C below the clearing temperature; alkaline potassium permanganate in Pyrex glass. the former were more precise and were reported. Results were also reported in ESTIMATED ERROR: Composition: within 0.01 wt % the presence of sodium nitrate, halides, sulfate and thiocyanate. Temperature: $\pm 0.05^{\circ}C$ **REFERENCES**: 1. Lund, H.; Bjerrum, J. Ber. 1931, 64B, 210.

0.0330

0.0412

0.0474

0.0611

0.0650

(continued next page)

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      COMPONENTS:
      EVALUATOR:

      (1) 1-Butanol; C<sub>4</sub>H<sub>10</sub>0; [71-36-3]
      Reber, L.A.; McNabb, W.M.; Lucasse, W.A.

      (2) Water; H<sub>2</sub>0; [7732-18-5]
      J. Phys. Chem. <u>1942</u>, 46, 500-15.
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EXPERIMENTAL VALUES (continued)

Mutual solubility of 1-butanol (1) and water (2)

Alcohol-rich phase		Water-rich phase	
t∕°c	g(1)/100g sln	x_1 (compiler)	$g(1)/100g \ sln \qquad x_1 \ (compiler)$
124.10	39.62	0.1376	
124.20	-	-	24.34 0.0725
124.30	36.83	0.1242	
124.35	-	-	31.81 0.1019
124.40	-	-	30.52 0.0965
124.40	-	-	32.96 0.1068

The critical solution temperature was reported as 124.40° C.

The addition of all salts led to an increase in temperature of complete miscibility, and this effect was more marked the lower the proportion of water and the greater the salt concentration. 1-Butanol

(2) Water;		COMPONENTS:		ORIGINAL MEASUREMENTS:		
APTABLES .	(1) 1-Butanol; C ₄ H ₁₀ 0; [71-36-3] (2) Water; H ₂ 0; [7732-13-5]		Othmer, D.F.; Bergen, W.S.; Shlechter, N.; Bruins, P.F. Ind. Eng. Chem. <u>1945</u> , 37, 890-4.			
VARIABLES: Temperature: 26 and 50 ⁰ C		PREPARED BY: A. Maczynski				
XPERIMENTAL	VALUES:					
		al solubility of	1-butanol (1) and w	ater (2)		
$t/^{\circ}$ C g(1)/100g sln		x_1 (compi				
			(2)-rich phase			
26	6.5	80.2	0.017	0.496		
50	6.1	79	0.015	0.48		
		AUXILIARY	INFORMATION			
	ATUS/PROCEDURE: t or synthetic me were reported in	thod (ref 1,2)	SOURCE AND PURITY ((1) commercial ma			
No details		the paper.	carefully fra	ctionated; C, purity not specified.		

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) 1-Butanol; C ₄ H ₁₀ 0; [71-36-3]	Booth, H.S.; Everson, H.E.
(2) Water; H ₂ 0; [7732-18-5]	Ind. Eng. Chem. <u>1948</u> , 40, 1491-3.
VARIABLES:	PREPARED BY:
One temperature: 25 ⁰ C Sodium xylene sulfonate	S.H. Yalkowsky; S.C. Valvani; A.F.M. Barton
EXPERIMENTAL VALUES:	
It was reported that the solubility of 1-but	anol in water was 9.1 mL(1)/100 mL(2) at 25° C.
The corresponding figure in 40% sodium xylend > 400 mL(1)/100 mL solvent.	
AUXILIARY	INFORMATION
METHOD/APPARATUS/PROCEDURE: A known volume of solvent (usually 50 mL) in a tightly stoppered calibrated Babcock tube was thermostatted. Successive measured quantities of solute were added and equilibrated until a slight excess of solute remained. The solution was centrifuged, returned to the thermostat bath for 10 min, and the volume of excess solute measured directly. This was a modification of the method described in ref 1.	SOURCE AND PURITY OF MATERIALS: (1) "CP or highest grade commercial" (2) distilled.
	ESTIMATED ERROR: Solubility within 0.1 mL/100 mL. REFERENCES: 1. Hanslick, R.S. Dissertation, Columbia University, <u>1935</u> .

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) 1-Butanol, C ₄ H ₁₀ 0; [71-36-3]	Hansen, R.S.; Fu, Y.; Bartell, F.E.
(2) Water; H ₂ 0; [7732-18-5]	J. Phys. Chem. <u>1949</u> , 53, 769-85.
VARIABLES:	PREPARED BY:
One temperature: 25 [°] C	S.H. Yalkowsky; S.C. Valvani; A.F.M. Barton

At equilibrium at 25.0° C the proportion of 1-butanol in the water-rich phase was reported to be 7.41 g(1)/100g sln, a concentration of 0.985 mol (1)/L sln.

The corresponding mole fraction solubility calculated by the compiler is $x_1 = 0.0191$.

AUXILIARY	INFORMATION
METHOD/APPARATUS/PROCEDURE: An excess of the alcohol was added to re- distilled water in a mercury-sealed flask	SOURCE AND PURITY OF MATERIALS: (1) refluxed 4h over magnesium and iodine, distilled with 60cm glass packed
which was shaken mechanically for 48 h in an air chamber thermostatted to $25.0 \pm 0.1^{\circ}$ C. The flask was then allowed to stand for 3 h in the airbath, after which a portion of the water-rich phase was removed by means of a hypodermic syringe and was compared inter- ferometrically with the most concentrated alcohol solution which could be prepared conveniently. The solubility determination was associated with a study of multimolecu- lar absorption from binary liquid solutions.	reflux column; b.p. 117 [°] C/745 mm Hg
	(2) distilled laboratory water, redistilled from alkaline permanganate solution.
	ESTIMATED ERROR: Temperature: 0.1 [°] C
	Solubility: deviation from mean of three determinations ±0.03 wt%.
	REFERENCES :

COMPONENTS:		ORIGINAL MEASUREMENTS:
(1) 1-Butanol; C ₄ H ₁₀ ; [71-36-3]		Donahue, D.J.; Bartell, F.E.
4 10		J. Phys. Chem. <u>1952</u> , 56, 480-4.
(2) Water; H ₂ O; [7732-18-5]		
VARIABLES:		PREPARED BY:
One temperature: 25°C		A.F.M. Barton
EXPERIMENTAL VALUES:		L
	Density Mu	futual solubility of 1-butanol (1) and water (2)
	g mL ⁻¹	x_1 g(1)/100g sln (compiler)
Alcohol-rich phase	0.8432	- 0.500 80.5
Water-rich phase	0,9860	0.0188 ^{<i>a</i>} 7.3
^{a} From ref 1 and 2		
	AUXILIARY	INFORMATION
METHOD / APPARATUS / PROCEDURE :		SOURCE AND PURITY OF MATERIALS:
Mixtures were placed in glass	stoppared	(1) "best reagent grade";
flasks and were shaken intermi	ittently for at	
least 3 days in a water bath. phase was analyzed for water of	The organic content by	(2) "purified"
the Karl Fischer method and the phase was analyzed interferome	ne aqueous	
The solubility measurements for	ormed part of a	1
study of water-organic liquid tensions.	interfacial	
		ESTIMATED ERROR:
		Temperature: $\pm 0.1^{\circ}$ C
		REFERENCES:
		1. Butler, J.A.V.; Thomson, D.W.;
		Maclennan, W.H. <i>J. Chem. Soc.</i> <u>1933</u> , 674.
		2. Hansen, R.S.; Fu, Y.; Bartell, F.E.
		J. Phys. Chem. <u>1949</u> , 53, 769.
1		1

COMPONENTS:		DRIGINAL MEASUREMENTS:
(1) 1-Butanol; C ₄ H ₁₀ ; [71-36-3	1	Erichsen, L. von
	-	Naturwissenschaften 1952, 39, 41-2.
(2) Water; H ₂ 0; [7732-18-5]		
VARIABLES: Temperature: 0-50 [°] C		PREPARED BY:
Temperature: 0-50 C		A. Maczynski; Z. Maczynska
EXPERIMENTAL VALUES:		
Solub	ility of 1-bu	utanol (1) in water (2)
t/ ^o C	x_1	g(1)/100g sln (compiler)
0 0.0	271	10.28
10 0.0	230	8.83
20 0.0	197	7.63
30 0.0	179	7.41
40 0.0	167	6.53
50 0.0	163	6.38
	AUXILIARY	INFORMATION
METHOD / APPARATUS / PROCEDURE :		SOURCE AND PURITY OF MATERIALS:
The synthetic method was used.		(1) not specified.
No details were reported in the p	aper.	(2) not specified.
		ESTIMATED ERROR:
		Not specified.
		REFERENCES :

COMPONENTS:			ORIGINAL MEASUREMENTS:	
	; c ₄ H ₁₀ 0; [71-36- ₂ 0; [7732-18-5]	3]	Erichsen, L. von Brennst. Chem. <u>1952</u> , 3	3, 166-72.
(1) """	2°, []			
VARIABLES:			PREPARED BY:	
Temperature:	0 - 125 [°] C		S.H. Yalkowsky; Z. Mac	zynska
EXPERIMENTAL VALUES:			······	
	Mutual sc	lubility of	l-butanol(1) and water	(2)
t/ ^o c	(2)-rich ph	ase	(1)-rich ph	ase
	g(1)/100g sln	x_1	g(1)/100g sln	x_1
0	10.32	0.0271	81.05	0.5112
10	8.68	0.0230	80.50	0.5061
20	7.56	0.0197	80.00	0.4980
30	7.06	0.0179	79.37	0.4861
40	6.72	0.0167	78.60	0.4717
50	6.55	0.0163	77.59	0.4562
60	6.52	0.0162	76.29	0.4381
70	6.67	0.0166	74.57	0.4152
80	6.90	0.0175	72.40	0.3890
90	7.50	0.0195	69.90	0.3600
100	8.82	0.0232	66.70	0.3290
110	11.05	0.0295	61.85	0.2875
120	15.45	0.0440	53.35	0.2180
125	23.50	0.0710	43.10	0.1490
The UCST	is 125.3 ⁰ C			
		AUXILIARY	INFORMATION	
METHOD /APPARATU	S/PROCEDURE:		SOURCE AND PURITY OF MA	TERIALS:
The synthetic	method was used.			or industrial product; emically free from
glass ampoules	nts were carried ou which were placed ok equipped with two	in an	isomers; b.p.116.6-116.7° n _D ²⁰ 1.3996.	-
windows. Clo a thermocouple	oud points were mea wound up around t ent being repeated	sured with he ampoule;	(2) not specified.	
			ESTIMATED ERROR:	
			Not specified.	
			REFERENCES:	

COMPONENTS :	ORIGINAL MEASUREMENTS:
(1) 1-Butanol; C ₄ H ₁₀ 0; [71-36-3]	McCants, J.F.; Jones, J.H.; Hopson, W.H.
(2) Untown H O. [7720 18 5]	Ind. Eng. Chem. <u>1953</u> , 45, 454-6.
(2) Water; H ₂ 0; [7732-18-5]	
VARIABLES:	PREPARED BY:
One temperature: 37.7 [°] C	A. Maczynski
EXPERIMENTAL VALUES:	
The solubility of 1-butanol in water at 37.7	C was reported to be 6.7 g (1)/100g sln.
The corresponding mole fraction, $x_1^{}$, calculat	ed by the compiler is 0.017.
-	
The solubility of water in 1-butanol at 37.7 ⁰	C was reported to be 21.2 $g(2)/100g sln$.
The corresponding mole fraction, x_{γ} , calculat	
2	· · · · · · · · · · · · · · · · · · ·
AUXILIARY	INFORMATION
METHOD /APPARATUS / PROCEDURE :	SOURCE AND PURITY OF MATERIALS:
The titration method described by Washburn	(1) Carbide and Carbon Co;
et al. (ref 1) was used.	technical product without further purification
	$n_{\rm p}^{20}$ 1.3988;
	purity not specified.
	(2) distilled.
	ESTIMATED ERROR:
	Not specified.
	REFERENCES:
	 Washburn, E.R.; Graham, C.L.; Arnold, G.R.; Trausue, L.F J. Am. Chem. Soc. <u>1940</u>, 62, 1454.

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) 1-Butanol; C ₄ H ₁₀ 0; [71-36-3]	Jones, J.H.; McCants, J.F.
(2) Water; H ₂ 0; [7732-18-5]	Ind. Eng. Chem. <u>1954</u> , 46, 1956-8.
VARIABLES:	PREPARED BY:
One temperature: 100 ⁰ F (37.8 ⁰ C)	S.H. Yalkowsky; S.C. Valvani; A.F.M.Barton

At equilibrium at 100° F (37.8°C) the proportion of 1-butanol in the alcohol-rich phase was reported to be 79.7 g(1)/100g sln and the proportion of 1-butanol in the water-rich phase was reported to be 7.2 g(1)/100g sln.

The corresponding mole fraction solubility values calculated by the compiler are $x_1 = 0.489$ and $x_1 = 0.0185$ respectively. The refractive indexes, $n_D^{38.3}$, were reported as 1.3871 and 1.3393, respectively.

AUXILIARY	INFORMATION

METHOD / AP PARATUS / PROCEDURE :	SOURCE AND PURITY OF MATERIALS:
The cloud point method by titrating, patterned after that described in ref 1, was used. The system under study was the ternary 1-butanol/1-hexanone/water.	(1) U.S.I.C. "approved" grade; $n_{\rm D}^{20}$ 1.3991, d_4^{20} 0.810
	(2) distilled; n_D^{20} 1.3330
	ESTIMATED ERROR: Temperature: controlled to within 0.1 ⁰ C.
	REFERENCES;
	 Washburn, E.R.; Hnizda, V.; Vold, R. J. Am. Chem. Soc. <u>1931</u>, 53, 3237.

COMPONENTS :	ORIGINAL MEASUREMENTS:
	CRIGINIE PERSONEPENIS.
(1) 1-Butanol; C ₄ H ₁₀ 0; [71-36-3]	Skrzec, A.E.; Murphy, N.F.
(2) Network 17 0: [7720.10.5]	Ind. Eng. Chem. <u>1954</u> , 46, 2245-7.
(2) Water; H ₂ 0; [7732-18-5]	
VARIABLES:	PREPARED BY:
One temperature: 26.7 [°] C	A. Maczynski
EXPERIMENTAL VALUES:	
The solubility of 1-butanol in water at 26.7°	C was reported to be 7.30 $g(1)/100g$ sln.
The corresponding mole fraction, x_1 , calculat	
The corresponding more fraction, "1, carculat	
The solubility of water in 1-butanol at 26.7	
The corresponding mole fraction, x_2 , calculat	ed by the compiler is 0.515.
	INFORMATION
METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
Probably the titration method was used. (This method was described for the determin-	 Commercial Solvents Corp., technical grade;
ation of mutual solubilities in ternary	used as received;
systems but nothing is reported on the binary system determination).	
	(2) not specified.
	ESTIMATED ERROR:
	Temperature: $\pm 0.5^{\circ}$ C.
	REFERENCES :
	I. Contraction of the second sec

2 Four-carbon Alcohols		
COMPONENTS :	ORIGINAL MEASUREMENTS:	
(1) 1-Butanol; C ₄ H ₁₀ O; [71-36-3]	Hayashi, M.; Sasaki, T.	
	Bull. Chem. Soc. Jpn. <u>1956</u> , 29, 857-9.	
(2) Water; H ₂ O [7732-18-5]		
VARIABLES:	PREPARED BY:	
One temperature: 30.0°C	S.H. Yalkowsky; S.C. Valvani; A.F.M. Barton	
Tween 80 concentration EXPERIMENTAL VALUES:	L	
The proportion of 1-butanol in the aqueous phase at 30.0° C was reported to be 7.01 g(1)/100g sln. The corresponding mole fraction calculated by the compiler is $x_1 = 0.0180$.		
The solubility of the alcohol in dilute solutions of Tween 80, obtained by extrapolating to zero turbidity the linear relation between turbidity and solute concentration in the surfactant solution, was less than that in pure water but increased with increasing concentration of Tween 80.		

AUXILIARY	INFORMATION
METHOD/APPARATUS/PROCEDURE: The mixture was well shaken at a temperature below 30.0°C and then stood in the thermostat for 24 h. After the excess solute particles cleared, a transparent saturated solution was obtained which was taken from the bottom of the vessel by a siphon. A known amount of this solution (about 20 g) was titrated with Tween 80 solution. Concentration was determined by comparison of turbidity to standard samples.	potassium carbonate, distilled over
	ESTIMATED ERROR: Solubility: ± 0.4% "possible error" REFERENCES:

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) 1-Butanol; C ₄ H ₁₀ 0; [71-36-3]	Kakovskii, I.A.
(2) Water; H ₂ 0; [7732-18-5]	Proc. Intern. Congr. Surface Activity, 2nd, London <u>1957</u> , 4, 225-37.
VARIABLES:	PREPARED BY:
One temperature: 25 [°] C	S.H. Yalkowsky and S.C. Valvani
EXPERIMENTAL VALUES:	,,,,,

The solubility of 1-butanol in water at 25° C was reported to be 1.07 mol L⁻¹ (79.3 g(1)/L sln: compiler).

AUXILIARY	INFORMATION

METHOD / AP PARATUS / PROCEDURE :	SOURCE AND PURITY OF MATERIALS:
No experimental details given.	Not specified.
	ESTIMATED ERROR:
	Not specified,
	REFERENCES :
L	l

COMPONENTS :	ORIGINAL MEASUREMENTS:
	CRIGINIE PERSOREPENIS.
(1) 1-Butanol; C ₄ H ₁₀ 0; [71-36-3]	Rao, R.M.; Rao, V.C.
	J. Appl. Chem. <u>1957</u> , 7, 659-66.
(2) Water; H ₂ 0; [7732-18-5]	
VARIABLES:	PREPARED BY:
One temperature: 27 ⁰ C	A. Maczynski
EXPERIMENTAL VALUES:	
The solubility of 1-butanol in water at 27 ⁰ C	was reported to be 7.0 $g(1)/100g \ sln$.
The corresponding mole fraction, x_1 , calculat	ted by the compiler is 0.018.
The solubility of water in 1-butanol at 27 ⁰ C	was reported to be 19.9 g(2)/100g sln.
The corresponding mole fraction, x_2 , calculat	ted by the compiler is 0.505.
The corresponding more fraction, w ₂ , carear	
AUXILIARY	INFORMATION
METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
The method of appearance and disappearance	(1) Merck reagent grade;
of turbidity described in ref 1 was used.	distilled; b.p. 117.7°C, d ³⁰ 0.8018, n ³⁰ 1.3940.
No details were reported in the paper.	b.p. 117.7 C, a 0.8018, n 1.3940.
	(2) not specified.
	ESTIMATED ERROR:
	Not specified.
	REFERENCES :
	1. Othmer, D.F.; White, R.E.; Trueger, E.
	Ind. Eng. Chem. <u>1941</u> , 33, 1240.
L	

ł	COMPONENTS:	ORIGINAL MEASUREMENTS:
	(1) 1-Butanol; C ₄ H ₁₀ 0; [71-36-3] (2) Water; H ₂ 0; [7732-18-5]	Kinoshita, K.; Ishikawa, H.; Shinoda, K. Bull. Chem. Soc. Japan <u>1958</u> , 31, 1081-4.
	VARIABLES:	PREPARED BY:
	One temperature: 25 [°] C	S.H. Yalkowsky; S.C. Valvani; A.F.M. Barton.

At equilibrium at 25.0°C the concentration of 1-butanol in the water-rich phase was reported to be 0.97 mol(1) L^{-1} . The weight percentage solubility was reported as 7.4 g(1)/100g sln, and the corresponding mole fraction solubility calculated by the compiler is $x_1 = 0.0191$.

AUXILIARY	INFORMATION
METHOD /APPARATUS / PROCEDURE: The surface tension in aqueous solutions of alcohols monotonically decreases up to their saturation concentration and remains constant in the beterogeneous region (ref 1-4). Surface tension was measured by the drop weight method, using a tip 6 mm in diameter. The measurements were carried out in a water thermostat at 25 ± 0.05 °C. From the (surface tension)-(logarithm of concentra- tion) curves the saturation points were determined as the intersections of the curves with the horizontal straight lines	 SOURCE AND PURITY OF MATERIALS: (1) purified by vacuum distillation through 50-100cm column; b.p. 11°C (pressure uncertain) (2) not stated.
passing through the lowest experimental points.	 Temperature: ±0.05°C. Solubility: within 4%. 1. Motylewski, S. Z. Anorg. Chem. <u>1904</u>, 38, 410. 2. Taubamann, A. Z. Physik. Chem. <u>1932</u>, A161, 141. 3. Zimmermann, H.K., Jr. Chem. Rev. <u>1952</u>, 51, 25. 4. Shinoda, K.; Yamanaka, T.; Kinoshita, K. J. Phys. Chem. <u>1959</u>, 63, 648.

COMPONENTS :	ORIGINAL MEASUREMENTS:
(1) 1-Butanol; C ₄ H ₁₀ 0; [71-36-3]	Venkataratnam, A.; Rao, R.I.
(2) Water; H ₂ 0; [7732-18-5]	J.Sci. Ind. Res. <u>1958</u> , 17B, 108-10.
2	
VARIABLES:	PREPARED BY:
One temperature: 30 [°] C	A. Maczynski
	-
EXPERIMENTAL VALUES:	
The solubility of 1-butanol in water at 30° C	
The corresponding mole fraction, $x_1^{}$, calculation	ed by the compiler is 0.017.
The solubility of water in 1-butanol at 30 ⁰ C	was reported to be 20.0 g(2)/100g sln.
The corresponding mole fraction, $x_2^{}$, calculation	ed by the compiler is 0.507.
· · · · · · · · · · · · · · · · · · ·	
AUXILIARY	INFORMATION
METHOD /APPARATUS / PROCEDURE :	SOURCE AND PURITY OF MATERIALS:
The method of appearance and disappearance of turbidity described in ref 1 was used.	<pre>(1) Merck and Co.; used as received;</pre>
	used as received; b.p. 117.2°C, n ³⁰ 1.3930, d ³⁰ 0.7996 g/ml.
No details were reported in the paper.	(2) distilled;
	free from carbon dioxide.
	ESTIMATED ERROR:
	Not specified.
	REFERENCES :
	1. Othmer, D.F.; White, R.E.; Trueger, E.
	Ind. Eng. Chem. <u>1941</u> , 33, 1240.

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) 1-Butanol; C ₄ H ₁₀ 0; [71-36-3]	Petriris, V.E.; Geankopolis, C.J.
	J. Chem. Eng. Data <u>1959</u> , 4, 197-8.
VARIABLES:	PREPARED BY:
One temperature: 25 [°] C	A. Maczynski
EXPERIMENTAL VALUES:	
The solubility of 1-butanol in water at 25 ⁰ C	was reported to be 7.0 $g(1)/100g$ sln.
The corresponding mole fraction, x_1 , calculat	
The corresponding hore fraction, w ₁ , careata	
The solubility of water in 1-butanol at 25 ⁰ C	was reported to be 20.7 $g(2)/100g sln$.
The corresponding mole fraction, x_{2} , calculat	
2	
	INFORMATION
METHOD / APPARATUS / PROCEDURE :	SOURCE AND PURITY OF MATERIALS:
The titration method was used.	 Baker, analytical reagent grade; used as received;
No details were reported in the paper.	purity not specified.
	(2) not specified.
	ESTIMATED ERROR:
	Not specified.
	REFERENCES:

COMPONENTE	
COMPONENTS :	ORIGINAL MEASUREMENTS:
(1) 1-Butanol; C ₄ H ₁₀ 0; [71-36-3]	Ababi, V.; Popa, A.
(2) Water; H ₂ O; [7732-18-5]	An. Stiint. Univ."Al. I. Cuza"Iasi. <u>1960</u> , 6, 929-42.
VARIABLES:	PREPARED BY:
One temperature: 25 [°] C	A.Maczynski
EXPERIMENTAL VALUES:	
The solubility of 1-butanol in water at 25° C The corresponding mole fraction, x_1 , calculat	
The corresponding more fraction, w ₁ , carculat	by the compiler is 0.010.
The solubility of water in 1-butanol at 25 ⁰ C	
The corresponding mole fraction, x_2 , calculated and the corresponding mole fraction x_2 , x_2 , x_3 , x_2 , x_3	ed by the compiler is 0.506.
	INFORMATION
METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
The turbidimetric method was used.	 Merck analytical reagent; used as received.
Ternary solubility methods were described in the paper but nothing was reported for binary solubilities.	(2) not specified.
	ESTIMATED ERROR:
	Not specified.
	REFERENCES :

COMP ONENTS :	ORIGINAL MEASUREMENTS:	
COTT UNENTS .		
(1) 1-Butanol; C ₄ H ₁₀ 0; [77-36-3]	Smirnova, N.A.; Morachevskii, A.G.	
(2) Water; H ₂ 0; [7732-18-5]	Zh. Prikl. Khim. (Leningrad) <u>1963</u> , 36, 2391-7.	
VARIABLES:	PREPARED BY:	
One temperature: 20 ⁰ C	A. Maczynski	
EXPERIMENTAL VALUES:		
The solubility of 1-butanol in water at 20°	C was reported to be 8.1 g(1)/100g sln.	
The corresponding mole fraction, $x_1^{}$, calculated by the compiler is 0.021.		
The solubility of water in 1-butanol at 20 ⁰	C was reported to be 20.1 g(2)/100g sln.	
The corresponding mole fraction, $x_2^{}$, calculation,	ated by the compiler is 0.509.	
	INFORMATION	
METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:	
The density method was used.	(1) CP reagent; treated with 5% solution of KMnO4,	
The density was measured to an accuracy of	dried over potassium and distilled;	
0.0001g cm ⁻³ .	$n_{\rm D}^{20}$ 1.3993, d_4^{20} 0.8097.	
No additional details were reported in the	(2) not specified.	
paper.	(2) not specified.	
	ESTIMATED ERROR:	
	Not specified.	
	REFERENCES :	

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) 1-Butanol; C ₄ H ₁₀ 0; [71-36-3]	Ratouis, M.; Dodé, M.
(2) Water; H ₂ 0; [7732-18-5]	Bull. Soc. Chim. Fr. <u>1965</u> , 3318-22.
VARIABLES:	PREPARED BY:
Temperature: 25-30 ⁰ C Ringer solution also studied	S.C. Valvani; S.H. Yalkowsky; A.F.M.Barton
EXPERIMENTAL VALUES:	
Proportion of 1-butanol(1) in water-rich phase
t/ ⁰ C g(1)/100g s	ln x ₁ (compiler)
25 7.34	0.0189
30 6.99	0.0180
Proportion of 1-butanol(1) in water-rich phase (Ringer solution)	
$t/{}^{0}C$ g(1)/100g s	ln
25 6.87	
30 6.70	
AUXILIARY	INFORMATION
METHOD APPARATUS / PROCEDURE :	SOURCE AND PURITY OF MATERIALS:
In a round bottomed flask, 50 mL of water and a sufficient quantity of alcohol were introduced until two separate layers were formed. The flask assembly was equilibrated by agitation for at least 3 h in a constant temp bath. Equilibrium solubility was attained by first supersaturating at a slightly lower temperature (solubility of alcohols in water is inversely proportional to temperature) and then equilibrating at	 n_D 1.39745 (2) twice distilled from silica apparatus or ion exchanged with Sagei A20
the desired temperature. The aqueous layer was separated after an overnight storage in a bath. The alcohol content was determined by reacting the aqueous solution with potassium dichromate and titrating the excess dichromate with ferrous sulfate solution in the presence of phosphoric acid and diphenylamine barium sulfonate as an indicator.	

COMPONENTS:	ORIGINAL MEASUREMENTS:
	N . I malana D
(1) 1-Butanol; C ₄ H ₁₀ O; [71-36-3]	Meeussen, E.; Huyskens, P.
(2) Water; H ₂ 0; [7732-18-5]	J. Chim. Phys. <u>1966</u> , 63, 845-54.
(2) water, n_2^{0} , $[7752-10-5]$	
VARIABLES: One temperature: 25 ⁰ C	PREPARED BY: A. Maczynski
One temperature: 25 C	A. Haczynski
EXPERIMENTAL VALUES:	0
The mole fraction solubility of water in 1-bu	itanol at 25°C was reported to be $x_2 = 0.492$.
The corresponding mass percentage calculated	by the compiler is 19.05 g(2)/100g sln.
	INFORMATION
METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
The interferometric method of Brown and Bury	 commercial product for chromatography; purified;
(ref 1) modified by Guillerm (ref 2) was used.	purified; purity not specified.
A Rayleigh M75 interference refractometer with a M160 attachment was employed.	(2) not specified.
Pycnometric densities of the solutions were	(2) not specifica.
used to evaluate solubility concentrations.	
	ESTIMATED ERROR: Temperature: ± 0.05°C
	Solubility : ± 0.002 mol(2)dm ⁻³ sln (type of error not specified).
	REFERENCES :
	1. Brown, F.S.; Bury, C.R.; J. Chem. Soc. <u>1923</u> , 123, 2430.
	2. Guillerm, S., Doctoral thesis, 1963.

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) 1-Butanol; C ₄ H ₁₀ 0; [71-36-3]	Lesteva, T.M.; Ogorodnikov, S.K.; Tyvina, T.N.
(2) Water; H ₂ 0; [7732-18-5]	Zh. Prikl. Khim. (Leningrad) <u>1968</u> , 41, 1159-63.
VARIABLES:	PREPARED BY:
Temperature: 20 and 75 ⁰ C	A. Maczynski
EXPERIMENTAL VALUES:	
Mutual solubility of	1-butanol (1) and water (2)
t/ ⁰ C g(1)/100g sln	x_1
(2)-rich phase (1)-rich pha	ase (2)-rich phase (1)-rich phase
20.0 4.9 80.3	0.012 0.498
75.0 5.2 75.8	0.013 0.432
AUXILIARY	INFORMATION
METHOD / APPARATUS / PROCEDURE :	SOURCE AND PURITY OF MATERIALS:
The titration method was used. No details were reported in the paper.	<pre>(1) source not specified; CP reagent; purity not specified.</pre>
	(2) not specified.
	ESTIMATED ERROR:
	Not specified.
	REFERENCES :

COMPONENTS:	ORIGINAL MEASUREMENTS: *Hanssens, I.
(1) 1-Butanol; $C_4 H_{10}^{0}$; [71-36-3]	Associatie van normale alcoholen en hun affiniteit voor water en organische solventen Doctoraatsproefschrift, Leuven, <u>1969</u> .
(2) Water; H ₂ 0; [7732-18-5]	Huyskens, P. Mullens, J.; Gomez, A.; Tack, J.
	Bull. Soc. Chim. Belg. <u>1975</u> , 84, 253-62.
VARIABLES:	PREPARED BY:
One temperature: 298K	M.C. Haulait-Pirson; A.F.M. Barton
EXPERIMENTAL VALUES:	L
The solubility of l-butanol(1) in the water- and the solubility of water(2) in the alcoho 9.261 mol(2)/L sln.	rich phase was reported as 0.926 mol(1)/L sln, L-rich phase was reported as
The corresponding values on a weight/volume 166.9 g(2)/L sln (compiler).	basis are 68.6 g(l)/L sln, and
(The temperature was unspecified in the these published paper).	is, but reported as 298 K in the 1975
AUXILIARY	INFORMATION
	INFORMATION SOURCE AND PURITY OF MATERIALS:
METHOD/APPARATUS/PROCEDURE:	INFORMATION SOURCE AND PURITY OF MATERIALS: (1) Merck p.a.
METHOD/APPARATUS/PROCEDURE: (1) and (2) were equilibrated using a cell described in ref 1. The Rayleigh M75 inter ference refractometer with the cell M160 for liquids was used for the determination of the concentrations. Cell thicknesses were	SOURCE AND PURITY OF MATERIALS: (1) Merck p.a. (2) distilled
METHOD/APPARATUS/PROCEDURE: (1) and (2) were equilibrated using a cell described in ref 1. The Rayleigh M75 inter ference refractometer with the cell M160 for liquids was used for the determination of	SOURCE AND PURITY OF MATERIALS: (1) Merck p.a. (2) distilled
METHOD/APPARATUS/PROCEDURE: (1) and (2) were equilibrated using a cell described in ref 1. The Rayleigh M75 inter ference refractometer with the cell M160 for liquids was used for the determination of the concentrations. Cell thicknesses were 1, 3 and 10 cm depending on the concentratio range. Standard solutions covering the whole range of concentrations investigated	SOURCE AND PURITY OF MATERIALS: (1) Merck p.a. (2) distilled
METHOD/APPARATUS/PROCEDURE: (1) and (2) were equilibrated using a cell described in ref 1. The Rayleigh M75 inter ference refractometer with the cell M160 for liquids was used for the determination of the concentrations. Cell thicknesses were 1, 3 and 10 cm depending on the concentratio range. Standard solutions covering the whole range of concentrations investigated	SOURCE AND PURITY OF MATERIALS: (1) Merck p.a. (2) distilled
METHOD/APPARATUS/PROCEDURE: (1) and (2) were equilibrated using a cell described in ref 1. The Rayleigh M75 inter ference refractometer with the cell M160 for liquids was used for the determination of the concentrations. Cell thicknesses were 1, 3 and 10 cm depending on the concentratio range. Standard solutions covering the whole range of concentrations investigated	SOURCE AND PURITY OF MATERIALS: (1) Merck p.a. (2) distilled ESTIMATED ERROR: soly ± 0.00036 - 0.05 mol/L sln, depending
METHOD/APPARATUS/PROCEDURE: (1) and (2) were equilibrated using a cell described in ref 1. The Rayleigh M75 inter ference refractometer with the cell M160 for liquids was used for the determination of the concentrations. Cell thicknesses were 1, 3 and 10 cm depending on the concentratio range. Standard solutions covering the whole range of concentrations investigated	SOURCE AND PURITY OF MATERIALS: (1) Merck p.a. (2) distilled ESTIMATED ERROR: soly ± 0.00036 - 0.05 mol/L sln, depending on the concentration

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) 1-butanol; C ₄ H ₁₀ O; [71-36-3]	*Mullens, J.
(2) Water; H ₂ O; [7732-18-5]	Alcoholassociaten, Doctoraatsproefschrift, Leuven, 1971.
2	Huyskens, P.; Mullens, J.; Gomez, A.; Tack,J.
	Bull. Soc. Chim. Belg. 1975, 84, 253-62.
VARIABLES:	PREPARED BY:
One temperature: 25 [°] C	M.C. Haulait-Pirson; A.F.M. Barton
EXPERIMENTAL VALUES:	l

At 25° C the solubility of 1-butanol(1) in the water-rich phase was reported as 0.926 mol(1)/L sln, and the solubility of water(2) in the alcohol-rich phase was reported as 9.261 mol(2)/L sln.

The corresponding values on a weight/volume basis are 68.6 g(1)/L sln, and 166.9 g(2)/L sln (compiler).

	INFORMATION
METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
The partition of the two components was made using a cell described in ref 1. The Rayleigh Interference Refractometer M154 was used for the determination of the concen- trations. Standard solutions covering the whole range of concentration investigated were used for	<pre>(1) Merck product (p.a.) (2) distilled</pre>
the calibration.	
	ESTIMATED ERROR:
	Soly ± 0.001 mol(1)/L sln.
	REFERENCES: 1. Meeussen, E.; Huyskens,P. J. Chim. Phys. <u>1966</u> , 63, 845.

ORIGINAL MEASUREMENTS:
Vochten, R.; Petre, G. J. Colloid Interface Sci. <u>1973</u> , 42, 320-7.
PREPARED BY: S.H. Yalkowsky; S.C. Valvani, A.F.M. Barton
-

The concentration of 1-butanol in the water-rich phase at equilibrium at 15° C was reported to be 1.1 ± 0.1 mol(1)/L sln. This corresponds to 81.5 g(1)/L sln (compiler).

AUXILIARY	INFORMATION
METHOD / APPARATUS / PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
The solubilities were obtained from surface tensions, measured by the static method of Wilhelmy (platinum plate). The apparatus consisted of an electrobalance (R.G. Cahn) connected with a high impedance null detector (FLUKE type 845 AR). An all-Pyrex vessel was used.	 purified by distillation and preparative gas chromatography; b.p. 117.5°C/760 mm Hg triply distilled from permanganate solution
	ESTIMATED ERROR: Temperature: ± 0.1 [°] C Solubility: (probably std deviation) ±0.1 mol(1)/L sln.
	REFERENCES:

COMPONENTS:	ORIGINAL MEASUREMENTS:		
1) 1-Butanol; C ₄ H ₁₀ 0; [71-36-3] (2) Water; H ₂ 0; [7732-18-5]	Korenman, I.M.; Gorokhov, A.A.; Polozenko,G.N Zh. Fiz. Khim. <u>1974</u> , 48, 1810-2; *Russ. J. Phys. Chem. <u>1974</u> , 48, 1065-7. Zh. Fiz. Khim. <u>1975</u> , 49, 1490-3; Russ. J. Phys. Chem. <u>1975</u> , 49, 877-8.		
VARIABLES:	PREPARED BY: A.F.M.Barton		
One temperature: 25 [°] C			

At equilibrium at 25.0° C the concentration of 1-butanol in the water-rich phase was reported to be 1.05 mol (1)/L sln, and the concentration of water in the alcohol-rich phase was reported to be 9.70 mol (2)/L sln.

The corresponding solubilities on a mass/volume basis, calculated by the compiler, are 77.8 g(1)/L sln, and 174.8 g(2)/L sln respectively.

AUXILIARY	INFORMATION	
ME THOD /APPARATUS / PROCEDURE :	SOURCE AND PURITY OF MATERIALS:	
The two liquids were shaken in a closed vessel at $25.0 \pm 0.1^{\circ}$ C until equilibrium was established. The solubility of the alcohol in the aqueous phase was determined on a Tsvet-1 chromatograph with a flame-ionization detector. The sorbent was a polyethylene glycol adipate deposited on Polychrom-1. The solubility of water in the alcohol was determined on a UKh-2 universal chromato- graph under isothermal conditions. The study formed part of an investigation of salting out by alkali halides of higher		
alcohol-water systems.	ESTIMATED ERROR: Temperature; ± 0.1 [°] C Solubility: not stated; the results shown are the arithmetic mean of four experiments.	
	REFERENCES :	

COMPONENTS:		ORI	GINAL MEASUREMENTS:		
(1) 1-Butanol; C ₄ H ₁₀ 0; [71-36-3]			Prochazka, 0.; Sushka, J.; Pick, J. Coll. Czech. Chem. Comm. <u>1975</u> , 40, 781-6.		
(2) Water; H	2 ² 0; [7732–13–5]				
ARIABLES:		PRE	PARED BY:		
Temperature:	83–124 [°] C	Α.	Maczynski		
XPERIMENTAL VA	LUES:			<u>,</u>	
	Mutual s	solubility of 1-b	utanol (1) and water	(2)	
t∕°c	g(1)/10	00g sln	x_1 (compiler)		
	(2)-rich phase	(1)-rich phase	(2)-rich phase		
82.7	7.3	-	0.019	-	
87.1	-	70.5	-	0.367	
90.1	-	69.3	-	0.360	
94.0	8.3	-	0.022	-	
98.5	8.9	-	0.023	-	
98.7	-	66.6	-	0.326	
105.2	-	63.4	-	0.296	
106.1	-	62.9	-	0.292	
107.2	10.3	-	0.027	-	
110.2	-	60.4	-	0.270	
111.6	11.7	-	0.031	-	
114.0	12.6	-	0.034	-	
115.2	-	56.8	-	0.242	
117.3	14.9	-	0.041	-	
				(continued next page	
		AUXILIARY INF	ORMATION		
METHOD/APPARATU	JS/PROCEDURE:	SO	URCE AND PURITY OF MAT	ERIALS:	
The turbidity	method was used.	(1	.) Analytical grade r		
The apparatus	with visual indic	ation of	distilled over forty-plate bubble cup column; b.p. 117.9°C/760 torr, $n_{\rm D}^{25}$ 1.3974, d_4^{25} 0.3057.		
turbidity was	described in ref	1. No more			
additional det paper.	ails were reporte	d in the			
F-F			(2) redistilled.		
		ES	TIMATED ERROR:		
			Not specified.		
		RF	FERENCES :		
			Matous, J.; Novak, Pick, J. <i>Coll. Cz</i> <u>1972</u> , <i>37</i> , 2653.		

COMPONENTS:		ORIG	ORIGINAL MEASUREMENTS:		
(1) 1-Butanol; C ₄ H ₁₀ 0; [71-36-3]		5-3] Pro	Prochazka, O.; Sushka, J.; Pick, J.		
(2) Water;	H ₂ 0; [7732-18-5]	Col	l. Czech. Chem. Comm	n., <u>1975</u> , 40, 781-6	
EXPER IMENTAL	VALUES (continued)				
t∕°C	g(1)/10	DOg sln	$x_1(com)$	piler)	
	(2)-rich phase	(1)-rich phase	(2)-rich phase	(1)-rich phase	
119.3	-	52.6	-	0.212	
119.8	-	52.1	-	0.209	
121.0	-	50.0	-	0.195	
121.7	18.4	-	0.052	-	
121.9	18.6	-	0.053	-	
123.1	20.8	45.5	0.060	0.169	
123.9	-	41.4	-	0.146	
124.1	26.1	-	0.079	-	
124.2	-	38.0	-	0.130	
124.3	29.7	36.5	0.093	0.123	
124.4	31.8	34.0	0.102	0.111	
124.4	32.5	32.5	0.105	0.105	

(1) 1-Butanol; C ₄ H ₁₀ 0; [71-36-3] (2) Water; H ₂ 0; [7732-18-5] VARIABLES: One temperature: 25°C A. Maczynski EXPERIMENTAL VALUES: The proportion of 1-butanol(1) in the water-rich phase at equilibrium at 25°C was reported to be 7.4 g(1)/100g sln. The corresponding mole fraction solubility, x ₁ , calculated by the compiler, is 0.019. The proportion of water(2) in the alcohol-rich phase at equilibrium at 25°C was reported to be 20.49 g(2)/100g sln. The corresponding mole fraction solubility, x ₂ , calculated by the compiler, is 0.513. METHOD/APPARATUS/PROCEDURE: The determinations were carried out using a separating frumel with a thermostatic facket. The extractor was loaded with (1) and (2) and quantitative gravity separation, samples were withdram from the anguous phase. The concentration of (2) in (1) was derived from a material balance based upon starting quantities and compositions. Each of the determinations were carried out solve from the anguest phase. The concentration of (2) in (1) was derived from a material balance based upon starting quantities and compositions. Each of the determinations was carried out solve from the method is described also in ref 1. ESTIMATED EREOR: The method is described also in ref 1.	COMPONENTS:	ORIGINAL MEASUREMENTS:
(2) Water; H ₂ 0; [7732-18-5] VARIABLES: One temperature: 25°C A. Maczynski EXPERIMENTAL VALUES: The proportion of 1-butanol(1) in the water-rich phase at equilibrium at 25°C was reported to be 7.4 g(1)/100g sln. The corresponding mole fraction solubility, x ₁ , calculated by the compiler, is 0.019. The proportion of water(2) in the alcohol-rich phase at equilibrium at 25°C was reported to be 20.49 g(2)/100g sln. The corresponding mole fraction solubility, x ₂ , calculated by the compiler, is 0.513. METHOD APPARATUS/PROCEDURE: The determinations were carried out using a fater an extended period of mixing and quantitative gravity separation, samples were withrown from the aqueous phase. The concentration of (1) in (2) was determined by concentration of (1) in (2) was determined by concentration of (1) in (2) was determined by concentration of (2) in (2) was determined by concentratin concentration of (2) in (2) was determined	(1) 1-Butanol; C ₄ H ₁₀ 0; [71-36-3]	
One temperature: 25°C A. Maczynski EXPERIMENTAL VALUES: The proportion of 1-butanol(1) in the water-rich phase at equilibrium at 25°C was reported to be 7.4 g(1)/100g sln. The corresponding mole fraction solubility, x ₁ , calculated by the compiler, is 0.019. The proportion of water(2) in the alcohol-rich phase at equilibrium at 25°C was reported to be 20.49 g(2)/100g sln. The corresponding mole fraction solubility, x ₂ , calculated by the compiler, is 0.513. METHOD /APPARATUS/PROCEDURE: The determinations were carried out using a separating funnel with a thermostatic jacket. The extractor was loaded with (1) and (2) and after an extended period of mixing and quantities gravity separation, samples were withdrawn from the aqueous phase. The concentration of (2) in (1) was detreminated from a material balance based upon starting quantities and compositions. Each of the determinations was carried out several times. The method is described also in ref 1. REFERENCES: 1. De Santis, R.; Marrelli, L.; Muscetta, P.N. J. Chem. Eng. Exts.,		
EXPERIMENTAL VALUES: The proportion of 1-butanol(1) in the water-rich phase at equilibrium at 25°C was reported to be 7.4 g(1)/100g sln. The corresponding mole fraction solubility, #1, calculated by the compiler, is 0.019. The proportion of water(2) in the alcohol-rich phase at equilibrium at 25°C was reported to be 20.49 g(2)/100g sln. The corresponding mole fraction solubility, #2, calculated by the compiler, is 0.513. METHOD APPARATUS/PROCEDURE: The determinations were carried out using a separating funnel with a thermostatic jackst. SOURCE AND PURITY OF MATERIALS: The determinations were carried out using a guantitive gravity separation, samples were withdrawn from the aqueous phase. The concentration of (1) in (2) was determined by colorimetrio analysis (double-bean Lange colorimetrio of the curue complex. The concentration of was carled out several times. The method is described also in ref 1. ESTIMATED ERROR: Temperature; ± 0.1°C. REFERENCES: The method is described also in ref 1.	VARIABLES:	PREPARED BY:
The proportion of 1-butanol(1) in the water-rich phase at equilibrium at $25^{\circ}C$ was reported to be 7.4 g(1)/100g sln. The corresponding mole fraction solubility, x_1 , calculated by the compiler, is 0.019. The proportion of water(2) in the alcohol-rich phase at equilibrium at $25^{\circ}C$ was reported to be 20.49 g(2)/100g sln. The corresponding mole fraction solubility, x_2 , calculated by the compiler, is 0.513. METHOD/APPARATUS/PROCEDURE: The determinations were carried out using a separating found. With a thermostatic jacket. The extractor was loaded with (1) and (2) and after an extended period of mixing and quantitative gravity separation, samples were withdrawn from the aqueous phase. The concentration of (1) in (2) was determined by colorimetric analysic (double-beam Lange colorimetric) of the crime complex. The concentrations was carried out several times The method is described also in ref 1. REFERENCES: 1. De Santis, R.; Morrelli, L.; Mussetta, P.N. J. Chem. Erg. Data,	One temperature: 25 [°] C	A. Maczynski
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AUXILIARY INFORMATION AUXILIARY INFORMATION METROD/APPARATUS/PROCEDURE: The determinations were carried out using a separating funnel with a thermostatic jacket. The extractor was loaded with (1) and (2) and after an extended period of mixing and quantitative gravity separation, samples were withdrawn from the aqueous phase. The concentration of (1) in (2) was determined by colorimeter) of the cerium complex. The concentration of (2) in (1) was derived from a material balance based upon starting quantities and compositions. Each of the determinations was carried out several times. The method is described also in ref 1. SOURCE AND PURITY OF MATERIALS: (1) Carlo Erba analytical purity; fractionated before use. (2) doubly distilled. (2) doubly distilled. ESTIMATED ERROR: Temperature: ± 0.1°C. REFERENCES: (1) De Santis, R.; Marrelli, L.; Muscetta, P.N. J. Chem. Eng. Exta,		rich phase at equilibrium at 25 ⁰ C was reported
AUXILIARY INFORMATION METHOD/APPARATUS/PROCEDURE: The determinations were carried out using a separating funnel with a thermostatic jacket. The extractor was loaded with (1) and (2) and fater an extended period of mixing and quantitative gravity separation, samples were withdrawn from the aqueous phase. The concentration of (1) in (2) was determined by colorimetric analysis (double-beam Lange colorimetri) of the ceriun complex. The concentration of (2) in (1) was detived from a material balance based upon starting quantities and compositions. Each of the determinations was carried out several times. The method is described also in ref 1. SOURCE AND PURITY OF MATERIALS: (1) Carlo Erba analytical purity; fractionated before use. (1) Carlo Erba analytical purity; fractionated before use. (2) doubly distilled. (2) REFERENCES: (2) De Santis, R.; Marrelli, L.; Muscetta, P.N. J. Chem. Eng. Data,	The corresponding mole fraction solubility, a	$x_1^{}$, calculated by the compiler, is 0.019.
AUXILIARY INFORMATION METHOD APPARATUS/PROCEDURE: The determinations were carried out using a separating funnel with a thermostatic jacket. The extractor was loaded with (1) and (2) and after an extended period of mixing and quantitative gravity separation, samples were withdrawn from the aqueous phase. The concentration of (1) in (2) was determined by colorimeter) of the cerium complex. The concentration based upon starting quantities and compositions. Each of the determinations was carried out several times. The method is described also in ref 1. REFERENCES: 1. De Santis, R.; Marrelli, L.; Muscetta, P.N. J. Chem. Eng. Data,		ch phase at equilibrium at 25 ⁰ C was reported
METHOD /APPARATUS/PROCEDURE: SOURCE AND PURITY OF MATERIALS: The determinations were carried out using a separating funnel with a thermostatic jacket. The extractor was loaded with (1) and (2) and after an extended period of mixing and quantitative gravity separation, samples were withdrawn from the aqueous phase. The concentration of (1) in (2) was determined by colorimeter) of the cerium complex. The concentration of (2) in (1) was derived from a material balance based upon starting quantities and compositions. Each of the determinations was carried out several times. The method is described also in ref 1. ESTIMATED ERROR: Temperature: ± 0.1°C. REFERENCES: 1. De Santis, R.; Marrelli, L.; Muscetta, P.N. J. Chem. Eng. Data,	The corresponding mole fraction solubility,	$x_2^{}$, calculated by the compiler, is 0.513.
METHOD /APPARATUS/PROCEDURE: SOURCE AND PURITY OF MATERIALS: The determinations were carried out using a separating funnel with a thermostatic jacket. fractionated before use. The extractor was loaded with (1) and (2) and after an extended period of mixing and quantitative gravity separation, samples were withdrawn from the aqueous phase. The concentration of (1) in (2) was determined by colorimeter) of the cerium complex. The concentration of (2) in (1) was derived from a material balance based upon starting quantities and compositions. Each of the determinations was carried out several times. The method is described also in ref 1. ESTIMATED ERROR: Temperature: ± 0.1°C. REFERENCES: 1. De Santis, R.; Marrelli, L.; Muscetta, P.N. J. Chem. Eng. Data,		
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	The determinations were carried out using a separating funnel with a thermostatic jacket The extractor was loaded with (1) and (2) and after an extended period of mixing and quantitative gravity separation, samples were withdrawn from the aqueous phase. The concentration of (1) in (2) was determined b colorimetric analysis (double-beam Lange colorimeter) of the cerium complex. The concentration of (2) in (1) was derived from a material balance based upon starting quantities and compositions. Each of the determinations was carried out several times	 (1) Carlo Erba analytical purity; fractionated before use. (2) doubly distilled. (2) doubly distilled. (2) ESTIMATED ERROR: Temperature: ± 0.1°C. REFERENCES: 1. De Santis, R.; Marrelli, L.; Muscetta, P.N. J. Chem. Eng. Data,

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) 1-Butanol; C ₄ H ₁₀ 0; [71-36-3]	De Santis, R.; Marrelli, L.; Muscetta, P.N.
(2) Water; H ₂ 0; [7732-18-5]	J. Chem. Eng. Data <u>1976</u> , 21, 324-7.
	Marrelli, L.
	Chem. Eng. J., <u>1979</u> , 18, 225-32.
VARIABLES:	PREPARED BY:
Temperature: 20-40 [°] C	A. Maczynski; S.H. Yalkowsky; S.C. Valvani
EXPERIMENTAL VALUES:	

Mutual solubility of butanol (1) and water (2)

t/ ^o C	g(1)/100g sln		$x_1^{}$ (compile	er)
	(2)-rich phase	(1)-rich phase	(2)-rich phase	(1)-rich phase
20	7.8	80.0	0.020	0.493
30	7.1	79.4	0.018	0.484
40	6.6	78.6	0.017	0.476

AUXILIARY	INFORMATION
METHOD /APPARATUS / PROCEDURE :	SOURCE AND PURITY OF MATERIALS:
The measurements of the solubility limits have been carried out at 20, 30, and 40° C using separator funnels with a thermostatic jacket for temperature control (±0.1 °C). Extractors were loaded with equal quantities of solution at concentrations between zero and the saturation value in the water. After an extended period of mixing and a	 Carlo Erba, analytical purity; refractionated. doubly distilled.

Extractors wer of solution at and the satura After an exten quantitative gravity separation, samples were withdrawn from both phases. Equilibrium compositions were determined by analyzing the alcohol in the aqueous phase. Alcohol in the aqueous phase was determined ESTIMATED ERROR: by colorimetric analysis (double beam Lange Temperature: ± 0.1 °C colorimeter) of the cerium complex. Each of the determinations was carried out Solubility standard deviation: The method is with several repetitions. ±0.5 wt percent also described in ref 1.

REFERENCES:

 De Santis, R.; Marrelli, L.; Muscetta, P.N. Chem. Eng. J. <u>1976</u>, 11, 207-14.

COMPONENTS:	<u></u>		ORIGI	NAL MEASUREMENTS:	
(1) 1-Butanol; C ₄ H ₁₀ 0; [71-36-3]		Lavrova, O.A.; Lesteva, T.M.			
	• = "		Zh.	Fiz. Khim. <u>197</u> 6, 5	50, 1617; Dep. Doc.
(2) Water;	H ₂ 0; [7732-18-5]		VINI	<i>TI</i> 3813-75.	
VARIABLES:			PREPA	RED BY:	
Temperature:	40 and 60 ⁰ C		A. M	aczynski	
EXPERIMENTAL V	ALUES:				
	Mutual	solubility of	l-but	anol(1) and water ((2)
t∕°c	g(1)/100	g sln		x_1 (comp	iler)
	(2)-rich phase	(1)-rich pha	ise	(2)-rich phase	(1)-rich phase
40	6.6	78.50		0.017	0.4701
60	6.45	76.31		0.016	0.4391
		AUXILIARY	INFOR	MATION	
METHOD/APPARA	TUS/PROCEDURE:		SOUR	CE AND PURITY OF MA	TERIALS ;
	n method was used.	e paper.	(1)		
				MATED ERROR: Not specified. RENCES:	

	Four-carbon Alcohols					
OMPONENTS:	ONENTS :			ORIGINAL MEASUREMENTS:		
(1) 1-Butanol; C ₄ H ₁₀ 0; [71-36-3]			Aoki,	Aoki, Y.; Moriyoshi, T.		
(2) Water; H ₂ 0; [7732-18-5]			J. Cher	n. Thermodyn. <u>1978</u> , 2	20, 1173-9 _.	
ARIABLES:			PREPARE	D BY:		
Temperatur	e: 303-3	398K		alvani; S.H. Yalkows	ky: A F M Barton.	
Pressure:	1-2450 a	atm (0.1-25 MPa)	G.T. H		ky, A.F.M.Darton,	
XPERIMENTA	L VALUES	:	<u></u>			
		Mutual solubil:	ity of l-butano	1 (1) and water (2)		
<i>Т /</i> К	p/atm	g(1)/100)g sln	$x_1^{(comp}$	iler)	
		(2)-rich phase	(1)-rich phase	(2)-rich phase	(1)-rich phase	
302.95	1	7.0	79.3	0.0180	0.482	
302.95	500	9.0	77.7	0.0235	0.459	
302.95	970	9.6	76.9	0.0252	0.447	
302.95	1150	10.2	76.3	0.0269	0.439	
302.95	1240	11.0	76.1	0.0292	0.436	
302.95	1500	11.2	75.0	0.0298	0.422	
302.95	2000	12.7	74.0	0.0342	0.409	
302.95	2250	13.9	72.5	0.0377	0.391	
302.95	2450	14.3	72.2	0.0390	0.387	
322.75	1	6.9	77.7	0.0177	0.459	
322.75	500	8.6	76.0	0.0224	0.435	
322.75	1000	9.8	74.4	0.0257	0.414	
322.75	1240	10.6	73.5	0.0280	0.403	
322.75	1550	11.0	73.2	0.0292	0.399	
322.75	2040	12.6	72.2	0.0339	0.387	
				(con	tinued next page)	
		AU	XILIARY INFORMA	TION		
METHOD/APPA	ARATUS/PR	OCEDURE :	SOURCE	AND PURITY OF MATER	IALS:	
for previ butanol. cut-off g capacity placed ir mechanica bath (± 0 least 12 6 h at th a sample Subsequent the conte lower lay Methanol samples h	ious stud Both co glass syr used as n a stain ally shak 0.02 K). h and th e desire of the u ntly the ents allo yer sampl as a mix before re e mass ra	ies on 2-butanol and mponents were placed inge of about 20 cm a sample vessel, wh less steel pressure en in an oil thermo After stirring fo en standing for ano d temperature and p pper layer was with pressure vessel was wed to settle, and ed. ing agent was added fractometric analys tio of sample to m	d iso- d in a 3 ich was vessel stat r at ther ressure drawn. moved, the to the is ethanol REFERE 1. Ma	est grade reagent"; ied by refluxing over stilling twice; ⁵ = 1.3973, d ²⁵ = 0. -ionized, distilled inO ₄ and then redisti ⁵ = 1.3327 TED ERROR: bility: mean error w ± 0.28 g(1)/ NCES: priyoshi, T.; Kanesh hara, K.; Yabumoto, hermodyn. <u>1975</u> , 7, 5	8062 g cm ³ from alkaline iled; within '100g sln mina, S.; K. J. Chem.	

			1-Butanol		
COMPONENTS:			ORIGINA	L MEASUREMENTS:	
(1) 1-Butanol; C ₄ H ₁₀ 0; [71-36-3]			Aoki,	Y.; Moriyoshi, T.	
(2) Wate:	r; H ₂ O;	[7732-18-5]	I Cha	m. Thermodyn. 1978	3 10 1173-9
	2		J. Che	m. 1neimoayn. 1970	, 10, 1175- 7 .
EXPERIMEN	TAL VALU	ES (continued)	- <u> </u>		
<i>T</i> / K	p /atm	g(1)/10	Og eln	2 (2000	vilor)
	1		(1)-rich phase	x _l (comp (2)-rich phase	(1)-rich phase
322.75	2250	12.7	71.5		÷
322.75	2450	13.2		0.0342	0.379
3 32.65	1	7.0	70.7 76.1	0.0356	0.370
3 32.65	500	7.5		0.0180	0.436
332.65	1000	8.6	74.5	0.0193	0.415
332.65			73.2	0.0224	0.399
332.65	1500 2010	9.3	71.7	0.0243	0.381
	2010	9.5	70.5	0.0249	0.368
332.65	2180	10.8	70.0	0.0286	0.362
332.65	2250	10.8	69.2	0.0286	0.353
332.65	2400	11.3	69.0	0.0302	0.351
332.65	2450	11.5	69.0	0.0306	0.351
342.65	1	6.7	75.0	0.0171	0.422
342.65	670	7.8	72.5	0.0202	0.391
342.65	1700	10.2	69.5	0.0269	0.357
342.65	2040	10.7	68.5	0.0283	0.346
342.65	2450	11.9	66.6	0.0318	0.327
362.65	1	7.5	69.7	0.0193	0,359
362.65	1000	10.7	65.4	0.0283	0.315
362.65	1040	-	65.4	-	0.315
362.65	1290	11.3	64.9	0.0302	0.310
362.65	1700	13.2	63.5	0.0356	0,297
362.65	2000	14.5	62.6	0.0396	0.289
362.65	2180	15.5	62.3	0.0427	0.287
362.65	2450	16.1	61.4	0.0446	0.278
372.45	1	9.5	66.8	0.0249	0.328
372.45	1000	12.3	62.8	0.0330	0.291
372.45	1290	12.7	62.3	0.0342	0,287
372.45	1570	13.7	60.7	0.0371	0.273
372.45	1800	15.6	60.3	0.0430	0.270
372.45	1970	16.7	58.9	0.0465	0.258
372.45	2450	18.5	55.2	0.0522	0.231
380.05	1	10.6	62.7	0.0280	0.290
380.05	500	11.5	60.9	0.0306	0.274
380.05	1000	13.2	59.0	0.0356	0.259
380.05	1500	15.8	57.4	0.0436	
380.05	2000	16.7	54.5	0.0458	0.247
380.05	2300	20.3			0.226
380.05	2450	25.5	52.3	0.0583	0.210
382.95	1	11.0	44.9 61 7	0.0768	0.165
382.95	500	11.0	61.7	0.0292	0.281
	500	11.7	60.1	0.0318 (cont	0.268 inued next page)

COMPONENT	 IS :		ORIGINA	ORIGINAL MEASUREMENTS;		
		H ₁₀ 0; [71-36-3]	Aoki,	Aoki, Y.; Moriyoshi, T.		
(2) Water; H ₂ 0; [7732-18-5]				J. Chem. Thermodyn. <u>1978</u> , 10, 1173-9.		
(2) wate	r; n ₂ 0; [//32-10-3]	J. Che	m. 1'hermoayn. <u>1978</u>	<u>8</u> , <i>10</i> , 1173-9.	
EXPERIME	NTAL VALU	ES (continued)		· · · · · · · · · · · · · · · · · · ·		
<i>Т</i> /к	p/atm	g(1)/10	Og sln	$x_1(comp)$	iler)	
		(2)-rich phase	(1)-rich phase	(2)-rich phase	(1)-rich phase	
382.95	1000	13.9	58.3	0.0377	0.254	
382.95	1500	16.5	56.4	0.0458	0.239	
382.95	1570	17.2	56.3	0.0481	0.238	
382.95	1700	17.3	55.8	0.0484	0.235	
382.95	1900	18.0	54.1	0.0506	0.223	
382.95	2000	19.6	52.5	0.0559	0.212	
382.95	2100	23.1	48.9	0.0680	0.189	
382.95	2200	31.6	41.0	0.1009	0.145	
384.45	1700	19.4	54.6	0.0552	0.227	
384.45	1800	20.0	52.4	0.0573	0.211	
384.45	1900	22.5	49.9	0.0659	0.195	
384.45	2000	30.8	41.0	0.0976	0.227	
386.15	1500	20.2	53.5	0.0579	0.218	
386.15	1570	22.2	51.8	0.0649	0.207	
386.15	1670	27.5	46.0	0.0844	0.172	
387.15	1500	26.4	46.1	0.0802	0.172	
388.15	1000	17.8	53.2	0.0500	0.216	
388.15	1090	18.0	53.0	0.0506	0.215	
388.15	1200	19.0	51.8	0.0539	0.207	
388.15	1360	25.9	45.5	0.0783	0.169	
388.15	1400	31.2	40.2	0.0992	0.141	
390.35	800	18.0	52.9	0.0506	0.214	
390.35	900	19.0	50.1	0.0539	0.196	
390.35	1000	25.2	45.7	0.0757	0.170	
391.25	1	14.5	55.6	0.0396	0.233	
391.25	300	15.6	54.6	0.0430	0.227	
391.25	500	16.7	53.7	0.0465	0.220	
391.25	600	18.0	53.5	0.0506	0.218	
391.25	720	19.7	51.8	0.0562	0.207	
391.25	770	21.6	48.5	0.0627	0.187	
391.25	790	23.5	44.1	0.0695	0.160	
392.45	450	25.5	45.5	0.0768	0.169	
392.45	500	30.0	39.8	0.0944	0.139	
392.95	1	17.2	53.7	0.0481	0.220	
392.95	270	21.2	49.7	0.0613	0.194	
392.95	340	26.3	46.3	0.0798	0.173	
392.95	350	27.1	44.7	0.0829	0.164	
395.25	1	18.2	47.7	0.0513	0.182	
395.25	150	25.1	41.9	0.0753	0.149	
395.2 5	200	32.3	36.8	0.1039	0.124	
					ntinued next page)	

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) 1-Butanol; C ₄ H ₁₀ 0; [71-36-3]	Aoki, Y.; Moriyoshi, T.
(2) Water; H ₂ 0; [7732-18-5]	J. Chem. Thermodyn. <u>1978</u> , 10, 1173-9

EXPERIMENTAL VALUES (continued)

T/K	p/atm	g(1)/100g sln		$x_1^{(comp}$	iler)
		(2)-rich phase	(1)-rich phase	(2)-rich phase	(1)-rich phase
395.85	1	18.9	48.0	0.0536	0.183
397.05	1	21.8	44.9	0.0635	0.165
397.45	1	24.7	41.8	0.0739	0.148
397.75	1	27.9	38.8	0.0859	0.134

Properties of the critical solutions

p_{c}^{\prime}/atm	_{Tc} (UCST)/κ	x_{1c}
1	397.85	0.110
204	395.25	0.113
380	392.95	0.117
500	392.45	0.115
820	391.25	0.118
1000	390.65	0.118
1030	390.35	0.118
1390	388,15	0.118
1500	387.65	0.120
1710	386.15	0.122
2000	384.35	0.122
2010	384.45	0.121
2200	382.95	0.121
2450	381.15	0.123
2500	380.05	0.125

 $(d \ \underline{r}/dp) = -(12.0 \pm 0.5) \times 10^{-3} \text{ K atm}^{-1} \text{ at } p < 400 \text{ atm}$ -(7.0 ± 0.7) x 10⁻³ K atm⁻¹ at 800 < p < 2500 atm

$$-(7.0 \pm 0.7) \times 10$$
 K atm at 800

$$(dx_{1,c}/dT) = -(4.0 \pm 0.5) \times 10^{-4} \text{ K}^{-1}$$

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) 1-Butanol; C ₄ H ₁₀ 0; [71-36-3] (2) Water; H ₂ 0; [7732-18-5]	Nishino, N.; Nakamura, M. Bull. Chem. Soc. Japan <u>1978</u> , 51, 1617-20; <u>1981</u> , 54, 545-8.
VARIABLES:	PREPARED BY:
Temperature: 275-360 K	G.T. Hefter

The mutual solubility of (1) and (2) in mole fractions are reported over the temperature range in graphical form. Graphical data are also presented for the heat of solution at infinite dilution of (1) in (2) and for the heat of evaporation of (1).

AUXILIARY	INFORMATION
METHOD/APPARATUS/PROCEDURE: The turbidimetric method was used. Twenty to thirty glass ampoules containing aqueous solutions of ca . 5 cm ³ of various concentra- tions near the solubility at room tempera- ture were immersed in a water thermostat. The distinction between clear and turbid ampoules was made after equilibrium was established (ca . 2h). The smooth curve drawn to separate the clear and turbid regions was regarded as the solubility curve.	 SOURCE AND PURITY OF MATERIALS: (1) G.R. grade (various commercial sources given); dried over calcium oxide; kept in ampoules over magnesium powder. (2) Deionized, refluxed for 15 h with potassium permanganate then distilled.
	ESTIMATED ERROR: Not stated.
	REFERENCES :

		1-Bu	tanol	87
COMPONENTS:			ORIGINAL MEASUREMENTS:	
(1) 1-Butanol; C ₄ H ₁₀ O; [71-36-3]			Lyzlova, R.V.	
(2) Water; H ₂ 0; [7732-18-5]			Zhur. Prikl. Khim. (Lenis 545–50.	ngrad) <u>1979</u> , 52,
			*J. App. Chem. USSR <u>1979</u>	, <i>52</i> , 509–14.
VARIABLES:		······	PREPARED BY:	
Temperatur	re: 20° C and 90° C		A.F.M. Barton	
EXPERIMENTA	L VALUES:	;	L	
	Mutual s	olubility of 1-b	utanol(1) and water(2)	
t/°c	<i>x</i> ₁		g(1)/100g sln	(compiler)
A1	-		se Alcohol-rich phase	Water-rich phase
20	0.478	0.021	79.0	8,1
90	0.360	0.020	69.8	7.7
		AUXILIARY	INFORMATION	
METHOD/APPA	ARATUS/PROCEDURE:		SOURCE AND PURITY OF MATE	ERIALS:
The analytical method was used, samples being withdrawn from coexisting liquid phases at equilibrium for analysis by refractometry. An IRF-23 refractometer measured the refractive index correct to 0.000 02. The study was concerned with phase equilibria in the ternary system 1-butanol/2-methyl-1- propanol/water, and only a few experiments dealt with mutual solubilities in the binary systems.			dried over freshly distilled twice wit fractionating colum $n_{\rm D}^{20}$ 1.39920 d_4^{20} 0.8	h 1.5 m gĺasš-packed m;
1			ESTIMATED ERROR:	

Not specified for binary systems; error below \pm 1% for water and \pm 1.5% for alcohol ratios in ternary systems.

REFERENCES:

COMPONENTS:	ORIGINAL MEASUREMENTS:
	Singh, R.P.; Haque, M.M.
(1) 1-Butanol; C ₄ H ₁₀ 0; [71-36-3]	Indian J. Chem. 1979, 17A, 449-51.
(2) Water; H ₂ 0; [7732-18-5]	Incluse of orests, 1713, 178, 443-51.
	· · · · · · · · · · · · · · · · · · ·
VARIABLES:	PREPARED BY:
One temperature: 30 ⁰ C	A.F.M. Barton
EXPERIMENTAL VALUES:	
Mutual solubility of 1-b	outanol(1) and water(2) at 30 ⁰ C
mol(2)/mol(1	$\begin{array}{ccc} 1 & x_1 & g(1)/100g \ \text{sln} \\ & (\text{compiler}) \end{array}$
alcohol-rich phase 1.0339	0.4920 79.9
water-rich phase 56.505	0.01677 6.56
AUXILIARY	INFORMATION
ME THOD /APPARATUS / PROCEDURE :	SOURCE AND PURITY OF MATERIALS:
Titrations of one component with the other (ref 1) were carried out in well-stoppered volumetric flasks. The shaking after each addition was done ultrasonically for at least 30 min. These results formed part of a study of the ternary system 1-butanol/ methanol/water.	 B.D.H. AR; purified; density and refractive index checked conductivity water from all-glass still
	ESTIMATED ERROR:
	Temperature: ± 0,1 ⁰ C Solubility: each titration repeated at least three times.
	REFERENCES: 1. Simonsen, D.R.; Washburn, E.R. J. Am. Chem. Soc. <u>1946</u> , 68, 235.

COMPONENTS :	ORIGINAL MEASUREMENTS:			
(1) 1-Butanol; C ₄ H ₁₀ 0; [71-36-3]	Fu, C.F.; King, C.L.; Chang, Y.F.; Xeu, C.X.			
(2) Water; H ₂ 0; [7732-18-5]	Hua Kung Hsueh Pao <u>1980</u> (3), 281-92.			
VARIABLES:	PREPARED BY:			
One temperature: 93 ⁰ C	C.F. Fu			
EXPERIMENTAL VALUES:				
The proportion of 1-butanol in the water	-rich phase at equilibrium at 92.8 ⁰ C was reported			
	to be 6.87 g(1)/100g sln. The corresponding mole fraction solubility, x_1 , is 0.0176.			
	-			
The proportion of water in the alcohol-rich phase at 92.8° C was reported to be				
30.80 g(2)/100g sln. The corresponding mole fraction solubility, x_2 , is 0.6467.				

AUXILIARY	INFORMATION
METHOD/APPARATUS/PROCEDURE: The turbidimetric method was used. Homogenous solutions were prepared and boiled at 760 mm Hg in a specially designed flask attached to a condenser of negligible hold- up compared with the volume of liquid solution. The solution was stirred by a magnetic stirrer and titrated with (1) or (2). The end point of titration was judged both by cloudiness and constancy of boiling temperature.	 SOURCE AND PURITY OF MATERIALS: (Some information not in the published paper has been supplied by the compiler) (1) Beijing Chemicals reagent; used as received; b.p. 117.1°C (760 mm Hg) n¹⁵_D 1.3992, d¹⁵₄ 0.8091. (2) distilled.
	ESTIMATED ERROR: (Supplied by compiler) Temperature: ± 0.02 ⁰ C Solubility: 0.4%
	REFERENCES :

	COMPONENTS :			ORIGINAL MEASUREMENTS:		
			Tokunaga, S.; Manabe, M.; Koda, M.			
(1) 1-Butanol; C ₄ H ₁₀ O; [71-36-3] (2) Water; H ₂ O; [7732-18-5]			Niihama Kogyo Koto Semmon Gakko Kiyo, Rikogaku Hen (Memoirs Niihama Technical College, Sci,and Eng.) <u>1980</u> , 16, 96–101.			
					VARIABLES:	
Temperature:	15 - 35 [°] C		A.F.M. Bar	ton		
EXPERIMENTAL VAI	LUES:	<u></u>				
	So	olubility of water i	n the alcoho	1-rich phase		
	t/ ^o c	g(2)/100g sln	<i>x</i> 2	mol(1)/mol(2)		
	15	19.9	0.506	0.983		
	20	20.1	0.509	0.969		
	25	20.4	0,513	0,955		
	35	21.1	0.523	0.929		
		AUXILIARY	INFORMATION			
(~ 10 mL) were stoppered vess 10-12 h in a v	of l-butano stirred m sel and all vater therm	E: 1 (~ 5 mL) and water agnetically in a owed to stand for	SOURCE AND (1) dist: no in chron	PURITY OF MATERIALS: illed; mpurities detectable by gas matography. nized; illed prior to use,		

COMPONENTS :	ORIGINAL MEASUREMENTS:
<pre>(1) 1-Butanol; C₄H₁₀0; [71-36-3] (2) Water; H₂0; [7732-18-5]</pre>	Lutugina, N.V., Reshchetova, L.I. <i>Vestnik Leningr. Univ.</i> <u>1972</u> , 16, 75-81.
VARIABLES: One temperature: 92.7 [°] C	PREPARED BY: C.F. Fu and G.T. Hefter

The solubility of 1-butanol in the water-rich phase at 92.7° C was reported to be 0.020 mole fraction.

The solubility of 1-butanol in the alcohol-rich phase at 92.7° C was reported to be 0.360 mole fraction.

The corresponding mass solubilities calculated by the compilers are 7.7 g(1)/100g sln and 69.8 g(1)/100g sln.

AUXILIARY INFORMATION				
METHOD/APPARATUS/PROCEDURE: Vapor-liquid-liquid equilibrium still des- cribed in ref 1 was used for liquid-liquid equilibrium determination at boiling point. Immediately after cutting off heating and stopping of violent boiling, samples were taken from both layers for analysis. Analytical method was described in detail.	<pre>SOURCE AND PURITY OF MATERIALS: (1) Source not specified; distilled over a column of 20 theoretical plates (according to C₆H₆ - CC2₄); b.p. 117.5°C (760 mm Hg), n²⁰_D 1.3993, d²⁰₄ 0.8098 (2) distilled. (2) distilled. ESTIMATED ERROR: Not specified REFERENCES: 1. Morachevskii, A.G.; Smirnova, N.A. Zh. Prikl. Khim. <u>1963</u>, 36, 2391.</pre>			

COMPONENTS:	ORIGINAL MEASUREMENTS:	
(1) 1-Butanol-d; C ₄ H ₉ DO; [4712-38-3]	Rabinovich, I.B., Fedorov, V.D.,	
	Pashkin, N.P., Avdesnyak, M.A.,	
(2) Water-d ₂ ; D ₂ 0; [7789-20-0]	Pimenov, N. Ya.	
	Dokl. Adad. Nauk SSSR <u>1955</u> , 105, 108-11.	
VARIABLES:	PREPARED BY:	
Temperature: 40-130°C	G. Jancso.and G.T. Hefter.	
EXPERIMENTAL VALUES:		
Effect of deuteration o	n solubility of l-butanol in water	
t/ ^o C 1	$00(L_{\rm H} - L_{\rm D})/L_{\rm H}^{\alpha}$	
40	42	
66	35	
80	32	
100	29	
103	24	
108	30	
125	67 ^b	
${}^{b}_{This}$ value refers to a temperature that control the l-butanol-H $_{2}^{0}$ system.	rresponds to within ± 0.5 K to the UCST of	
	(continued next page)	
AUXILIARY	INFORMATION	
METHOD /APPARATUS / PROCEDURE :	SOURCE AND PURITY OF MATERIALS;	
The synthetic method (cloud-clear points) of Alexejew (ref 1) was used which consists in observing the temperature at which a measured weight of one liquid is visually soluble in a measured weight of the other liquid.	 (1) 1-butanol-d was prepared by the hydrolysis of the aluminium salt of the ordinary butanol with D₂O. The OD group of the product had² a deuterium content of > 99 at. %. (2) D₂O, 99.0 - 99.8 at. % D, source not given. 	
	ESTIMATED ERROR: Solubility: not specified Temperature: ±0.02 [°] C	

```
      COMPONENTS:
      ORIGINAL MEASUREMENTS:

      (1) 1-Butanol-d; C<sub>4</sub>H<sub>9</sub>DO; [4712-38-3]
      Rabinovich, I.R., Fedorov, V.D.,

      (2) Water-d<sub>2</sub>; D<sub>2</sub>O; [7789-20-0]
      Pashkin, N.P., Avdesnyak, M.A.,

      Pimenov, N. Ya.
      Dokl. Akad. Nauk SSSR 1955, 105, 108-11.
```

EXPERIMENTAL VALUES: (continued)

The upper critical solution temperature of 1-butanol and H_2^0 is 125.1°C, compared with 131.1°C for 1-butanol-d and D_2^0 .

Mutual solubilities for the 1-butanol-H $_2^0$ system were also determined but only graphical data were given (Δ in Figure 1).

The literature reference for the data of Hill and Malisov (o) is not given but is presumably that listed as ref 4 in the Critical Evaluation.

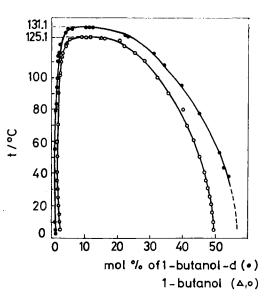


Fig. 1. Mutual solubilities of $CH_3CH_2CH_2CH_2OD(1)$ in $D_2O(2)$ (•) and $CH_3CH_2CH_2OH(1)$ in $H_2O(2)$ (Δ ,o)

CONDONENTS	· · · · · ·	EVALUATOD -	1		
COMPONENTS: (1) 2-Butanol (sec-butanol): $(H \cap H)$		EVALUATOR:			
(1) 2-Butanol (<i>sec-butanol</i>); C ₄ H ₁₀ 0;		G.T. Hefter, School of Mathematical and			
[78-92-2]		-	Physical Sciences, Murdoch University,		
(2) Water; H ₂ 0; [7732-18-5]		Perth, Western Australia. November 1982.			
CRITICAL EVALUATION:		L			
The solubility in the 2-butan	ol (1) - water	(2) system has been rep	ported in a form		
suitable for critical evaluat					
Reference	T/K	Solubility	Method		
Alexejew (ref 1)	283-376	mutual	synthetic/analytical		
Dolgolenko (ref 3)	250-388	mutual	synthetic		
Evans (ref 6)	293	mutual	volumetric		
Altsybeeva $et al.$ (ref 7)	293-353	mutual	analytical		
Morachevskii and Popovich	283-368	(1) in (2)	refractometric		
(ref 8) Ratouis and Dode (ref 9)	298 & 303	(1) in (2)	analytical		
Shakhud <i>et al.</i> (ref 12)	293 - 333	mutual	titration		
Moriyoshi <i>et al.</i> (ref 13)	283-383	mutual	refractometric		
De Santis <i>et al</i> . (ref 14) Becke and Quitzch (ref 15)	298 298	mutual mutual	analytical refractometric		
The original data are given i Evaluation. Data sheets have not been pre and Russo (ref 10) and Rabino contain original data	pared for the g	graphical data of Timme	rmans (ref 2), Schneider		
contain original data. Solubilities in the system 2-butanol- d , C_4H_9 OD, and water- d_2 , D_2O , are given in the data sheet for Rabinovich <i>et al.</i> (ref 16) following the 2-butanol/water system data sheets.					
In the Critical Evaluation the data of Mullens $et \ all$.(ref ll) in weight/volume fractions are excluded from consideration because no density information was included.					
Of the data obtained by Dolgolenko (ref 3) only the highest boiling fraction (b.p. 99.0 - 99.5°C, see data sheet) has been considered in the Critical Evaluation as the physical properties of that fraction correspond most closely to those reported for 2-butanol by other workers (ref 8,12). This is consistent with the view of the original author (ref 3).					
The data of Becke and Quitzch (ref 15), the water-rich phase data of Dolgolenko (ref 3), Altsybeeva <i>et al.</i> (ref 7) and De Santis <i>et al.</i> (ref 14), and the alcohol-rich phase data of Alexejew (ref 1) disagree markedly from all other studies and are rejected.					
The data point at 333 K, water-rich phase, in the otherwise satisfactory study by Moriyoshi <i>et al.</i> (ref 13) is also in marked disagreement with other studies and has been rejected.					
All other data are included i by graphical interpolation or asterisk (*). "Best" values	extrapolation	5			
		(continued	nevt nage)		

(continued next page)

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COMPONENTS:	EVALUATOR:
(1) 2-Butanol (<i>sec-butanol</i>); C ₄ H ₁₀ 0; [78-92-2]	G.T. Hefter, School of Mathematical and Physical Sciences, Murdoch University,
(2) Water; H ₂ 0; [7732-18-5]	Perth, Western Australia. November 1982.

CRITICAL EVALUATION: (continued)

The uncertainty limits (σ_n) attached to these "best" values do not have statistical significance. They are to be regarded only as a convenient representation of the spread of the reported values and not as error limits.

It will be noted from the tables following that there are serious disagreements among the solubility data reported by independent workers for the system 2-butanol-water. This is reflected in the large σ_n values.

No one study or any of the averaged values can be singled out for recommendation and clearly this sytem requires a careful and thorough re-investigation over the entire temperature range. The values given in the following tables should be regarded as *tentative* only, until further independent studies can be made.

This situation is surprising since the 2-butanol-water system possesses some interesting features. At atmospheric pressures the solubility curve is strongly "waisted" at low temperatures (ref 2,3) and, depending on the purity of the 2-butanol, may even show a closed miscibility loop (ref 3)! This loop is unusually sensitive to pressure (ref 4,13) and disappears entirely at about 830 atm (the hypercritical point: see below).

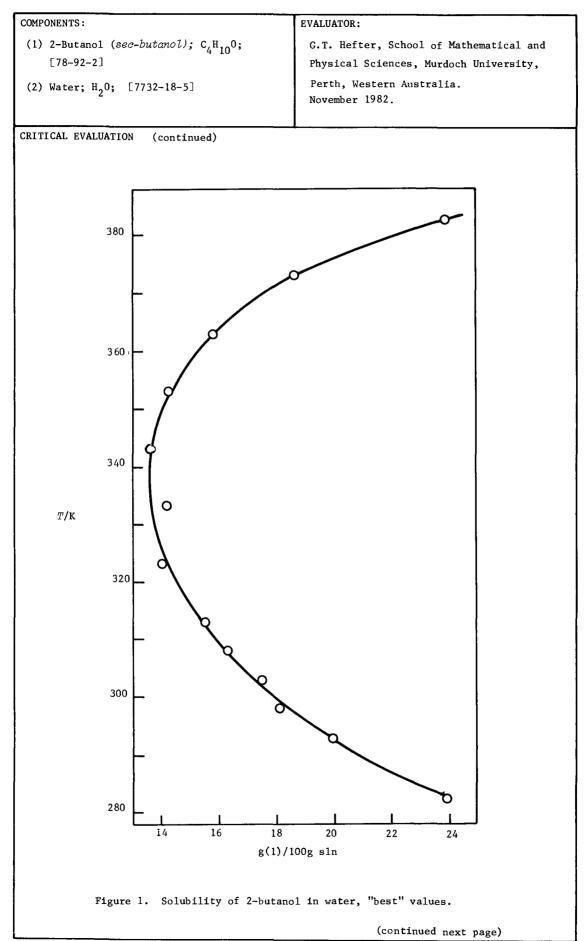
The crucial effect of alcohol purity on the solubility curve (ref 3) may of course be the reason for the lack of agreement between independent workers already noted and supports the need for further precise studies of this sytem supported by modern methods of analysis and purity determination.

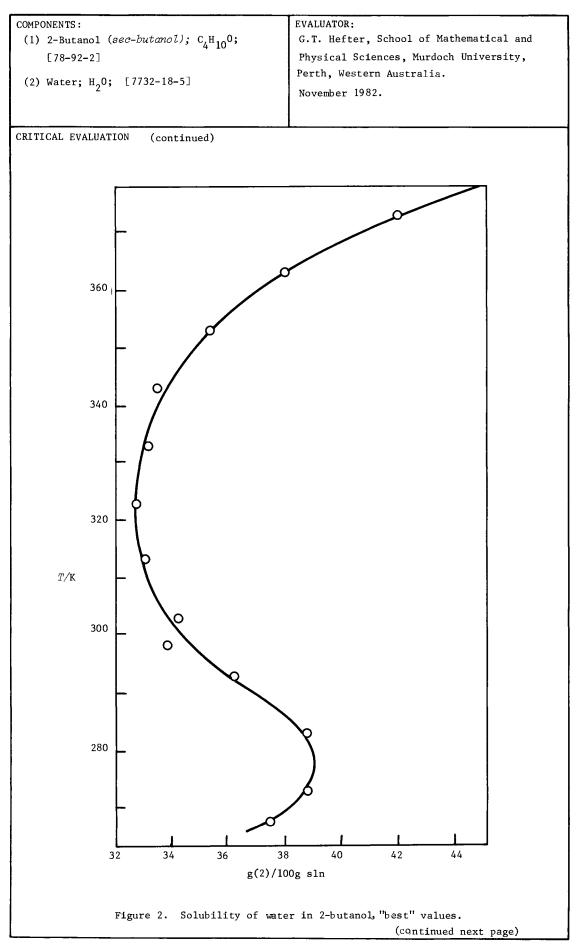
The solubility of 2-butanol (1) in water (2)

T/K	Solubility, g(1)/100g sln	
	Reported values "Best	" values $(\pm \sigma_n)$
283	23.9 (ref 13)	23.9
293	19.8 (ref 8), 19.62 (ref 12), 20.2 (ref 13)	19.9 ± 0.2
298	19.0 [*] (ref 1), 18.5 (ref 6), 17.70 (ref 9), 17.0 [*] (ref 13)	18.1 ± 0.8
303	17.0 [*] (ref 1), 17.9 (ref 13)	17.5 ± 0.5
308	16.0 [*] (ref 1), 16.5 (ref 9)	16.3 ± 0.3
313	15.3 [*] (ref 1), 15.6 (ref 8), 16.24 (ref 12), 14.9 (ref 13)	15.5 ± 0.5
323	14.8 [*] (ref 1), 13.2 (ref 13)	14.0 ± 0.8
333	14.5 [*] (ref 1), 14.0 (ref 8), 13.98 (ref 12)	14.2 ± 0.2
343	14.6 [*] (ref 1), 12.9 (ref 13)	13.8 ± 0.9
353	15.1 [*] (ref 1), 14.0 (ref 8), 13.8 (ref 13)	14.3 \pm 0.6
363	16.0 [*] (ref 1), 15.5 (ref 13)	15.8 ± 0.3
373	18.9 [*] (ref 1), 18.3 (ref 13)	18.6 ± 0.3
383	23.9 (ref 13)	23.9

(I) 2-Buta	-1 (acc but moths C H O	EVALUATOR:	
(1) 2-Butanol (<i>sec-butanol</i>); C ₄ H ₁₀ 0; [78-92-2]		G.T. Hefter, School of Mathematical and Physical Sciences, Murdoch University,	
(2) Water; H ₂ 0; [7732-18-5]		Perth, Western Australia. November 1982.	
CRITICAL EV	ALUATION (continued)	<u> </u>	
	The solubility o	f water (2) in 2-butanol (1)	
T/K		Solubility, g(2)/100g sln	
	Reported val	ues "Best" values (±ơ	
268	37.5 [*] (ref 3)	37.5	
273	38.8 [*] (ref 3)	38.8	
283	38.4 [*] (ref 3), 39.1 (ref 13)	38.8 ± 0.4	
293	35.8 [*] (ref 3), 35.6 (ref 6), 36.	1 (ref 7), 36.8 (ref 8),	
		36.52 (ref 12) 36.2 (ref 13) 36.2 ± 0.4	
298	34.7 [*] (ref 3), 33.9 [*] (ref 13), 33	$3.1 (ref 14)$ 33.9 ± 0.7	
303	34.0 [*] (ref 3), 34.5 (ref 13)	34.3 ± 0.3	
313	33.4 [*] (ref 3), 33.0 (ref 7), 33.	5 (ref 8), 33.0 [*] (ref 12),	
		32.8 (ref 13) 33.1 ± 0.3	
323	33.1 [*] (ref 3), 32.5 (ref 13)	32.8 ± 0.3	
333	33.3 [*] (ref 3), 33.4 (ref 7) 33.8	(ref 8), 32.64 (ref 12),	
		33.1 (ref 13) 33.2 ± 0.4	
343	33.8 [*] (ref 3), 33.8 (ref 7), 32.	8 (ref 13) 33.5 ± 0.5	
353	35.0 [*] (ref 3), 36.2 (ref 8), 34.	7 (ref 13) 35.3 ± 0.6	
363	37.7 [*] (ref 3), 38.2 (ref 13)	38.0 ± 0.3	
373	41.5[*](ref 3), 42.3 (ref 13)	41.9 ± 0.4	
383	49.0 [*] (ref 3), 49.3 (ref 13)	49.2 ± 0.2	
Timmermans	, 0.1-80 MPa) on the lower and upp	13) have determined the effects of pressure wer critical solution temperatures. Their	
-	e in reasonable agreement (T_{c} diff	ers by ca. r = 5k/.	
results ar Moriyoshi	et al. (ref 13) have also determin $(0.1-80 \text{ MPa})$ and the "hypercritica	eed the mutual solubility of (1) and (2) at 1 point", i.e. where the closed solubility	
results ar Moriyoshi 1-800 atm	et al. (ref 13) have also determin $(0.1-80 \text{ MPa})$ and the "hypercritica	ed the mutual solubility of (1) and (2) at	
results ar Moriyoshi 1-800 atm	et al. (ref 13) have also determin $(0.1-80 \text{ MPa})$ and the "hypercritica	ed the mutual solubility of (1) and (2) at	
results ar Moriyoshi 1-800 atm	et al. (ref 13) have also determin $(0.1-80 \text{ MPa})$ and the "hypercritica	ed the mutual solubility of (1) and (2) at	
results ar Moriyoshi 1-800 atm	et al. (ref 13) have also determin $(0.1-80 \text{ MPa})$ and the "hypercritica	ed the mutual solubility of (1) and (2) at	
results ar Moriyoshi 1-800 atm	et al. (ref 13) have also determin $(0.1-80 \text{ MPa})$ and the "hypercritica	ed the mutual solubility of (1) and (2) at	
results ar Moriyoshi 1-800 atm	et al. (ref 13) have also determin $(0.1-80 \text{ MPa})$ and the "hypercritica	ed the mutual solubility of (1) and (2) at	
results ar Moriyoshi 1-800 atm	et al. (ref 13) have also determin $(0.1-80 \text{ MPa})$ and the "hypercritica	ed the mutual solubility of (1) and (2) at	
results ar Moriyoshi 1-800 atm	et al. (ref 13) have also determin $(0.1-80 \text{ MPa})$ and the "hypercritica	ed the mutual solubility of (1) and (2) at	

(continued next page)





COMPO	NENTS :	EVALUATOR:	
(1)	2-Butanol (sec-butanol); C ₄ H ₁₀ 0;	G.T. Hefter, School of Mathematical and	
	[78-92-2]	Physical Sciences, Murdoch University,	
(2) Water; H ₂ 0; [7732-18-5] Perth, Western Australia.			
(2)	waler, 1120, 17732-10-51	November 1982.	
CRITI	CAL EVALUATION (continued)		
	rences		
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13.	Moriyoshi, T.; Kaneshina, S.; Aihara, K <u>1975</u> , 7, 537.	.; Yabumoto, K. J. Chem. Thermodyn.	
14.	De Santis, R.; Marrelli, L.; Muscetta, H	P.N. Chem. Eng. J. <u>1976</u> , 11, 207.	
15.	Becke, A.; Quitzch, G. Chem. Tech. 1977	<i>, 29</i> , 49 .	
16.	Rabinovich, I.B.; Fedorov, V.D.; Pashkin Dokl. Akad/Nauk SSSR <u>1955</u> , 105, 108.	n, N.P.; Avdesnyak, M.A.; Pimenov, N, Ya.	
l			

COMPONENT	S:			ORIGINAL	MEASUREMENT	rs:
(1) 2-Butanol; (sec-butanol); C ₄ H ₁₀ 0;		Alexejew, W.				
[78-92-2]						
		[7732-18-5]		Ann. Ph	ys. Chem. <u>1</u>	886, 28, 305-38.
	2					
VARIABLES				DREDARED		
		0		PREPARED		aczynska; A. Szafranski
Temperat	ure: 10-	103 °C			,,	,,
EXPERIMENTAL VALUES:						
		Mutual	solubility of	2-butano	1(1) and wa	ter (2)
t,	∕°c	g(1)/100	g sln		$x_1(\text{com})$	piler)
	(2)-	-rich phase	(1)-rich phas	se (2)	-rich phase	(1)-rich phase
10	0.1	-	55.2		-	0.230
20	D .9	-	60.3		-	0.270
24	ł	20.1	-		0.0576	-
28	3.5	-	62.4		-	0.287
32	2	17.1	-		0.0477	
34	4	15.9	-		0.0439	~
50	ó	14.7	~		0.0402	-
72	2	14.7	-		0.0402	-
77	7.1	-	62.4		-	0.287
84	4.5	~	60.3		-	0.270
88	3.3	15.9	-		0.0439	-
90	5.1	-	55.2		-	0.230
91	7.5	-	54.9		-	0.228
9	7.6	17.1	-		0.0477	~
10	1.5	20.1	-		0.0576	-
102	2.5	-	48.8		-	0.188
			AUXILIARY	INFORMAT	ION	
METHOD /AJ	PARATUS/PI	ROCEDURE :		SOURCE A	ND PURITY O	F MATERIALS:
		or analytica only when the		(1) no	t specified	•
		emperature.	5010011109	(2) no	t specified	
Into a 1	ared glass	s tube (1) was	s introduced			
and weig	ghed, then	(2) was added	l through a			
	ry funnel. ed. fastene		is sealed, c of a mercury	[
thermome	eter and re	epeatedly heat	ed and			
		(or glycerol) respectivel) bath until 7 homogeneous			
and turl			, Ç	ESTIMAT	ED ERROR:	
				110	t specified	•
				REFEREN	CESI	
				NETEKEN	620;	
				1		

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) 2-Butanol (<i>sec-butanol</i>); C ₄ H ₁₀ 0;	Dolgolenko, W.
[78-92-2]	Z. Phys. Chem. <u>1908</u> , 62, 499-511.
(2) Water; H ₂ 0; [7732-18-5]	
2	
VARIABLES: Temperature: -23 - 115 ⁰ C	PREPARED BY:
Temperature: $-23 - 115$ C Distillation fractions of (1): 98.0-99.5°C	G.T. Hefter
Distillation fractions of (1): 98.0-99.5 C	
EXPERIMENTAL VALUES:	
The mutual solubility of 2-butanol and water	ring determined for three beiling rence
fractions of 2-butanol. As quite considerab	5 5
by the author for all three fractions are give	· ·
, , , , , , , , , , , , , , , , , , ,	
mutual solubility data for a separate sample	
N.P. Ipatiew; the data are similar to those i	ii iaure a.
Note that the third distillation fraction (Ta	ble c) shows a closed solubility loop with
a lower critical solution temperature of ca 7	0 ⁰ C. This is attributed by the author
to contamination of the 2-butanol by tertiary	-butanol or iso -butanol. The upper
critical solution temperature varies from ca.	
t/ ^o C g(1)/100g s1	ln x ₁
(2)-rich phase (1)-	-rich phase (2)-rich phase (1)-rich phase
a. First distillation fraction of 2-butanol	
B.p. 98.0-97.6°C at 760.8 mm Hg; d_4^{20} 0.8059	96
	35.76 - 0.119
7.0 -	43.36 - 0.157
8.6 -	- 0.0934 -
9.9 29.76	(continued next page)
AUXILIARY	INFORMATION
METHOD / APPARATUS / PROCEDURE :	SOURCE AND PURITY OF MATERIALS:
The synthetic method of Alexejew (ref 1)	(1) Kahlbaum;
was used. The two components were care-	dried with barium oxide then
fully weighed into glass tubes which were fitted into a wooden holder and placed	fractionated.
in a large beaker or, for low temperature	(2) not specified.
work, a Dewar flask. The temperature was then lowered and raised whilst the tubes	Other details given in the data tables.
were shaken and the turbidity temperature	
was noted until consistent results were obtained. See also comments above.	
obtained. See also comments above.	
	ESTIMATED ERROR:
1	
	Temperature: 0.05 ⁰ C
	Temperature: 0.05 ⁰ C
	Temperature: 0.05 ⁰ C Composition: See data
	Temperature: 0.05 [°] C Composition: See data REFERENCES:
	Temperature: 0.05 [°] C Composition: See data REFERENCES:
	Temperature: 0.05 [°] C Composition: See data REFERENCES:

<u> </u>					
COMPONENTS:	u + m o 1, $C = 0$,		MEASUREMENTS :		
(1) 2-Butanol (<i>sec-b</i> [78-92-2]	4 ^{10⁰}	Dolgolenk			
		2. Phys.	Chem. <u>1908</u> , 62, 49	9-511.	
(2) Water; H ₂ 0; [77	32-18-5]				
EXPERIMENTAL VALUES	(continued)				
t/ ^o C					
	g(1)/10	Ug sln	x	x_1	
	(2)-rich phase	(1)-rich phase	(2)-rich phase	(1)-rich phase	
11.2	28.55	-	0.0885	-	
11.3	-	48.92	-	0.189	
15.7	-	53.77	-	0.220	
17.2	-	55.02	-	0.229	
21.9	21.77	-	0.0634	-	
22.4	-	58.19	-	0.253	
26.5	-	59.89	-	0.261	
29.9	18.77	-	0.0532	-	
32.5	18.15	-	0.0512	-	
37.3	-	62.96	-	0.292	
38.3	-	63.18	-	0.294	
46.3	15.51	-	0.0427	-	
53.5	14.83	-	0.0406	-	
58.0	14.59	-	0.0399	-	
71.7	-	63.18	_	0.294	
73.0	14.59	62.96	0.0399	0.292	
77.6	14.83	-	0.0406	-	
83.8	15.51	-	0.0427	-	
85.7	-	59.89	_	0.266	
90.3	-	58.19	-	0.253	
95.2	18.15	-	0.0512	-	
96.0	-	55.02	-	0.229	
96.9	18.77	-	0.0532	-	
97.7	-	53.77	-	0.220	
103.0	21.77	-	0.0634	_	
103.2	_	48.92	-	0.189	
105.7	-	43.36	-	0.157	
106.8	28.55	_	0.0885	-	
106.9	-	35.76	-	0.119	
107.0	29.76	_	0.0934	-	

COMPONENTS: (1) 2-Butanol (<i>sec-butanol</i>); C ₄ H ₁₀ 0; [78-92-2]		Dolgolenko,	ORIGINAL MEASUREMENTS: Dolgolenko, W. Z. Phys. Chem. <u>1908</u> , 62, 499-511.		
(2) Water; H ₂ 0;	[7732–18–5]				
EXPERIMENTAL VALU	ES (continued)				
b. Second distil	lation fraction of 2-but	anol:			
b.p. 98.6-99.0 ⁰ C	at 760.8 mm Hg, d_4^{20} 0.	80619.			
t/ ^o c	$g(1)/100g sln$ x_1				
•		(1)-rich phase	-	(1)-rich phase	
-17 2		_	0.0770	_	
-17.2 -8.8	25.54 27.10	_	0.0829	_	
	27.10	- 50 75	0.0029	-	
-6.2	- 70	58.75	-	0.257	
-5.4	27.70	-	0.0852	-	
-3.0	-	56.90	-	0.243	
1.3	-	55.73	-	0.234	
2.3	27.70	-	0.0852	-	
4.3	-	55.73	-	0.234	
4.7	27.10	-	0.0829	-	
9.0	25.54	56.90	0.0770	0.243	
13.9	-	58.75	-	0.257	
15.0	22.89	-	0.0673	-	
19.8	20.87	-	0.0603	-	
21.2	-	61.49	-	0.280	
24.7	-	62.50	-	0.288	
29.4	17.90	-	0.0503	-	
30.1	-	63.81	-	0.300	
37.5	16.16	-	0.0448	-	
41.3	15.50	-	0.0426	-	
77.2	-	63.81	-	0.300	
83.1	-	62.50	-	0.288	
85.8	-	61.49	-	0.280	
88.1	15.50	-	0.0426	-	
91.9	16.16	-	0.0448	-	
93.5	-	58.75	-	0.257	
97.3	-	56.90	-	0.243	
97.9	17.90	-	0.0503	-	
99.4	-	55.73	-	0.234	
100.0	-	55.24	-	0.231	
100.1	-	55.20	-	0.231	
103.0	-	52,99	-	0.215	
104.1	20.87	-	0.0603	-	
105.0	-	51.01	-	0.202	
106.5	22.89	-	0.0673	-	
107.0	-	47.97	-	0.183	
108.2 108.9	25.54	- 42.49	0.0770	- 0.152	
		76,77			
		• • • • • • • • • • • • • • • • • • • •	(continued	l next page)	

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COMPONENTS: (1) 2-Butanol (<i>sec-butanol</i>); C ₄ H ₁₀ 0; [78.02-2]		Dolgolen		511
[78-92-2] (2) Water; H ₂ 0; [77	32-18-5]	2. Fny8.	Chem. <u>1908</u> , 62, 499-	511.
EXPERIMENTAL VALUES	(continued)			<u></u>
t/ ^o c	g(1)/100)g sln	<i>x</i> ₁	
, -			l (2)-rich phase	(l)-rich pha
100.0	27.70	-	0.0829	
109.0	27.70	- 40.08	0.0829	- 0.140
109.2 109.3	- 29.20	40.08	0.0911	0.140
109.4	30.20	36.16	0.0951	0.121
c. Third distillati	on fraction of 2	2-butanol:		
b.p. 99.0-99.5 [°] C at				
	4	•		
-23.4	20.28	-	0.0582	-
-21.0	22.81	-	0.0670	-
-14.9	23.89	-	0.0709	-
-7.5	-	63.65	-	0.299
-2.3	-	61.63	-	0.281
0.7	-	61.09	_	0.276
1.2	23.89	-	0.0709	_
5.9	-	61.09	-	0.276
6.2	22.81	_	0.0670	_
10.0	_	61.63	-	0.281
14.4	20.28	_	0.0582	-
18.0	19.02	_	0.0540	_
18.2	_	63.65	_	0.299
27.6	_	65.64	-	0.317
33.1	15.32	-	0.0421	-
40.2	_	66.68	-	0.327
44.9	13.60	-	0.0369	-
62.0	-	66.68	-	0.327
76.2	_	65.64	_	0.317
85.5	13.60	-	0.0369	-
85.8	-	63.65	-	0.299
92.0	-	61.63	-	0.233
93.4	-	61.09	-	0.276
95.5	15.32	-	0.0421	-
97.0	-	59.73	-	0.265
105.1	_	55.18	-	0.230
106.4	19.02	-	0.0540	-
106.9	-	53.79	-	0.221
109.1	20.28	-	0.0582	-
111.4	_	49.71	-	0.194
112.1	22.81	48.45	0.0670	0.186
				next page)

COMPONENTS: (1) 2-Butanol (<i>sec</i> - [78-92-2]	butanol); C ₄ H ₁₀ 0;	Dolgoler	MEASUREMENTS: 1ko, W. <i>Chem</i> . <u>1908</u> , 62, 49	9-511
(2) Water; H ₂ 0; [7	732-18-5]		, , , , , , , , , , , , , , ,	.
EXPERIMENTAL VALUES	(Continued)	···		<u></u>
t/°c	g(1)/100g	g sln	x	
			(2)-rich phase	•
112.9	23.89	-	0.0709	_
113.4	-	45.27	-	0.167
113.5	25.18	-	0.0756	-
114.0	-	43.31	-	0.157
114.3	27.60	-	0.0848	-
114.5	-	40.09	-	0.140
114.8	31.23	-	0.0994	-
114.9	35.20	-	0.117	-
<pre>d. <u>2-Butanol suppl</u> b.p. 98.5-98.8^oC at</pre>	$750.4 \text{ mm Hg;} d_4^{20}$	0.80656	0.078/	
~8.4	25.95	-	0.0786	-
-5.7	-	61.46	-	0.280
-4.3	26.33	-	0.0800	-
-3.5	-	60.34	-	0.270
-2.6	26.33	-	0.0800	-
-2.3 1.02	- 25.95	59.88	-	0.266
2.22	23.95	- 59.16	0.0786	-
2.32	_	59.16	-	0.261
8.02	_	59.88	_	0.261 0.266
8.07	23.96	-	0.0712	0.200
9.72	-	60.34	0.0712	0.270
13.22	_	61.46	-	0.270
14.97	21.46	-	0.0623	-
20.30	19.59	_	0.0560	_
28.47	17.2	-	0.0482	-
91.6	-	61.46	_	0.280
94.5	-	60.34	-	0.270
95.4	-	59.88	-	0.266
97.5	-	59.16	-	0.261
99.5	17.2	-	0.0482	-
99.9	-	57.89	-	0.251
.03.0	-	56.20	-	0.238
.05.3	19.59	-	0.0560	-
108.1	21.46	-	0.0623	-
111.4	23.96	-	0.0712	-
112.5	25.95	-	0.0786	-
112.7	26.33		0.0800	

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COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) 2-Butanol; (<i>sec-butanol</i>); C ₄ H ₁₀ O; [78-92-2]	Timmermans, J.
(2) Water; H ₂ 0; [7732-18-5]	Arch. Neerl. Sci. Exactes Nat. 1922, A6(3),
(2) value, (2) , $(7732-10-5)$	147; J. Chim. Phys. Physicocim. Biol. <u>1923</u> ,
	20, 491.
VARIABLES:	PREPARED BY:
Temperature: (-9) - 114 ⁰ C Pressure: 0.1-81 MPa (1-800 atm)	A. Maczynski; G.T. Hefter
EXPERIMENTAL VALUES:	
p/atm p/MPa (compiler) lower	critical upper critical rature/ ⁰ C temperature/ ⁰ C
	8.45 113.8
	5.3 105.3
120 12.1	
	7.8 –
	4.8 –
	0.8 – 6.7 –
	2.7 85.3
	9.6 81.3
	8.6 73.5
	omogeneous at all temperatures
	subgeneous at all temperatures
$dT_c/dp (LCST)^a = + 0.064 \text{ K atm}^{-1}$	
$dT_c/dp (UCST)^{\alpha} = -0.045 \text{ K atm}^{-1}$	
^a Not reported in original papers but calculate	ed in ref 1.
AUXILIARY	INFORMATION
ME THOD /APPARATUS / PROCEDURE :	SOURCE AND PURITY OF MATERIALS:
The method and apparatus were described in an earlier reference which is not identified in the paper.	(1) source not specified; b.p. 99.50 \pm 0.01°C, d_{L}^{0} 0.82263 \pm 0.00002.
	4
	(2) not specified.
	ESTIMATED ERROR:
	Not exection
	Not specified.
	REFERENCES:
	 Moriyoshi, T.; Kaneshina, S.; Aihara, K.; Yabumoto, K. J. Chem. Thermodynamics <u>1975</u>, 7, 537.
	l

COMPONENTS:	ORIGINAL MEASUREMENTS:
<pre>(1) 2-Butanol; (sec-butanol); C₄H₁₀0; [78-92-2] (2) Water; H₂0; [7732-18-5]</pre>	Evans, T.W. Anal. Chem. <u>1936</u> , 8, 206-8.
	PREPARED BY:
One temperature: 20 ⁰ C	A. Maczynski
EXPERIMENTAL VALUES:	
The solubility of 2-butanol in water at 20° C	was reported to be $18.5 g(1)/100g sln.$
The corresponding mole fraction, x_1 , calculat	_
The solubility of water in 2-butanol at 20 ⁰ C	was reported to be 35.6 $g(2)/100g$ sin
The corresponding mole fraction, x_1 , calculat	ed by the compiler is 0.695.
	IN DO DALATION
	INFORMATION
METHOD / APPARATUS / PROCEDURE :	SOURCE AND PURITY OF MATERIALS:
Hill's method (ref 1) was used.	(1) not specified.
Weighed amounts of (1) and (2) were introduced into centrifuge tubes and shaken	(2) not specified.
until equilibrium was reached. The phases were allowed to separate and the volumes of	
the upper and lower layers were read. The experiment was then repeated with a different	
ratio of the starting materials. The	
mutual solubility data were calculated from phase volumes and weights.	
	ESTIMATED ERROR:
	Solubility: 0.1-0.2% (type of error not specified).
	REFERENCES :
	1. Hill. A.E. J. Am. Chem. Soc. <u>1923</u> , 45, 1143.
	1

08		Four-Garbe	on Alcohols	
COMPONENTS:			ORIGINAL MEASUREMENT	rS :
 (1) 2-Butanol; (sec-butanol); C₄H₁₀0; [78-92-2] (2) Water; H₂0; [7732-18-5] 			Altsybeeva, A.I.; Morachevskii, A.G. Zh. Fiz. Khim. <u>1964</u> , 38, 1574-9. Altsybeeva, A.I.; Belousov, V.N.; Ovtraht, H.V.; Morachevskii, A.G. Zh. Fiz. Khim.	
VARIABLES:			<u>1964, 38, 1242-7.</u> PREPARED BY:	
Temperature:	20–70 ⁰ С		A. Maczynski	
EXPERIMENTAL V	ALUES:			······
	Mutua	l solubility in	the system 2-butanol	(1) and water (2)
t/ ^o c	x	1	g(1)/100g s1	n(compiler)
	(2)-rich phase	(1)-rich phase	(2)-rich phase	(1)-rich phase
20	0.058	0.301	20	63.9
40	0.046	0.330	17	67.0
60	0.039	0.326	14	66.6
70	0.039	0.322	14	66.2
		AUXILIARY	INFORMATION	
METHOD / APPARA	TUS/PROCEDURE:	<u> </u>	SOURCE AND PURITY O	F MATERIALS:
Probably the	analytical metho	od was used.	(1) not specified	;
were describe ternary syste but nothing w	metric and densin ed for the analys em 2-butanol/wate was specified for solubility in th	sis of the er/2-butanone, the determin-	(2) not specified	
			ESTIMATED ERROR:	
			ESTIMATED ERROR: Not specified	
			Not specified	

		2-DUL				
COMPONENTS :			ORIGINAL MEASUREMENT	S:		
 2-Butanol; [78-92-2] Water; H₂ 			Morachevskii, A.G.; Popovich, Z.P. Zh. Prik1.Khim. <u>1965</u> , 38, 2129-31. PREPARED BY:			
/ARIABLES:						
Temperature: 2	0–85 [°] C		A. Maczynski; Z. Ma	aczynska		
EXPERIMENTAL VAL	UES:	I	·····	<u> </u>		
	Mutua	l solubility of	2-butanol (1) and wa	ter (2)		
t/ ^o c	g(1)/100	g sln	$x_1(comp$	iler)		
(2)-rich phase	(1)-rich phase	e (2)-rich phase	(1)-rich phase		
20	19.8	63.2	0,0566	0.294		
40	15.6	66.5	0.0430	0.325		
60	14.0	66.2	0.0381	0.332		
80	14.0	63.8	0.0381	0.300		
85	15.0	62.0	0.0411	0,284		
		A11XT1 1 ARY	INFORMATION			
METHOD/APPARATUS	/PROCEDURE :		SOURCE AND PURITY OF	F MATERIALS:		
The analytical method was used. A mixture of (1) and (2) was placed in a thermostatted bath and stirred for an hour. After some time (a few minutes to two hours) each phase was sampled. The compositions of the phases were determined by refraction using an IRF-22 refractometer.		 source not spepurified; b.p. 99.52°C, 0.1-0.15% of wanalysis. not specified. ESTIMATED ERROR:	ecified; $n_{\rm D}^{20}$ 1.3970, d_4^{20} 0.8067, water by Karl Fischer			
			Solubility : ± 0.	05 [°] C 3 g(1)/100 sln (type of ror not specified.)		

COMPONENTS:	ORIGINAL MEASUREMENTS:		
(1) 2-Butanol (<i>sec-butanol</i>); C ₄ H ₁₀ 0;	Ratouis, M.; Dodé, M.		
[78-92-2]	Bull. Soc. Chim. Fr. 1965, 3318-22		
(2) Water; H ₂ 0; [7732-18-5]	<i>babb. bbc. onum. 11. <u>1909</u>, 9940 22.</i>		
VARIABLES:	PREPARED BY:		
Temperature: 25-30 ⁰ C Ringer solution also studied	S.C. Valvani; S.H. Yalkowsky; A.F.M. Barton		
EXPERIMENTAL VALUES:			
Solubility of 2-butan	ol in water-rich phase		
t/ ⁰ C g(1)/100g s	ln x _l (compiler)		
25 17.70	0.0497		
35 16.50	0.0458		
Solubility of 2-butan	ol in Ringer solution		
$t/{}^{0}C$ g(1)/100g s	ln		
25 15.79			
30 14.90			
AUXILIARY	INFORMATION		
METHOD / APPARATUS / PROCEDURE :	SOURCE AND PURITY OF MATERIALS:		
METHOD/APPARATUS/PROCEDORE: In a round bottom flask, 50 mL of water and a sufficient quantity of alcohol were introduced until two separate layers were formed. The flask assembly was equilibrat- ed by agitation for at least 3 h in a con- stant temperature bath. Equilibrium solub- ility was attained by first supersaturation at a slighly lower tempature (solubility of alcohols in water is inversely proportional to temperature) and then equilibriating at the desired temperature. The aqueous layer was separated after an overnight storage in a bath. The alcohol content was determined by reacting the aqueous solution with potassium dichromate and titrating the excess dichromate with ferrous sulfate solution in the presence of phosph- oric acid and diphenylamine barium sulfonate as an indicator.	 (1) Prolabo, Paris; redistilled with 10:1 reflux. b.p. 99.1°C/762.9 mm Hg n²⁵_D 1.39534 (2) twice distilled from silica apparatus or ion exchanged with Sagei A20. 		

COMPONENTS:	ORIGINAL MEASUREMENTS:
 (1) 2-Butanol (sec-butanol); C₄H₁₀O; [78-92-2] (2) Water; H₂O; [7732-18-5] 	 *Mullens, J. Alcoholassociaten, Doctoraatsproefschrift, Leuven, <u>1971</u>. Huyskens, P.; Mullens, J.; Gomez, A.; Tack,J. Bull, Soc. Chim. Belg. <u>1975</u>, 84, 253-62.
VARIABLES:	PREPARED BY:
One temperature: 25 [°] C	M.C. Haulait-Pirson; A.F.M. Barton

EXPERIMENTAL VALUES:

At equilibrium at 25° C the concentration of 2-butanol(1) in the water-rich phase was reported as 2.449 mol(1)/L sln, and the concentration of water(2) in the alcohol-rich phase was reported as 7.825 mol(2)/L sln.

The corresponding solubilities on a mass/volume basis are 181.5 g(1)/L sln and 141.0 g(2)/L sln (compiler).

AUXILIARY	INFORMATION
METHOD /APPARATUS / PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
The partition of the two components was made using a cell described in ref 1. The Rayleigh Interference Refractometer M154 was used to determine the concentrations. Standard solutions covering the whole range of concentration investigated were used for the calibration.	<pre>(1) Merck (p.a.) (2) distilled</pre>
	ESTIMATED ERROR:
	Solubility ± 0.001 mol(1)/L sln.
	REFERENCES:
	 Meeussen, E.; Huyskens, P. J. Chim. Phys. <u>1966</u>, 63, 845.

12	Four-carbon Alcohols				
COMPONENTS:			ORIGINAL M	EASUREMENTS:	
<pre>(1) 2-Butano1; (sec-butano1); C₄H₁₀0; [78-92-2] (2) Water; H₂0; [7732-18-5]</pre>			ORIGINAL MEASUREMENTS: Shakhud, ⁷ h.N.; Markuzin, N.P.; Storonkin, A.V. Vestn. Leningr. Univ. Ser. Fiz. Khim. <u>1972</u> (10) 85-8; 89-92.		
/ARIABLES: Temperature: 20-			PREPARED BY: A. Maczynski		
•					
XPERIMENTAL VALUE	S:				
	Mutual	solubili	ty of 2-bu	tanol (1) and water ((2)
t∕°C	∞ ₁ (2)-rich phase		phase	g(1)/100g s: (compile: (2)-rich phase	r)
20	0.056	0.29	7	19.62	63.48
40	0.045	0.34	0	16.24	67.94
40	0.045	0.32	1	16.24	66.05
60	0.038	0.33	4	13.98	67.36
			<u></u>		
	A	AUXILIARY	INFORMATIC)N	
METHOD/APPARATUS/	PROCEDURE:		SOURCE AN	D PURITY OF MATERIAL	S:
The titration me	thod was used. Me in a round-bottom	asurement flask		ce not specified; e distilled;	
	rcury seal and imme	rsed	d ²⁰	0.8069, $n_{\rm D}^{20}$ 1.397	2.
reported in the		were	· ·	-	
			(2) twic	e distilled, $d_{ m D}^{ m 20}$ 1.3	332.
					<u> </u>
			ESTIMATED		
			-	ure: ± 0.02 ⁰ C	
			Solubili	ty: ± 1% (max. dev.)	
			REFERENCE	2S :	
			1		

COMPONENT	IS:			ORIGINAL MEASUREMENTS:			
<pre>(1) 2-Butanol; (sec-butanol); C₄H₁₀0; [78-92-2]</pre> (2) Water: H 0: [7732-18-5]				Moriyoshi, T.; Kaneshina, S.; Aihara, K.; Yabumoto, K. J. Chem. Thermodynamics 1975, 7, 537-45.			
(2) Water; H ₂ 0; [7732-18-5]				o. onen. in	<u></u>	<u></u> , , , ,	
VARIABLE	S :			PREPARED BY:		. <u></u>	
Tempera Pressur	ture: 283-38 e: 0.1-81	1 K MPa (1-80	00 atm)	A. Maczynsk:	i; Z. Maczynska	a; G.T. Hefter	
EXPERIMENTAL VALUES: Mutual solubility of			2-butano1(1)	2-butanol(l) and water (2)			
p/atm	p/MPa	T/K	(2)-rich	-	(1)-rich		
	(compiler)		g(1)/100g sln	x_1 (compiler)	g(1)/100g slr	n x _l (compiler)	
1	0.101	283.15	23.9*	0.0709	60.9*	0.274	
T	0,101	203.15	20.2	0.0579	63.8*	0.300	
		300.15	17.9*	0.0503	65.5*	0.316	
		313.15	14.9*	0.0498	67.2*	0.332	
		323.15	13.2*	0.0356	67.5*	0.335	
		333.15	12.8*	0.0344	66.9*	0.329	
		343.15	12.9	0.0347	67.2*	0.332	
		353.15	13.8*	0.0374	65.3	0.314	
		363.15	15.5*	0.0427	61.8*	0.282	
		373.15	18.3*	0.0516	57.7*	0.249	
		383.15	23.9	0.0709	50.7*	0.200	
				0 0001	56 0	0.236	
100	10.1	283.15	26.9	0.0821	56.0	0.262	
		293.15	22.8	0.0670	59.4	0.285	
		300.15	20.0	0.0573	62.1	0.305	
		313.15	16.5	0.0458	64.4		
		323.15	14.6	0.0399	65.3	0.314	
		333.15	13.9	0.0377	64.9	0.310 0.316	
		343.15	14.1	0.0383	65.5 64.0	0.302	
		353.15	15.1	0.0414 0.0474	60.1	0.268	
		363.15	17.0	0.0600	53.5*	0.218	
		373.15 380.55	20.8 25.6	0.0772	48.6	0.187	
		500,55	23.0			next page)	
			AllXTLTARY	INFORMATION			
METHOD /A	APPARATUS/PROC	EDURE:		SOURCE AND P	URITY OF MATER	IALS:	
				(1) source	not specified	:	
						ith freshly burned	
Both co	omponents were	e placed i	n a cut-off	lime,	distilled;		
glass s	syringe of abo	out 20 cm ³	capacity used				
as a sa	ample vessel,	which was	placed in a	$n_{\rm D}$	10.1		
	walled stainle						
			essure vessel			d from alkaline	
	nnected to a l			potass	ium permangana	te, redistilled.	
			nically shaken				
	oil thermosta		After stirring				
for at	least 6 h and	l then sta	nding for				
	r 6 h at the o			NOTIVITED	DDOD -		
	ature and pres		-	ESTIMATED EL	KKUK:		
upper	layer was take	en. Subs	equently, the	Temperature	e: ± 0.02 K		
pressu	re vessel was	moved, th	e contents	Solubility			
	d to settle, a		mples was made	1	(type of	error not specified	
sample	tometrically.	ara or sa	mpics was made	PPPPPP			
LELLAC	concernearity .			REFERENCES:			
				1			
				1			

Four-carbon Alcohols

COMPONENTS:				ORIGINAL MEASU	REMENTS:	
 (1) 2-But Γ78-9 	anol; (sec-ba 2-2]	utanol); (^C 4 ^H 10 ⁰ ;	Moriyoshi, T.; Yabumoto, K.	Kaneshina, S.	; Aihara, K.;
	; H ₂ 0; [77	32-18-5]		J. Chem. Thermo	odynamics <u>1975</u> ,	7, 537-45.
	2					
EXPERIMENT	AL VALUES (c	ontinued)		L =		
p/atm	p/MPa		(2)-r	ich phase	(1)-ric	h phase
L	(compiler)	T/K	g(1)/100g s	ln x _l (compiler)	g(1)/100g sln	x_{l} (compiler)
200	20.2	280 15	35.2*		45.9*	0.171
200	20.3	289.15	27 0	0.1166 0.0859	43.9 53.4	0.218
		293.15	27.9			
		300.15	23.4	0.0691	58.2 62.0	0.253 0.284
		313.15	18.4	0.0519		0.284
		323.15	16.2	0.0449	63.1	
		333.15	15.0	0.0411	63.2	0.294
		343.15	15.3	0.0420	64.1	0.303
		353.15	16.4	0.0455	62.7	0.290
		363.15	18.6	0.0526	58.2	0.253
		373.15	22.6*	0.0662	51.0*	0.202
		378.15	29.3	0.0915	46.1	0.172
300	30.4	298.15	33.0*	0.1069	47.5	0.180
300	50.4	300.15	28.9	0.0899	51.2	0.203
		313.15	20.5	0.0590	59.9	0.266
			17.9		61.2	0.200
		323.15		0.0503	61.7	0.281
		333.15	16.3	0.0452		
		343.15	16.5	0.0458	62.5	0.288
		353.15	17.8	0.0500	61.1	0.276
		363.15	20.4	0.0586	55.7	0.234
		373.15	33.2	0.1077	41.6	0.147
400	40.5	304.15	31.4*	0.1001	46.6*	0.175
		313.15	23.0	0.0677	57.8	0.250
		323.15	19.5	0.0556	59.4	0.262
		333.15	17.8	0.0500	60.1	0.268
		343.15	17.7	0.0497	60.7	0.273
		353.15	19.1	0.0543	59.2	0.261
		363.15	22.9*	0.0673	52.3	0.210
		368.15	28.9*	0.0899	46.1	0.172
500	50 .7	309.15	39.6*	0.1374	40.5*	0.142
500	5000	131.15	26.8	0.0817	52.8	0.214
		323.15	21.4	0.0620	57.0	0.244
		333.15	19.4	0.0552	58.2	0.253
		343.15	19.0	0.0539	58.5	0.255
		353.15	20.6	0.0593	56.4	0.239
		363.15	27.3	0.0836	47.1	0.178
600	60.8	316.15	32.4*	0.1043	45.9*	0.171
600	00.0		24.1	0.0716	53.0	0.215
		323.15		0.0718	55.4	0.232
		333.15	21.7		55.9	0.232
		343.15	21.0	0.0607 0.0670		0.235
		353.15 360.15	22.8 _* 31.2	0.0992	52.6 _* 43.1	0.155
700	71 0			0 1000	44.0	0.160
700	71.0	323.15	31.6	0.1009	44.0 51.4	0.204
		333.15	24.9	0.0746		
		343.15 353.15	23.9 26.9	0.0709 0.0821	52.5 46.9	0.212 0.177
000	01 1		30.8*	0 0076	44.4*	0 142
800	81.1	333.15	20.8 20.1 [*]	0.0976	44•4* / 6 3*	0.162
		338.15	29.1	0.0907	46.3	0.173
		343.15 348.15	29.1 [*] 31.8 [*]	0.0907 0.1018	46.1 43.3	0.172 0.156
*			all athon wal	ues obtained by :	intornalation (hu the origina
	direct measu ors) of direc			ues obtailled by	incerpolation (by the origina

2-Butanol

COMPONENTS:			ORIGINAL MEASUREMENTS:	
(1) 2-Butanol (sec-butanol): C.H.	.0:	Moriyoshi, T.; Kaneshina	, S.; Aihara, M.;
(1) 2-Butanol (<i>sec-butanol</i>); C ₄ H ₁₀ 0; [78-92-2]			Yabumoto, K.	
			J. Chem. Thermodynamics	1975, 7, 537-45
(2) Water; H ₂ 0:	[//32-18-5]			
EXPERIMENTAL VAI	UES (continued)			
	Propert	ies of the	critical solutions	
p/atm	T _c (lcst)/κ	x_{1c}	T_{c} (UCST)/K	x _{lc}
1	-	_	390.35	-
100	-	-	387.15	-
160 ^{<i>a</i>}	283.15 ^a	0.149 ^a	-	-
200	288,35	-	380.45	-
250 ^a	293.15 ^a	0.140 ^a	-	-
300	297.05	-	373.45	-
303 ^{<i>a</i>}	-	-	373.15 ^{<i>a</i>}	0.131 ^{<i>a</i>}
358 ^a	300 . 15 ^{<i>a</i>}	0.139 ^a	-	-
400	302.45	-	369.35	-
500	309.15	-	365.55	-
552 ^{<i>a</i>}	-	-	363.15 ^a	0.129 ^a
580 ^{<i>a</i>}	313 . 15 ^{<i>a</i>}	0.143 ^a	-	-
600	314.95	-	360 .95	-
700	322.05	-	355.45	-
714 ^{<i>a</i>}	323.15 ^a	0.134 ^a	-	-
751 ^{<i>a</i>}	-	-	353 . 15 ^{<i>a</i>}	0.133 ^a
800	330.65	-	350.15	-
830 ^a	333.15 ^a	0.130 ^a	-	-
840 ^a	-	-	343.15 ^{<i>a</i>}	0.131 ^{<i>a</i>}

^{α} Calculated by the authors using the "rectilinear diameter law". All other values obtained (by the authors) by graphical interpolation of the experimental results. The hypercritical point, where the closed solubility loop disappears, was estimated to occur at (340.0 ± 1.5) K, (845 ± 5) atm, and $x_1 = 0.131 \pm 0.002$

 $dT_c/dp(LCST) = +0.060 \text{ K atm}^{-1}$

 $dT_{c}/dp(UCST) = -0.046 \text{ K atm}^{-1}$ $dx_{1c}/dT \simeq 0 \text{ K}^{-1}$

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) 2-Butanol (sec-butanol); C ₄ H ₁₀ 0; [78-92-2]	De Santis, R.; Marrelli, L.; Muscetta, P.N. Chem. Eng. J., <u>1976</u> , 11, 207-14.
(2) Water; H ₂ 0; [7732-18-5]	Cherk. Eng. 5., 1970, 11, 207-14.
VARIABLES:	PREPARED BY:
One temperature: 25 [°] C	A. Maczynski

EXPERIMENTAL VALUES:

The proportion of 2-butanol(1) in the water-rich phase at equilibrium at $25^{\circ}C$ was reported to be 22.5 g(1)/100g sln.

The corresponding mole fraction solubility, x_1 , calculated by the compiler, is 0.0659.

The proportion of water(2) in the alcohol-rich phase at equilibrium at 25° C was reported to be 33.1 g(2)/100g sln.

The corresponding mole fraction solubility, $x_2^{}$, calculated by the compiler, is 0.671.

AUXILIARY	INFORMATION

METHOD / APPARATUS / PROCEDURE :	SOURCE AND PURITY OF MATERIALS:
The determinations were carried out using a separating funnel with a thermostatic jacket. The extractor was loaded with (1) and (2)	 Merck, analytical purity; fractionated before use
and after an extended period of mixing and quantitative gravity separation, samples were withdrawn from the aqueous phase. The concentration of (1) in (2) was determined by colorimetric analysis (double-beam Lange colorimeter) of the cerium complex. The concentration of (2) in (1) was derived from a material balance based upon starting quantities and compositions. Each of the determinations was carried out with several	
repetitions. The method is described in ref 1.	ESTIMATED ERROR: Temperature: ± 0.1 [°] C
	REFERENCES:
	 De Santis, R.; Marelli, L.; Muscetta, P.N. J. Chem. Eng. Data, 1976, 21, 324.
	-

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) 2-Butanol (sec-butanol); C ₄ H ₁₀ 0;	Becke, A.; Quitzch, C.
[78-92-2]	Chem. Tech., <u>1977</u> , 29, 49-51
(2) Water; H ₂ 0; [7732-18-5]	
(2) water, (2) , $[7752-10-5]$	
······································	
VARIABLES:	PREPARED BY:
One temperature: 25 [°] C	A. Maczynski
EXPERIMENTAL VALUES:	
The mole fraction of 2-butanol in the water-	deb phase at equilibrium at 25°C was
reported to be $x_1 = 0.035$, corresponding to	
-	
The mole fraction of water in the alcohol-ric	
to be $x_2 = 0.301$, corresponding to 9.47 g(2)	/100g sln (compiler).
Graphical data at 60° C were also presented.	
	INFORMATION
METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
The refractometric and the Karl-Fischer	(1) not specified
dead-stop titration methods were used.	(2) not specified
No more details are given in the paper.	
1	
	ESTIMATED ERROR:
	Solubility: 0.05-1% for (1) and (2) 0.3 - 1.3% for (2) in (1)
	(relative error)
	REFERENCES :

COMPONENTS:	ORIGINAL MEASUREMENTS:		
(1) 2-Butanol-d; C ₄ H ₉ DO; [4712-39-4]	Rabinovich, I.B., Fedorov, V.D.,		
(2) Water-d ₂ ; D ₂ 0; [7789-20-0]	Pashkin, N.P., Avdesnyak, M.A.,		
	Pimenov, N. Ya.		
	Dokl. Akad. Nauk SSSR <u>1955</u> , 105, 108–11.		
VARIABLES:	PREPARED BY:		
Temperature: 10-120 ⁰ C	G. Jancso and G.T. Hefter.		
EXPERIMENTAL VALUES:			
Effect of deuteration or	n solubility of 2-butanol in water		
t/ ^o c	$100(L_{\rm H} - L_{\rm D})L_{\rm H}^{\alpha}$		
10	9.0		
20	7.8		
26	7.0		
40	5.5		
66	4.7		
80	6.3		
100	14		
103	17		
108	22		
	(continued next page)		
AUXILIARY	INFORMATION		
METHOD/APPARATUS/PROCEDURE: The synthetic method (cloud-clear points)	SOURCE AND PURITY OF MATERIALS: (1) 2-butanol-d was prepared by the		
of Alexejew (ref 1) was used which consists	hydrolysis of the aluminium salt of		
in observing the temperature at which a measured weight of one liquid is visually	the ordinary butanol with D_2^0 .		
soluble in a measured weight of the other liquid.	The OD group of the product had a deuterium content of > 99 at %.		
TTATA.	(2) D ₂ 0, 99.0 - 99.8 at %, source not given.		
	ESTIMATED ERROR:		
	Solubility: not specified		
	Temperature: ± 0.2 [°] C		
	REFERENCES :		
	1. Alexejew, W.J. J. Prakt. Chem. <u>1882</u> , 25, 518.		
	 Rabinovich, I.B. Influence of Isotopy on the Physicochemical Properties of Liquids. (In Russian). Nauka. Moscow 1968, p.261. 		

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COMPONENTS:

(1) 2-Butanol-d; C<sub>4</sub>H<sub>9</sub>DO; [4712-39-4]

(2) Water-d<sub>2</sub>; D<sub>2</sub>O; [7789-20-0]

Do
```

ORIGINAL MEASUREMENTS: Rabinovich, I.B., Fedorov, V.D., Pashkin, N.P., Avdesnyak, M.A., Pimenov, N. Ya. Dokl. Akad. Nauk SSSR <u>1955</u>, 105, 108-11.

EXPERIMENTAL VALUES (continued)

The upper critical solution temperature of 2-butanol - H_2^0 was reported to be 113.1°C, compared with 119.3°C for 2-butanol-d - D_2^0 .

The solubility diagram (Figure 1) was taken from ref 2. Mutual solubilities for the 2-butanol - H_2^0 system were also determined (\bullet). but only given in graphical form. The source of the literature data (o in Figure 1) is not given.

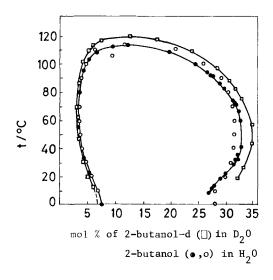
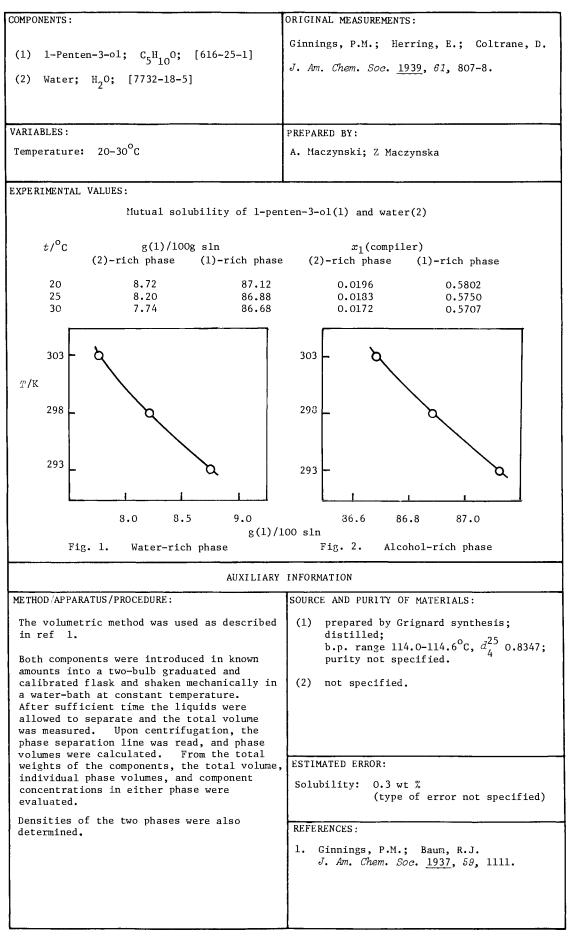
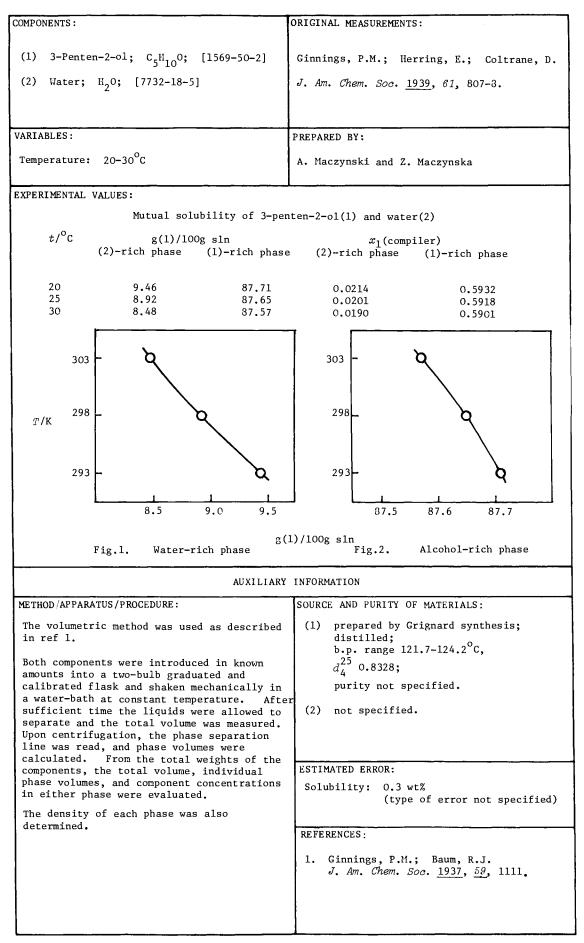
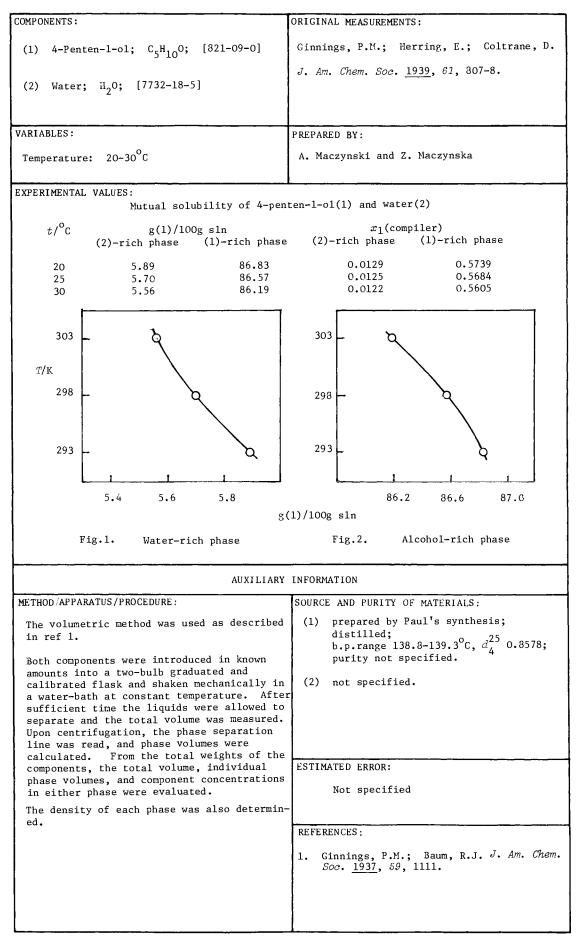


Fig. 1. Mutual solubilities of $C_4H_9OD(1)$ in $D_2O(2)$ ([) and of $C_4H_9OH(1)$ in $H_2O(2)$ (•,o).



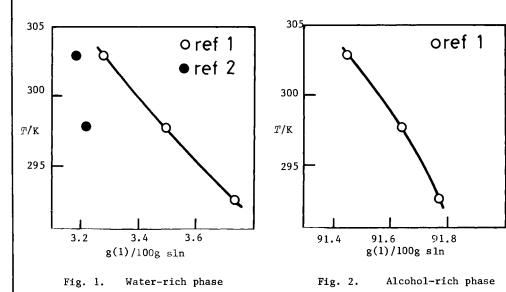




COMPONENTS:	EVALUATOR:
(1) 2,2-Dimethy1-1-propanol (neopentyl	A. Maczynski, Institute of Physical
alcohol, tert-butyl carbinol); C ₅ H ₁₂ 0;	Chemistry of the Polish Academy of Sciences,
[75-84-3]	Warsaw, Poland; and A.F.M. Barton, Murdoch
(2) Water; H ₂ O; [7732-18-5]	University, Perth, Western Australia.
(-,, -2-,	November 1982

CRITICAL EVALUATION:

Solubilities in the system comprising 2,2-dimethyl-1-propanol (1) and water (2) have been reported in two publications (Figures 1 and 2). Ginnings and Baum (ref 1) carried out measurements of the mutual solubilities of the components at 293, 298 and 303 K, by the volumetric method. Ratouis and Dode['] (ref 2) determined the solubility of (1) in (2) at 298 and 303 K by an analytical method and their value 3.22 ± 0.1 g(1)/100g sln at 298 K is in reasonable agreement with the value 3.50 ± 0.1 g(1)/100g sln of ref 1. Although the 303 K value of 3.19 ± 0.1 g(1)/100g sln is in agreement with the value 3.28 ± 0.1 g(1)/100g sln given in ref 1, information is so limited that all values are regarded as tentative.



Tentative values for the mutual solubilities of 2,2-dimethyl-l-propanol (1) and water (2)

T/K	Water-rich	Water-rich phase		Alcohol-rich phase	
	g(1)/100g sln	x_1	g(2)/100g sln	<i>x</i> 2	
293	3.7	0.0079	8.2	0.31	
298	3.5	0.0074	8.4	0.31	
303	3.3	0.0069	8.5	0.31	

References

1. Ginnings, P.M.; Baum, R. J. Am. Chem. Soc. 1937, 59, 1111.

2. Ratouis, M.; Dode, M. Bull. Soc. Chim. Fr. <u>1965</u>, 3318.

COMPONENTS:		ORIGINAL MEASUREMENTS:			
(1) 2,2-Dimethy1-1-propanol (neopentyl		Ginnings, P.M.; Baum, R.			
alcohol, tert-butylcarbinol); C ₅ H ₁₂ 0; [75-84-3]		J. Am. Chem. Soc. <u>1937</u> , 59, 1111-3.			
(2) Water; H	(2) Water; H ₂ 0; [7732-18-5]				
VARIABLES:	······································		PREPARED BY:		
Temperature	: 20-30 [°] C		A. Maczynski and Z. Maczynska		
EXPERIMENTAL	VALUES:	······································			
	Mutual solubility	of 2,2-dimethy	1-1-propanol(1) and	d water(2)	
t∕°c	g(1)/100g (2)-rich phase		x_1 (e (2)-rich phase	compiler) e (1)-rich phase	
20	3.74	91.77	0.00788	0.6950	
25	3.50	91.64	0.00736	0.6913	
30	3.28	91.46	0.00688	0.6863	
Relative density d_4 $t/^{\circ}C$ Water-rich phaseAlcohol-rich phase200.99360.8243250.99300.8216					
	30	0.9925	0.81		
	<u></u>	AUXILIARY			
AUXILIARY METHOD/APPARATUS/PROCEDURE: The volumetric method was used. Both components were introduced in known amounts into a two-bulb graduated and calibrated flask and shaken mechanically in a water-bath at constant temperature. After sufficient time the liquids were allowed to separate and the total volume was measured. Upon centrifugation, the phase separation line was read, and phase volumes were calculated. From the total weights of the components, the total volume individual phase volumes, and component concentrations in either phase were evaluated.		(2) Not specified.			

COMPONENTS:		ORIGINAL MEASUREMENTS:	
(1) 2,2-Dimethy1-1-propanol	(neope n t <u>y</u> l	Ratouis, M., Dode, M.	
alcohol, tert-butylcarbinol); C ₅ H ₁₂ 0; [75-84-3]		Bull. Soc. Chim. Fr. <u>1965</u> , 3318-22.	
(2) Water, H ₂ 0; [7732-18-5]			
VARIABLES:			
Temperature: 25-30 ⁰ C		PREPARED BY:	
-		S.C. Valvani; S.H. Yalkowsky; A.F.M. Barton.	
Ringer solution also studied			
Proportion	of (1) in water-	rich phase	
t/ ^o c	g(1)/100g sln	<pre>x₁ (compiler)</pre>	
25	3,22	0.00675	
30	3.19	0.00669	
30	2.84		
(Ringer solution)			
		ΙΝΕΟΡΜΑΤΙΟΝ	
	AUXILIARY	INFORMATION	
METHOD/APPARATUS/PROCEDURE:		SOURCE AND PURITY OF MATERIALS:	
In a round bottomed flask, 50 a sufficient quantity of alco duced until two separate laye)mL of water and whol were intro-	· · · · · · · · · · · · · · · · · · ·	
In a round bottomed flask, 50 a sufficient quantity of alco duced until two separate laye The flask assembly was equili agitation for at least 3 h in temp bath. Equilibrium solu attained by first supersatura slightly lower temperature (s alcohols in water is inversel to temperature) and then equil	OmL of water and chol were intro- ers were formed. lbrated by a a constant ubility was ating at a solubility of y proportional librating at the	SOURCE AND PURITY OF MATERIALS: (1) Fluka A.G.; Buchs S.G.; redistilled with 10:1 reflux;	
In a round bottomed flask, 50 a sufficient quantity of alco duced until two separate laye The flask assembly was equild agitation for at least 3 h in temp bath. Equilibrium solu attained by first supersatura slightly lower temperature (s alcohols in water is inversel to temperature) and then equil desired temperature. The aq separated after an overnight	OmL of water and obol were intro- ers were formed. Ubrated by a constant ubility was ating at a solubility of Ly proportional Librating at the ueous layer was storage in a	 SOURCE AND PURITY OF MATERIALS: (1) Fluka A.G.; Buchs S.G.; redistilled with 10:1 reflux; b.p. 112°C/755.3 mm Hg (2) twice distilled from silica apparatus 	
In a round bottomed flask, 50 a sufficient quantity of alco duced until two separate laye The flask assembly was equili agitation for at least 3 h in temp bath. Equilibrium solu attained by first supersatura slightly lower temperature (s alcohols in water is inversel to temperature) and then equil desired temperature. The aq separated after an overnight bath. The alcohol content w	OmL of water and ohol were intro- ers were formed. Ubrated by a constant ubility was ating at a solubility of y proportional librating at the ueous layer was storage in a ras determined	 SOURCE AND PURITY OF MATERIALS: (1) Fluka A.G.; Buchs S.G.; redistilled with 10:1 reflux; b.p. 112°C/755.3 mm Hg (2) twice distilled from silica apparatus or ion-exchanged with Sagei A20 ESTIMATED ERROR: 	
In a round bottomed flask, 50 a sufficient quantity of alco duced until two separate laye The flask assembly was equili agitation for at least 3 h in temp bath. Equilibrium solu attained by first supersature slightly lower temperature (s alcohols in water is inversel to temperature) and then equil desired temperature. The aq separated after an overnight bath. The alcohol content w by reacting the aqueous solut assium dichromate and titrati	OmL of water and ohol were intro- ers were formed. Ubrated by a constant ubility was ating at a solubility of by proportional librating at the ueous layer was storage in a vas determined fion with pot- ing the excess	 SOURCE AND PURITY OF MATERIALS: (1) Fluka A.G.; Buchs S.G.; redistilled with 10:1 reflux; b.p. 112°C/755.3 mm Hg (2) twice distilled from silica apparatus or ion-exchanged with Sagei A20 ESTIMATED ERROR: 	
In a round bottomed flask, 50 a sufficient quantity of alco duced until two separate laye The flask assembly was equild agitation for at least 3 h in temp bath. Equilibrium solu attained by first supersatura slightly lower temperature (s alcohols in water is inversel to temperature) and then equil desired temperature. The ag separated after an overnight bath. The alcohol content w by reacting the aqueous solut assium dichromate and titrati dichromate with ferrous sulfa the presence of phosphoric ac	OmL of water and obol were intro- ers were formed. Ubrated by a constant ubility was acting at a solubility of y proportional ibrating at the queous layer was storage in a ras determined tion with pot- ng the excess te solution in id and	 SOURCE AND PURITY OF MATERIALS: (1) Fluka A.G.; Buchs S.G.; redistilled with 10:1 reflux; b.p. 112°C/755.3 mm Hg (2) twice distilled from silica apparatus or ion-exchanged with Sagei A20 ESTIMATED ERROR: Solubility relative error of 2 determination 	
In a round bottomed flask, 50 a sufficient quantity of alco duced until two separate laye The flask assembly was equild agitation for at least 3 h in temp bath. Equilibrium solu attained by first supersatura slightly lower temperature (s alcohols in water is inversel to temperature) and then equil desired temperature. The aq separated after an overnight bath. The alcohol content w by reacting the aqueous solut assium dichromate and titrati dichromate with ferrous sulfa	OmL of water and obol were intro- ers were formed. Ubrated by a constant ubility was acting at a solubility of y proportional ibrating at the queous layer was storage in a ras determined tion with pot- ng the excess te solution in id and	 SOURCE AND PURITY OF MATERIALS: (1) Fluka A.G.; Buchs S.G.; redistilled with 10:1 reflux; b.p. 112°C/755.3 mm Hg (2) twice distilled from silica apparatus or ion-exchanged with Sagei A20 ESTIMATED ERROR: Solubility relative error of 2 determination less than 1% 	
In a round bottomed flask, 50 a sufficient quantity of alco duced until two separate laye The flask assembly was equild agitation for at least 3 h in temp bath. Equilibrium solu attained by first supersatura slightly lower temperature (s alcohols in water is inversel to temperature) and then equil desired temperature. The ag separated after an overnight bath. The alcohol content w by reacting the aqueous solut assium dichromate and titrati dichromate with ferrous sulfa the presence of phosphoric ac diphenylamine barium sulfonat	OmL of water and obol were intro- ers were formed. Ubrated by a constant ubility was acting at a solubility of y proportional ibrating at the queous layer was storage in a ras determined tion with pot- ng the excess te solution in id and	<pre>SOURCE AND PURITY OF MATERIALS: (1) Fluka A.G.; Buchs S.G.; redistilled with l0:1 reflux; b.p. 112°C/755.3 mm Hg (2) twice distilled from silica apparatus or ion-exchanged with Sagei A20</pre> ESTIMATED ERROR: Solubility relative error of 2 determination less than 1% Temperature: ± 0.05°C	
In a round bottomed flask, 50 a sufficient quantity of alco duced until two separate laye The flask assembly was equild agitation for at least 3 h in temp bath. Equilibrium solu attained by first supersatura slightly lower temperature (s alcohols in water is inversel to temperature) and then equil desired temperature. The ag separated after an overnight bath. The alcohol content w by reacting the aqueous solut assium dichromate and titrati dichromate with ferrous sulfa the presence of phosphoric ac diphenylamine barium sulfonat	OmL of water and obol were intro- ers were formed. Ubrated by a constant ubility was acting at a solubility of y proportional ibrating at the queous layer was storage in a ras determined tion with pot- ng the excess te solution in id and	<pre>SOURCE AND PURITY OF MATERIALS: (1) Fluka A.G.; Buchs S.G.; redistilled with l0:1 reflux; b.p. 112°C/755.3 mm Hg (2) twice distilled from silica apparatus or ion-exchanged with Sagei A20</pre> ESTIMATED ERROR: Solubility relative error of 2 determination less than 1% Temperature: ± 0.05°C	
In a round bottomed flask, 50 a sufficient quantity of alco duced until two separate laye The flask assembly was equild agitation for at least 3 h in temp bath. Equilibrium solu attained by first supersatura slightly lower temperature (s alcohols in water is inversel to temperature) and then equil desired temperature. The ag separated after an overnight bath. The alcohol content w by reacting the aqueous solut assium dichromate and titrati dichromate with ferrous sulfa the presence of phosphoric ac diphenylamine barium sulfonat	OmL of water and obol were intro- ers were formed. Ubrated by a constant ubility was acting at a solubility of y proportional ibrating at the queous layer was storage in a ras determined tion with pot- ng the excess te solution in id and	<pre>SOURCE AND PURITY OF MATERIALS: (1) Fluka A.G.; Buchs S.G.; redistilled with l0:1 reflux; b.p. 112°C/755.3 mm Hg (2) twice distilled from silica apparatus or ion-exchanged with Sagei A20</pre> ESTIMATED ERROR: Solubility relative error of 2 determination less than 1% Temperature: ± 0.05°C	

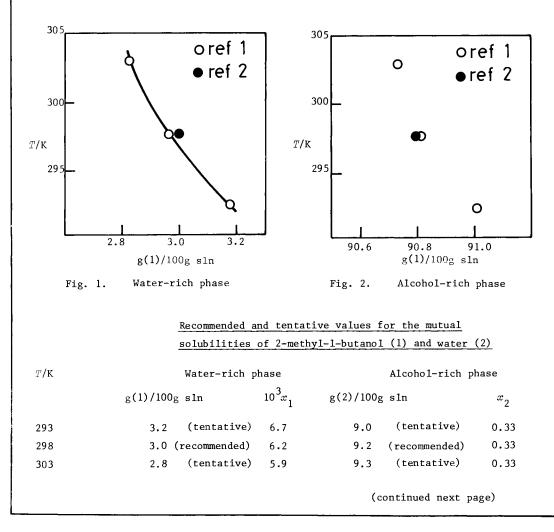
COMPONENTS:	EVALUATOR:
 2-Methyl-l-butanol ("active" amyl alcohol, sec-butylcarbinol); C₅H₁₂O; 	A. Maczynski, Institute of Physical Chemistry of the Polish Academy of Sciences,
[137-32-6]	Warsaw, Poland; and A.F.M. Barton, Murdoch
(2) Water; H ₂ 0; [7732-18-5]	University, Perth, Western Australia November 1982

CRITICAL EVALUATION:

Solubilities in the system comprising 2-methyl-1-butanol (1) and water (2) have been reported in three publications. Ginnings and Baum (ref 1) carried out measurements of the mutual solubilities of the components at 293, 298 and 303 K by the volumetric method. Crittenden and Hixon (ref 2), determined the mutual solubilities at 298 K, presumably by the titration method, while Ratouis and Dode (ref 3) analyzed the water-rich phase at 303 K.

For the water-rich phase (Figure 1) the value 3.0 $g(1)/100g \sin given$ in ref 2 at 298 K is in good agreement with ref 1, 2.97 $g(1)/100g \sin n$, and is recommended. The value 2.61 $g(1)/100g \sin n$ for the solubility of (1) in (2) given in ref 3 at 303 is not in good agreement with ref 1 and 2, and is excluded from consideration.

In the alcohol-rich phase (Figure 2), the value 90.8 g(1)/100g sln given in ref 2 at 298 K is in very good agreement with the value 90.81 g(1)/100g sln of ref 1, and is recommended. The temperature dependence reported in ref 1 is inconsistent with that of related systems, and this information is to be considered as tentative.



COMPONENTS:	EVALUATOR:	
 (1) 2-Methyl-l-butanol ("active" amyl alcohol, sec-butylcarbinol); C₅H₁₂0; [137-32-6] (2) Water; H₂0; [7732-18-5] 	A. Maczynski, Institute of Physical Chemistry of the Polish Academy of Sciences, Warsaw, Poland;and A.F.M. Barton, Murdoch University, Perth, Western Australia November 1982	
CRITICAL EVALUATION (continued)		
References		
1. Ginnings, P.M.; Baum, R. J. Am. Chem. S	Soc. <u>1937</u> , 59, 1111.	

2. Crittenden, E.D., Jr.; Hixon, A.N. Ind. Eng. Chem. <u>1954</u>, 46, 265.

3. Ratouis, M.; Dode, M. Bull. Soc. Chim. Fr. <u>1965</u>, 3318.

COMPONENTS:	,		ORIGINAL MEASUREMENTS	:	
 2-Methyl-l-butanol ("active" amyl alcohol, sec-butylcarbinol); C₅H₁₂0; 		Ginnings, P.M.; Baum, R. J. Am. Chem. Soc. <u>1937</u> , 59, 1111.			
-	[137-32-6] (2) Water; H ₂ 0; [7732-18-5]				
VARIABLES:	2, [7752 10-5]		PREPARED BY:		
Temperature:	20–30 ⁰ C		A. Maczynski; Z Macz	ynski.	
EXPERIMENTAL V	ALUES:		· · · · · · · · · · · · · · · · · · ·		
	Mutual solubil:	ity of 2-methy]	-1-butanol(1) and wat	er(2)	
t/°c	g(1)/100	sln	x_1 (compi	ler)	
07 0			-	(1)-rich phase	
20	3.18	91.05	0.00667	0.6752	
25	2.97	90.81	0.00621	0.6688	
30	2.83	90.74	0.00592	0.6669	
		Relative d	ensity, d_4		
	t/°c	Water-rich ph	ase Alcohol-ric	h phase	
	20	0.9943	0.8311		
	25	0.9930	0.8288		
	30	0,9928	0.8239		
		AUXILIARY	INFORMATION		
METHOD/APPARA	TUS/PROCEDURE:		SOURCE AND PURITY OF	MATERIALS:	
Both compone amounts into calibrated f in a water-b After suffic allowed to s was measured phase separa volumes were weights of t individual p	tion line was read	ed in known ated and echanically emperature. uids were otal volume gation, the d, and phase om the total e total volume, component	b.p. range 128 d_4^{25} 0.8108. (2) not specified. ESTIMATED ERROR: Temperature: ± 0.1 Solubility: bette	metallic calcium; .4-129.1°C,	

COMPO	NENTS:	ORIGINAL MEASUREMENTS:
COMIO	NEW 10 .	URIGINAL MEASUREMENTS:
(1)	2-Methyl-1-butanol ("active" amyl alcohol, sec-butylcarbinol); C ₅ H ₁₂ 0; [137-32-6]	Crittenden, E.D., Jr.; Hixon, A.N. Ind. Eng. Chem. <u>1954</u> , 46, 265-8.
(2)	Water; H ₂ 0; [7732-18-5]	
VARIA	BLES :	PREPARED BY:
One	temperature: 25 [°] C	A. Maczynski
EXPER	NIMENTAL VALUES:	
The	solubility of 2-methyl-1-butanol in wate:	r at 25° C was reported to be 3.0 g(1)/100 sln.
The	corresponding mole fraction, x_1 , calculat	ted by the compiler is 0.0063.
The	solubility of water in 2-methyl-l-butano	l at 25 ⁰ C was reported to be 9.2 g(2)/100g sln.
The	corresponding mole fraction $x_2^{}$, calculate	ed by the compiler is 0.33.
	AUXILIARY	INFORMATION
METH	OD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
for In by 1 a to com bur	sumably the titration method described ternary systems containing HCl was used. this method the solubility was determined oringing 100 ml samples of (1) or (2) to emperature $25^{\circ} \pm 0.10^{\circ}$ C and the second ponent was then added from a calibrated et, with vigorous stirring, until the ution became permanently cloudy.	 source not specified; purified; purity not specified. not specified.
		ESTIMATED ERROR: Solubility: 2% (alcohol-rich)-10% (water- rich) Temperature: ± 0.10°C (no further details) REFERENCES:

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COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) 2-Methyl-1-butanol ("active" amyl	Ratouis, M., Dode, M.
alcohol; sec-butylcarbinol);	Bull. Soc. Chim. Fr. 1965, 3318-22.
^C ₅ H ₁₂ ⁰ ; [137-32-6]	<u>1705</u> , 5510-22.
(2) Water, H ₂ 0; [7732-18-5]	
VARIABLES:	PREPARED BY:
One temperature: 30 ⁰ C	S.C. Valvani; S.H. Yalkowsky; A.F.M. Barton
Ringer solution also studied	
EXPERIMENTAL VALUES:	
The proportion of (1) in the water-rich phase	at equilibrium at 30° C was reported to
be 2.61 g(1)/100g sln.	
The corresponding mole fraction, calculated b	- 1
The proportion of (1) in the water-rich phase	
equilibrium at 30° C was reported to be 2.46 g	(1)/100g sln.
AUXILIARY	INFORMATION
METHOD APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
In a round bottomed flask, 50 mL of water and a sufficient quantity of alcohol were	(1) Prolabo, Paris;
introduced until two separate layers were	redistilled with 10:1 reflux; $n_{\rm D}^{25}$ 1.40780
formed. The flask assembly was equilib- rated by agitation for a least 3 h in a	
constant temp bath. Equilibrium solubility	(2) twice distilled from silica apparatus or ion-exchanged with Sagei A20
was attained by first supersaturating at a slightly lower temperature (solubility of	of ion exchanged with sager A20
alcohols in water is inversely proportional to temperature and then equilibrating at	
the desired temperature. The aqueous	
layer was separated after an overnight storage in a bath. The alcohol content	ESTIMATED ERROR:
was determined by reacting the aqueous solution with potassium dichromate and	Solubility: relative error of 2 determina-
titrating the excess dichromatewith ferrous	tions less than 1%
sulfate solution in the presence of phosphoric acid and diphenylamine barium	Temperature: ± 0.05°C
sulfonate as an indicator.	REFERENCES:
L	1

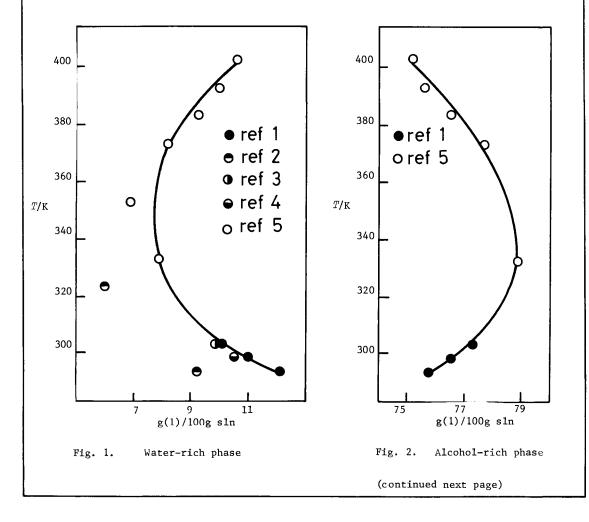
2-Methyl-2-butanol

COMPONENTS:	EVALUATOR:	
(1) 2-Methyl-2-butanol (tert-pentanol,	A. Maczynski, Institute of Physical	
tert-amyl alcohol, ethyldimethylcarbinol	Chemistry of the Polish Academy of Sciences,	
C ₅ H ₁₂ O; [75-85-4]	Warsaw, Poland;and A.F.M. Barton, Murdoch	
(2) Water; H ₂ 0; [7732-18-5]	University, Perth, Western Australia.	
(-, -, -, -, -, -, -, -, -, -, -, -, -, -	November 1982	

CRITICAL EVALUATION:

Solubilities in the system comprising 2-methyl-2-butanol (1) and water (2) have been reported in six publications. Ginnings and Baum (ref 1) carried out measurements of mutual solubility of the components at 293, 298 and 303 K by the volumetric method. Krupatkin (ref 2) determined the solubility of (1) in (2) at 293 and 323 K by the titration method. The water-rich phase was studied also by Ratouis and Dode (ref 3) (at 303 K by an analytical method) and Mullens (ref 4) (an interferometric method at one temperature) Moriyoshi and Aoki (ref 5) determined mutual solubilities between 333 and 402 K and up to 2450 atm (248 MPa) by refractometry. Hyde *et al.* (ref 6) determined the upper critical solution temperature and a "room temperature" solubility.

Data for the water-rich phase at atmospheric pressure are collected in Figure 1. The results of Krupatkin (ref 2) disagree with all others, and are not considered further. At 303 K the value 9.90 \pm 0.1 g(1)/100g sln of ref 3 is in good agreement with the value 10.10 \pm 0.1 g(1)/100g sln of ref 1, although in poor agreement with the values at 298 K of ref 1 and 4. The values of ref 1 at 293, 298 and 303 K are selected as tentative values. Above 332 K the graphically smoothed data of Moriyoshi and Aoki (ref 5), all that is available, are also regarded as tentative.



COMPONENTS		1	EVALUATOR				
(1) 2-Methyl-2-butanol (tert-pentanol, tert-amyl alcohol, ethyldimethylcarbinol)			A.Maczynski, Institute of Physical				
	Academy of Science						
C5H12	C ₅ H ₁₂ 0: [75-85-4] Sciences, Warsaw, Poland and A.F.M.						
(2) Water; H ₂ 0; [7732-18-5] Murdoch University, Perth, Western							
	2		Australia.				
November 1982							
CRITICAL EVA	LUATION (continued)						
The informa	tion on the alcohol-rich	phase is col	lected in Figure 2. At	t 293, 298 and			
303 K only	the data of Ginnings and	Baum (ref 1)	are available, and are	presented			
tentatively	Above 332 K the grap	hically smoot	hed data of Moriyoshi an	nd Aoki (ref 5)			
are regarde	ed as tentative.						
	abilities of (1) and (2)						
sheet of re	of 5. Information on th	is system is	inadequate, and further	study is required.			
	Tentative values f	or the mutual	solubilities				
	of 2-methy1-2-buta	nol (1) and v	vater (2)				
<i>т/</i> к	Water-ri	ch phase	Alcohol-r	Alcohol-rich phase			
178	g(1)/100g sln	-	$g(2)/100g sln \qquad x_2$				
	g(1)/100g 510	x_1	g(2)/100g 51n	[~] 2			
293	12.1	0.027	24.3	0.61			
298	11.0	0.025	23.7	0.60			
303	10.1	0.024	22.7	0.59			
313	9.0	0.020	22.1	0.58			
333	7.8	0.019	21.2	0.57			
353	7.7	0.017	21.4	0.57			
373	8.2	0.018	22.5	0.59			
393	9.9	0.022	24.1	0.61			
References							
L. Ginnings,	, P.M.; Baum, R. J. Am. C	hem. Soc. <u>19</u>	<u>37</u> , 59, 1111.				
2. Krupatkin	n, I.L. Zh. Obshch. Khim.	<u>1955</u> , 25, 1	371; J. Gen. Chem. USSR	<u>1955,</u> 25, 1815.			
3. Ratouis,	M.; Dode, M. Bull. Soc.	Chim. Fr. <u>19</u>	<u>965</u> , 3318.				
4. Mullens,	J. Alcoholassociaten, do	ctoraatsproe	schrift, Leuven, 1971;	Huyskens, P.;			
Mullen, S	J.; Gomez, A.; Tack, J.	Bull. Soc. Cl	nim. Belg. <u>1975</u> , 84, 253				
5. Moriyoshi, T.; Aoki, Y. J. Chem. Eng. Japan, <u>1978</u> , 11, 341.							
5. Hyde, A.	J.; Langbridge, D.M.; Law	rence, A.S.C	Disc. Faraday Soc. <u>19</u>	<u>54</u> , <i>18</i> , 239.			

COMPONENTS:	ORIGINAL MEASUREMENTS:		
 2-Methyl-2-butanol (tert-pentanol, tert-amyl alcohol, ethyldimethylcarbinol C₅H₁₂⁰; [75-85-4] 	Ginnings, P.M.; Baum, R. J. Am. Chem. Soc. <u>1937</u> , 59, 1111-13.		
(2) Water; H_2^0 ; [7732-18-5]			
VARIABLES:	PREPARED BY:		
Temperature: 20-30 ⁰ C	A. Maczynski		
EXPERIMENTAL VALUES:			
Mutual solubility of 2-met	hyl-2-butanol and water		
t/ ⁰ C g(1)/100g sln	x_1 (compiler)		
(2)-rich phase (1)-rich pha	ase (2)-rich phase (1)-rich phase		
20 12.15 75.74	0.02748 0.3894		
25 11.00 76.53	0.02463 0.3998		
30 10.10 77.31	0.02244 0.4104		
Relativ	ve density, d_{μ}		
t/ ⁰ C Water-rich pl	-		
20 0.9837	0.8662		
25 0 .9829	0.8552		
30 0,9828	0.8498		
AUXILIARY	INFORMATION		
METHOD / APPARATUS / PROCEDURE :	SOURCE AND PURITY OF MATERIALS:		
The volumetric method was used. Both components were introduced in known amounts into a two-bulb graduated and calibrated flask and shaken mechanically in a water-bath at constant temperature. After sufficient time the liquids were allowed to separate and the total volume was measured. Upon centrifugation, the phase separation line was read, and phase volumes were calculated. From the total weights of the components, the total volume, individual phase volumes, and component concentrations in either phase were evaluated.	 (1) from Grignard synthesis; distilled from metallic calcium; b.p. range 101.9-102.1°C, d₄²⁵ 0.8055; purity not specified. (2) not specified. (2) not specified. ESTIMATED ERROR: Temperature: ± 0.1°C Solubility : better than 0.1 wt % (type of error not specified) REFERENCES: 		

COMPONENTS:	ORIGINAL MEASUREMENTS:
 2-Methyl-2-butanol (tert-pentanol, tert-amyl alcohol, ethyldimethylcarbinol) C₅H₁₂O; [75-85-4] 	Hyde, A.J; Langbridge, D.M.; Lawrence, A.S.C. Disc. Faraday Soc. <u>1954</u> , 18, 239-58
(2) Water; H ₂ 0; [7732-18-5]	
VARIABLES:	PREPARED BY:
One temperature; ca 260.0°C	A. Maczynski; A.F.M. Barton
EXPERIMENTAL VALUES:	
The upper critical solution temperature was $45.0 \text{ g(1)}/100 \text{g} \text{ sln } (x_1 = 0.143, \text{ compiler}).$ The solubility of (1) in (2) at room tempera	
AUXILIARY	INFORMATION
METHOD /APPARATUS / PROCEDURE :	SOURCE AND PURITY OF MATERIALS:
Not specified	 not specified not specified
	ESTIMATED ERROR:
	Not specified
	REFERENCES :

COMPONENTS	•		OPTOTNAL MEASUE	DEMENITS .	
	· :hyl-2-butanol (<i>ter</i> ;	t novetore of toret	ORIGINAL MEASUREMENTS:		
		-	Krupatkin, I.L.		
	alcohol, ethyldime	ing icarbinol);	Zh. Obshch. Khim. 1955, 25, 1871-6;		
	0; [75-85-4]		*J. Gen. Chem.	USSR <u>1955</u> , 25, 1815–9.	
(2) Water	; H ₂ 0; [7732-18-5]]			
VARIABLES			PREPARED BY:		
Temperatu	re: 20 ⁰ C and 50 ⁰ C		S.H. Yalkowsky	; S.C. Valvani; A.F.M. Barton	
EXPERIMENT	TAL VALUES:	<u></u>			
	Mutual solubi	lity of 2-methyl-2	2-butanol (1) ar	nd water (2)	
t∕°c	Water-rich	phase	Alcohol-rich	n phase	
	g(1)/100g sln	x_1	g(1)/100g sln	x_1	
		(compilers)		(compilers)	
20	9.23	0.0204	85.20	0.541	
50	6	0.013	78.88	0.433	
ļ 					
		AUXILIARY	INFORMATION	<u> </u>	
METHOD /AP	PARATUS/PROCEDURE:		SOURCE AND PUR	ITY OF MATERIALS:	
a study 3-methy1	above formed part of the ternary syst -1-butanol. The in	em including	(1) distilled b.p. 102 ⁰	-	
the isothermal method, in ampoules with ground-glass stoppers in a water thermostat Samples of one component at the specified constant temperature were titrated with the other component until turbidity developed.			(2) distilled	twice	
			ESTIMATED ERRO	DR:	
			Not stated		
			DEFEDENCIE	·	
			REFERENCES :		

Ratouis, M.; Dode, M. Bull. Soc. Chim. Fr. <u>1965</u> , 3318. PREPARED BY: S.C. Valvani; S.H. Yalkowsky; A.F.M. Barton.
······································
ne water-rich phase at equilibrium at
lculated by the compiler is $x_1 = 0.0220$.
of a mixture with Ringer solution at (1)/100g sln.
INFORMATION
<pre>SOURCE AND PURITY OF MATERIALS: (1) Prolabo, Paris; redistilled with 10:1 reflux ratio; b.p. 102.4-102.5°C/757.7 mm Hg n²⁵ 1.40258 (2) twice distilled from silica apparatus or ion-exchanged with Sagei A20 ESTIMATED ERROR: Solubility: relative error of 2 determina- tions less than 1% Temperature: ± 0.05°C REFERENCES:</pre>

(1) 2-Methyl-2-butanol; (tert-pentanol,			
	* Mullens, J. Alcoholassociation, doctoraatsproetschrift		
tert-amyl alcohol, ethyl	Leuven, 1971.		
dimethylcarbinol), C ₅ H ₁₂ 0; [75-85-4]	Huyskens, P.; Mullens, J.; Gomez, A.; Tack, J.		
(2) Water; H ₂ 0; [7732-18-5]	Bull. Soc. Chim. Belg. <u>1975</u> , 84, 253-62.		
ARIABLES:	PREPARED BY:		
One temperature: 25°C	M.C. Haulait-Pirson; A.F.M. Barton.		
XPERIMENTAL VALUES: At equilibrium at 25 [°] C the concentration of phase was reported as 1.198 mol(1)/L sln, alcohol-rich phase was reported as 7.308 mol The corresponding solubilities on a mass/vol 131.7 g(2)/L sln (compiler).	and the concentration of water (2) in the $(2)/L \ sln.$		

AUXILIARY INFORMATION						
METHOD/APPARATUS/PROCEDURE: The partition of the two components was made using a cell described in ref 1. The Rayleigh Interference Refractometer M154 was used for the determination of the concentrations. Standard solutions covering the whole range of concentration investigated were used for the calibration.	<pre>SOURCE AND PURITY OF MATERIALS: (1) Merck (P.a.) (2) distilled ESTIMATED ERROR: Solubility: ±0.001 mol(1)/L sln. REFERENCES: 1. Meeussen, E.; Huyskens, P. J. Chim. Phys. <u>1966</u>, 63, 845.</pre>					

COMPONENTS:				ORIGINAL MEASUREMENTS:			
(1) 2-Methyl-2-butanol(tert-pentanol, tert-				Moriyoshi, T.; Aoki, Y.			
amyl alcohol, ethyldimethylcarbinol); C ₅ H ₁₂ 0; [75-85-4]			J. Chem. Eng. Jpn. <u>1978</u> , 11, 341-5.				
(2) Wateı	r;H ₂ 0; ũ	7732-18-5]					
VARIABLES:				PREPARED BY:			
Temperatur Pressure:		02 K 1-2450 atm)		A. Maczynski;	Z. Maczynski;	A.F.M. Barton	
EXPERIMENTA						(0)	
- 1-			-	hy1-2-butano1 (
T/K	p/atm	p/MPa (compiler)	g((2)-rich phase	1)/100g sln (1)-rich phase	(2)-rich phase	mpiler) (1)-rich phase	
332.65	1 500	0.1 50.7	7.9 9.0	78.9 77.5	0.0172 0.0198	0.433 0.413	
	1000	101.3	9.3	75.8	0.0205	0.390	
	1510 2000	153.0 202.7	10.3 11.2	74.2 72.7	0.0229 0.0251	0.370 0.352	
	2450	248.3	12.4	71.3	0.0281	0.337	
352.55	1	0.1	6.9	82.4	0.0149	0.489	
	500 816	50.7 82.7	7.5 8.1	80.1 78.9	0.0163 0.0177	0.451 0.433	
	1000	101.3	8.5	78.0	0.0186	0.433	
	1530	155.0	9.5	75.8	0.0210	0.390	
	2000	202.7	9.8	74.2	0.0217	0.370	
	2450	249.3	10.3	72.4	0.0241	0.349	
372.55	1	0.1	8.2	77.7	0.0179	0.416	
	500 748	50.7 75.8	9.6 10.0	76.5 75.4	0.0212 0.0222	0.399 0.376	
	965	97.8	10.0	74.9	0.0227	0.379	
	1020	103.4	10.2	74.7	0.0236	0.376	
	1034	104.8	10.6	-	0.0236	-	
	1224	124.0	-	74.5	-	0.374	
	1361	137.9	11.2	74.0	0.0251	0.368	
	1565 1864	158.6 188.9	11.5 12.5	73.6 72.9	0.0258 0.0284 (continued	0.363 0.355	
			AUXILIARY	INFORMATION	(continued	next page)	
METHOD /APP	ARATUS / PRO	CEDURE :		SOURCE AND PURITY OF MATERIALS:			
		method was use	d.	(1) source not specified, best grade			
				reagent;			
		conditions of t		dried by refluxing over freshly ignited			
		ures of (1) and st 24 h and th				en distilled twice;	
	e for anot		t a known	$n_{\rm D}^{23}$ 1.40	25, d ²⁵ 0.804	2 g cm ⁻ .	
		as added to the					
		ixing, the refr		(2) not spec	ified;		
		ulting solution			d in ref l.		
		K, and their c om a calibratio					
Detaila	of the ann	aratus and expe	rimental	ESTIMATED ERRO	R:		
		cribed in ref			± 0.05 K		
r			-		± 7 atm		
				Solubility: ± 0.32 g(1)/100 sln (mean error)			
				REFERENCES;		., 	
			REFERENCES: 1. Moriyoshi, T.; Aoki, Y.; Kamiyama, H.				
				J. Chem.	Thermodyn. 1	<u>.977</u> , 9, 495.	
1							

2-Methyl-2-butanol

COMPONENTS:				ORIGINAL MEASUREMENTS			
(1) 2-Methyl-2-butanol (tert-pentanol, tert-				Moriyoshi, T.; Aoki, Y.			
amyl alcohol, ethyldimethylcarbinol); C ₅ H ₁₂ 0; [75-85-4]				J. Chem. Eng. Jpn. <u>1978</u> , 11, 341-5.			
(2) Water; H ₂ ⁰ ; [7732-18-5]							
EXPERIMENTAL VALUES (continued)							
T/K	p/atm	<pre>p/MPa (compiler)</pre>	g(1) (2)-rich phase				
372.55	2000 2245 2450	202.7 227.5 248.3	12.7 13.5 13.8	72.0 70.7 69.6	0.0289 0.0309	0.344 0.330	
382.05	1 500 816 1000	0.1 50.7 82.7 101.3	9.3 9.8 10.6 11.2	76.5 75.4 74.5 74.2	0.0317 0.0205 0.0217 0.0236 0.0251	0.319 0.399 0.385 0.374 0.370	
	1225 1510 1864 2245	124.1 153.0 188.9 227.5	11.5 11.8 12.7 13.9	73.6 72.2 71.3 69.4	0.0258 0.0266 0.0289 0.0319	0.363 0.347 0.337 0.317	
391.85	2450 1 748 1000	248.3 0.1 75.8 101.3	14.5 10.0 11.5 11.6	68.5 75.6 74.0 73.6	0.0324 0.0222 0.0258 0.0261	0.308 0.388 0.368 0.363	
401.75	1500 2245 2450 1	152.0 227.5 248.3 0.1	12.7 14.5 14.8 10.7	71.8 69.0 69.1 75.2	0.0289 0.0335 0.0343 0.0239	0.342 0.313 0.304 0.383	
	500 1000 2000 2272 2450	50.7 101.3 202.7 230.2 248.3	11.6 12.6 14.4 14.8 15.6	74.0 72.9 69.4 68.3 67.7	0.0261 0.0286 0.0332 0.0343 0.0364	0.368 0.355 0.317 0.306 0.300	

The existence of an upper critical solution temperature was expected on the basis of the behaviour of some butanol-water systems, but was not observed under the conditions used in this study.

COMPONENTS:	EVALUATOR:				
 (1) 3-Methyl-1-butanol (isopentanol, isoamyl alcohol, isobutylcarbinol); C₅H₁₂O; [123-51-3] (2) Water; H₂O; [7732-18-5] CRITICAL EVALUATION 					
Solubilities in the water-rich phase of the swater (2) have been reported in the following		3-methyl-1-butanol (1) and			
Reference	Т/К	Method			
Coull and Hope (ref 5)	298	titration			
Mitsui and Sasaki (ref 7)	283	indirect from 3-component system			
Addison (ref 8)	293	surface tension			
Booth and Everson (ref 9)	298	titration			
Krupatkin (ref 12)	293, 333	titration			
Hayashi and Sasaki (ref 14)	303	turbidity			
Ratouis and Dode (ref 17)	303	analytical			
The mutual solubilities of (1) and (2) were	e measured in the	following works:			
Reference	Т/К	Method			
Brun (ref 3)	273	synthetic			
Kablukov and Malischeva (ref 4)	288-303	volumetric			
Ginnings and Baum (ref 6)	293-303	volumetric			
Crittenden and Hixon (ref 10)	298	titration			
Weiser and Geankopolis (ref 13)	298-323	titration			
Arnold and Washburn (ref 15)	283-313 syr	nthetic and analytical			
Lavrova and Lesteva (ref 18)	313, 333	titration			
Hyde <i>et al.</i> (ref 11) determined the upper critical solution temperature and a "room temperature" solubility.					

The remaining data have not been compiled: Fontein (ref 1) used mixed amyl alcohols; Fuhner (ref 2) carried out only preliminary experiments on this sytem; and Ito (ref 16) reported the critical solution temperature. The results of Coull and Hope (ref 5), Mitsui and Sasaki (ref 7) and Booth and Everson (ref 9) are in volume units without densities provided, and have not been compared with the other data. The data of Krupatkin (ref 12) are in disagreement with those of all other references, and are rejected.

Values for the solubility of (1) in (2) over the temperature range 283 to 333 K are listed as follows.

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(continued next page)

3-Methyl-1-butanol

		EVALUATOR:	
(1) 3-Methy]	-1-butanol (isopentanol, isoamyl	A. Maczynski, Institut	e of Physical
alcohol,	isobutylcarbinol); C ₅ H ₁₂ 0;	Chemistry of the Polis	h Academy of Sciences
[123-51-	-3]	Warsaw, Poland; and A.F	.M. Barton, Murdoch
(2) Water: F	1 ₂ 0; [7732-18-5]	University, Perth, Wes	
(-,, .	2, 2, 2, 2, 2, 2, 2, 2, 2, 2, 2, 2, 2, 2	November 1982	
CRITICAL EVAL	LUATION (continued)	•	
<i>т/</i> к	g(1)/100g si	ln	
	literature valu	ues	graphically determined values
273	3.95 (ref 3)		Values
283	2.8 (ref 15)		3.2
288	3.04 (ref 4)		3.0
293	2.82(ref 4), 2.85(ref 6), 2.6	56(ref 8), 6,20(ref 12)	2.8
298	2.67(ref 4), 2.67(ref 6), 2.7		2.0
	,,, _,	2.4 (ref 15)	2.7
303	2.56(ref 4), 2.53(ref 6), 2.5		2.6
313	2.2 (ref 15), 2.52 (ref 18)		2.4
323	4 (ref 12), 2.53 (ref 13)		2.3
333	2.20 (ref 18)		2.2
in good agre above 303 K	and 303 K the values of the solub ement, and were selected to estim all the data are in poor agreemen tentative.	nate the recommended valu	ref 4, 6, 10, 14 are les. Below 293 K ar
in good agre above 303 K regarded as For the alcol	ement, and were selected to estim all the data are in poor agreemer tentative. hol-rich phase, values of the sol	nate the recommended valuate, and the graphically e	ref 4, 6, 10, 14 are nes. Below 293 K ar estimated values are
in good agre above 303 K regarded as For the alcol	ement, and were selected to estim all the data are in poor agreemer tentative. hol-rich phase, values of the sol	nate the recommended valuat, and the graphically e ubility of (2) in (1) be	ref 4, 6, 10, 14 are nes. Below 293 K ar estimated values are
in good agre above 303 K regarded as For the alcol are tablulat	ement, and were selected to estim all the data are in poor agreemen tentative. hol-rich phase, values of the sol ed here.	nate the recommended valu nt, and the graphically e ubility of (2) in (1) be	ref 4, 6, 10, 14 are nes. Below 293 K ar estimated values are
in good agre above 303 K regarded as For the alcol are tablulat	ement, and were selected to estim all the data are in poor agreemen tentative. hol-rich phase, values of the sol ed here. g(1)/100g sl	nate the recommended valu nt, and the graphically e ubility of (2) in (1) be	cef 4, 6, 10, 14 are ues. Below 293 K ar estimated values are etween 283 and 333 K graphically determined
in good agre above 303 K regarded as For the alcol are tablulat <i>T</i> /K	ement, and were selected to estim all the data are in poor agreemen tentative. hol-rich phase, values of the sol ed here. g(1)/100g sl literature val	nate the recommended valu nt, and the graphically e ubility of (2) in (1) be	cef 4, 6, 10, 14 are ues. Below 293 K ar estimated values are etween 283 and 333 K graphically determined
in good agre above 303 K regarded as For the alcol are tablulat <i>T</i> /K 273	ement, and were selected to estim all the data are in poor agreemen tentative. hol-rich phase, values of the sol ed here. g(1)/100g sl literature val 91.0 (ref 3)	nate the recommended valu nt, and the graphically e ubility of (2) in (1) be	ref 4, 6, 10, 14 are ues. Below 293 K an estimated values are etween 283 and 333 K graphically determined values
in good agre above 303 K regarded as For the alcol are tablulat <i>T/K</i> 273 283	ement, and were selected to estim all the data are in poor agreemen tentative. hol-rich phase, values of the sol ed here. g(1)/100g sl literature val 91.0 (ref 3) 91.0 (ref 15)	nate the recommended valu at, and the graphically e Lubility of (2) in (1) be .n .ues	ref 4, 6, 10, 14 are ues. Below 293 K ar estimated values are etween 283 and 333 K graphically determined values 91.0
In good agread above 303 K regarded as For the alcologic are tablulate T/K 273 283 288	ement, and were selected to estim all the data are in poor agreemen tentative. hol-rich phase, values of the sol ed here. g(1)/100g sl literature val 91.0 (ref 3) 91.0 (ref 15) 90.67 (ref 4)	nate the recommended valu nt, and the graphically e Lubility of (2) in (1) be .n .ues	ref 4, 6, 10, 14 are tes. Below 293 K and estimated values are etween 283 and 333 K graphically determined values 91.0 90.7 90.4
in good agre above 303 K regarded as For the alcol are tablulat <i>T/K</i> 273 283 288 293	ement, and were selected to estim all the data are in poor agreement tentative. hol-rich phase, values of the soled here. g(1)/100g sl literature val 91.0 (ref 3) 91.0 (ref 15) 90.67 (ref 4) 90.40(ref 4), 90.53(ref 6), 8	nate the recommended valu nt, and the graphically e Lubility of (2) in (1) be .n .ues	ref 4, 6, 10, 14 are tes. Below 293 K ar estimated values are etween 283 and 333 K graphically determined values 91.0 90.7 90.4
in good agre above 303 K regarded as For the alcol are tablulat <i>T/K</i> 273 283 288 293	ement, and were selected to estim all the data are in poor agreement tentative. hol-rich phase, values of the soled here. g(1)/100g sl literature val 91.0 (ref 3) 91.0 (ref 15) 90.67 (ref 4) 90.40(ref 4), 90.53(ref 6), 8 90.13(ref 4), 90.39(ref 6), 9 89.85 (ref 5), 90.24 (ref 6)	hate the recommended valu ht, and the graphically of lubility of (2) in (1) bo n ues 5.46(ref 12) 0.9(ref 10), 90.25(ref 1	ref 4, 6, 10, 14 are les. Below 293 K ar estimated values are etween 283 and 333 K graphically determined values 91.0 90.7 90.4 3),
in good agree above 303 K regarded as For the alcol are tablulat <i>T/K</i> 273 283 288 293 298	ement, and were selected to estim all the data are in poor agreement tentative. hol-rich phase, values of the soled here. g(1)/100g sl literature val 91.0 (ref 3) 91.0 (ref 15) 90.67 (ref 4) 90.40(ref 4), 90.53(ref 6), 8 90.13(ref 4), 90.39(ref 6), 9	hate the recommended valu ht, and the graphically of lubility of (2) in (1) bo n ues 5.46(ref 12) 0.9(ref 10), 90.25(ref 1	ref 4, 6, 10, 14 are tess. Below 293 K and estimated values are etween 283 and 333 K graphically determined values 91.0 90.7 90.4 3), 90.2
in good agree above 303 K regarded as For the alcol are tablulat. <i>T/K</i> 273 283 288 293 298 303 313 323	ement, and were selected to estim all the data are in poor agreement tentative. hol-rich phase, values of the soled here. g(1)/100g sl literature val 91.0 (ref 3) 91.0 (ref 15) 90.67 (ref 4) 90.40(ref 4), 90.53(ref 6), 8 90.13(ref 4), 90.39(ref 6), 9 89.85 (ref 5), 90.24 (ref 6)	nate the recommended valu at, and the graphically of Lubility of (2) in (1) bo n ues 5.46(ref 12) 0.9(ref 10), 90.25(ref 1 90.2 (ref 15)	ref 4, 6, 10, 14 are les. Below 293 K ar estimated values are etween 283 and 333 K graphically determined values 91.0 90.7 90.4 3), 90.2 89.9
in good agree above 303 K regarded as For the alcol are tablulat <i>T/K</i> 273 283 288 293 298 303 313	ement, and were selected to estim all the data are in poor agreement tentative. hol-rich phase, values of the soled here. g(1)/100g sl literature val 91.0 (ref 3) 91.0 (ref 15) 90.67 (ref 4) 90.40(ref 4), 90.53(ref 6), 8 90.13(ref 4), 90.39(ref 6), 9 89.85 (ref 5), 90.24 (ref 6) 86.6 (ref 15), 89.3 (ref 18)	nate the recommended valu at, and the graphically of Lubility of (2) in (1) bo n ues 5.46(ref 12) 0.9(ref 10), 90.25(ref 1 90.2 (ref 15)	ref 4, 6, 10, 14 are les. Below 293 K ar estimated values are etween 283 and 333 K graphically determined values 91.0 90.7 90.4 3), 90.2 89.9 89.3
in good agree above 303 K regarded as For the alcol are tablulat <i>T/K</i> 273 283 288 293 298 303 313 323 333	ement, and were selected to estim all the data are in poor agreement tentative. hol-rich phase, values of the soled here. g(1)/100g sl literature val 91.0 (ref 3) 91.0 (ref 15) 90.67 (ref 4) 90.40(ref 4), 90.53(ref 6), 8 90.13(ref 4), 90.39(ref 6), 9 89.85 (ref 5), 90.24 (ref 6) 86.6 (ref 15), 89.3 (ref 18) 82.02 (ref 12), 88.5 (ref 13)	hate the recommended valu hat, and the graphically of hubility of (2) in (1) bo hues 5.46(ref 12) 0.9(ref 10), 90.25(ref 1 90.2 (ref 15)	ref 4, 6, 10, 14 are les. Below 293 K ar estimated values are etween 283 and 333 K graphically determined values 91.0 90.7 90.4 3), 90.2 89.9 89.3 88.6 88.0

(continued next page)

COMPON	ENTS:	EVALUATOR:			
(1) 3-	-Methyl-1-butanol (isopentanol, isoamyl	Z A. Maczynski, Institute of Physical			
1	lcohol, isobutylcarbinol); C ₅ H ₁₂ O;	Chemistry of the Polish Academy of Sciences,			
	123-51-3]	Warsaw, Poland; and A.F.M. Barton, Murdoch			
(2) Wa	ater; H ₂ 0; [7732-18-5]	University, Perth, Western Australia.			
		November 1982			
CRITIC.	AL EVALUATION (continued)				
	3-methyl-1-butanol (
ł	T/K Water-rich				
Į	g(1)/100g sln	$10^3 x_1$ g(2)/100g sln x_2			
	283 3.2 (tentative)	6.7 9.0 (tentative) 0.33			
ļ	288 3.0 (tentative)	6.3 9.3 (tentative) 0.33			
	2932.8 (recommended)	d) 5.8 9.6 (tentative) 0.34			
	298 2.7 (recommende				
	303 2.6 (recommende				
	313 2.4 (tentative)				
	333 2.2 (tentative)459 upper critical solution tem				
Refer	ences				
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5.	Coull, J.; Hope, H.B. J. Phys. Chem.	<u>1935,</u> 39, 967.			
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9.	Booth, H.S.; Everson, H.E. Ind. Eng.	Chem. <u>1948</u> , 40, 1491.			
10.	Crittenden, E.D., Jr.; Hixon, A.N. In	d. Eng. Chem. <u>1954</u> , 46, 265.			
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14.	Hayashi, M.; Sasaki, T. Bull. Chem. S	oc. Jpn, <u>1956</u> , 29, 857.			
15.	Arnold, V.W.; Washburn, E.R. J. Phys.	Chem. <u>1958</u> , 62, 1088.			
16.	Ito, K. Sci. Papers Inst. Phys. Chem.	Res. (Tokyo) <u>1961</u> , 55, 189.			
17.	Ratouis, M.; Dode, M. Bull. Soc. Chim	. Fr. <u>1965</u> , 3318.			
18.	Lavrova, O.A.; Lesteva, T.M. Zh. Fiz. 3813-75.	Khim. <u>1976</u> , 50, 1617; Dep. Doc. VINITI			

COMPONENTS :	ORIGINAL MEASUREMENTS:
(1) 3-Methyl-1-butanol (isopentanol, isoamyl	Brun, P.
alcohol, isobutylcarbinol); C5H ₁₂ 0;	C.R. Hebd. Seances Acad. Sci. 1925, 180,
[123-51-3]	1745-7; <u>1926</u> , <i>183</i> , 207-10.
(2) Water; H ₂ 0; [7732-18-5]	
VARIABLES:	PREPARED BY:
One temperature: 0°C	A.F.M. Barton

EXPERIMENTAL VALUES:

The mass percentage of 3-methyl-l-butanol (1) at equilibrium in the water-rich phase at 0°C was reported as 3.95 g(1)/100g sln, the corresponding mole fraction solubility, calculated by the compiler, is $x_1 = 0.00833$.

The mass percentage of 3-methyl-l-butanol in the alcohol-rich phase at equilibrium at 0°C was reported as 91.0 g(1)/100g sln; the corresponding mole fraction solubility calculated by the compiler is $x_1 = 0.674$.

Graphical results were reported in the 1925 paper for 40, 80, and 120°C.

AUXILIARY	INFORMATION
TOVITINU	INTOWNITON

METHOD / APPARATUS / PROCEDURE :	SOURCE AND PURITY OF MATERIALS:
The synthetic method was used, in which the turbidity temperature is determined for mixtures of known composition.	Not specified.
	ESTIMATED ERROR:
	Not specified.
	REFERENCES :

COMPONENTS:				ORIGINAL MEASUREMENTS:				
<pre>(1) 3-Methyl-1-butanol (isopentanol, isoamyl alcohol isobutylcarbinol); C₅H₁₂O; [123-51-3]</pre>								
(2)	Water;	н ₂ 0; [7732-	18-5]					
	IABLES: perature	: 15-30 [°] C			PREPARED BY S.H. Yalkow	: vsky; S.C. V	alvani; A.)	F.M. Barton
EVDE		VALUES:						
				·	3-methy1-1-1			
t/ ⁰	c		Mutual sol er-rich pha ^x 1 (compiler	se d/g cm ⁻³	·		l-rich pha	se d/gcm ⁻³
	с °1	Wat g(1)/100g	er-rich pha ^x 1	se d/g cm ⁻³	·	Alcoho g(2)/100g sln	l-rich phas	se d/gcm ⁻³
t/ ^o	°c °1 0.0306	Wat g(1)/100g sln	er-rich pha ^x 1	se $d/g \text{ cm}^{-3}$	°2	Alcoho g(2)/100g sln 9.310	ol-rich phan ^x 1 (compilen -	se d/gcm ⁻³ r)
t/ ⁰	°C °1 0.0306 0.0396	Wat g(1)/100g sln 3.081	er-rich pha ^x 1	se d/g cm ⁻³) 0.9934	^c 2 0.0773 0.0776	Alcoho g(2)/100g sln 9.310	ol-rich phas ^x 1 (compiles - -	d/g cm ⁻³ r) 0.8308
t/ ⁰ 15 15 15	°C °1 0.0306 0.0396	Wat g(1)/100g sln 3.081 3.086	er-rich pha ^x 1	se d/g cm ⁻³) 0.9934 0.9933	^c 2 0.0773 0.0776	Alcoho g(2)/100g sln 9.310 9.346	ol-rich phas ^x 1 (compiles - -	d/g cm ⁻³ r) 0.8308 0.8306
t/ ⁰ 15 15 15	°1 0.0306 0.0396 0.0294	Wat g(1)/100g sln 3.081 3.086 2.965 3.04	er-rich pha ^x 1 (compiler - - -	se d/g cm ⁻³) 0.9934 0.9933 0.9921	^c 2 0.0773 0.0776 0.0776	Alcoho g(2)/100g sln 9.310 9.346 9.347 9.33	ol-rich phas ^x 1 (compiles - - - -	d/g cm ⁻³ r) 0.8308 0.8306 0.8306
t/ ⁰ 15 15 15 15(C ³ 1 0.0306 0.0396 0.0294 mean)- 0.0283	Wat g(1)/100g sln 3.081 3.086 2.965 3.04	er-rich pha ^x 1 (compiler - - -	se d/g cm ⁻³ 0.9934 0.9933 0.9921 0.9929	^c 2 0.0773 0.0776 0.0776	Alcoho g(2)/100g sln 9.310 9.346 9.347 9.33 9.578	01-rich phan x ₁ (compilen - - 0.665 -	d/g cm ⁻³ c) 0.8308 0.8306 0.8306 0.8306 0.8306

0.665

-

-

-

0.8275

0.8245

0.8241

0.8241

25(mean)- 2.67	0.00558	0.9914		-	9.87	0.651	0.8242
					(cont	inued next	page)
		AUXILIARY	INFOR	MATION			
METHOD/APPARATUS/PROCEI The method is based o of the quantity of ea mixing and the volume equilibrium proposed but published first b Alcohol was poured in (calibrated within ± added from the buret liquids mixed by shak tube. After complet layers, the volumes a recorded, and the ref	n the measur ch liquid ta s of the lay by the prese y Hill (ref to the measu 0.01 cm^3). $(\pm 0.01 \text{ cm}^3)$ ing or rever e separation nd temperatu	aken for yers at ent authors l). uring tube Water was) and the rsing the into ure were	(1)	dried distil	led twice f 130.6-131.3 led with po ith barium	cous cupric From calcium 1 [°] C/760 mm 1 Dtassium pe	n. Hg rmanganate, distillate
density determined.			Tem the Solu app REFE	rmometer ubility arent f: RENCES:	e: tenth-de r used. : not stat rom experin	nental valu	ion from mean

2.82

2.703

2.711

2.610

20(mean)-

25 0.0268

25 0.0269

25 0.258

-

-

-

0.9924

0.9921

0.9916

0.9906

-

0.0812

0.0815

0.0815

9.60

9.853

9.887

9.885

0.00589

COMPONENTS:	ORIGINAL MEASUREMENTS:
 (1) 3-Methyl-1-butanol (isopentanol, isoamyl alcohol isobutylcarbinol); C₅H₁₂O; [123-51-3] (2) Water; H₂O; [7732-18-5] 	Kablukov, I.A., Malischeva, V.T. <i>J. Am. Chem. Soc.</i> <u>1925</u> , 47, 1553-61.

EXPERIMENTAL VALUES: (continued)

Mutual solubility of 3-methyl-1-butanol (1) and water (2)

$t/^{o}$	С	Water	-rich phase			Alco	hol-rich phase	
	c_1	g(1)/100g sln	x ₁ (compiler)	$d/g \text{ cm}^{-3}$	°2	g(2)/100g sln	<pre>x₁ (compiler)</pre>	d/g cm ⁻³
30	0.0257	2.594	-	0.9906	0.0832	10.13	-	0.8212
30	0.0257	2.599	-	0.9909	0.0834	10.16	-	0.8208
30	0.0246	2.491	-	0.9899	0.0834	10.16	-	0.8209
30(mean) -	2.56	0.00534	0.9904	-	10.15	0.644	0.8209

COMPONENTS:	ORIGINAL MEASUREMENTS:		
(1) 3-Methyl-1-butanol (isopentanol, isoamyl	Coull, J.; Hope, H.B.		
alcohol, isobutylcarbinol); C ₅ H ₁₂ O; [123-51-3]	J. Phys. Chem. <u>1935</u> , 39, 967-71		
(2) Water; H ₂ 0; [7732-18-5]			
VARIABLES:	PREPARED BY:		
One temperature: 25 ⁰ C	S.H. Yalkowsky; S.C. Valvani; A.F.M. Barton		
EXPERIMENTAL VALUES:			
The proportions by volume at equilibrium at 2	5° C of the alcohol and water were		
reported as 3.10 mL(1)/100mL sln in the water	-rich phase and 93.32 mL(1)/100mL sln		
in the alcohol-rich phase.			
Properties of homoger	neous mixtures of (1) and (2)		
mL(1)/100mL sln mL	(2)/100mL sln n ²⁵		
100.0	0.0 1.4058		
95.0	5.0 1.4033		
93.0	7.0 1.4018		
2.0	98.0 1.3346		
AUXILIARY	INFORMATION		
METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:		
The results from part of the investigation	(1) Baker A.C.S. reagent grade;		
of the ternary system including propanol,	fractionally distilled;		
(1), and (2). The alcohol sample (200 mL) was thoroughly agitated in a thermostat	b.p. 130.5°C		
while water was added until the first appearance of turbidity. The agitation was continued for 6-8h to ensure equilibrium In some cases (1) was added to water and	(2) not stated		
propanol.			
	ESTIMATED ERROR:		
	Temperature: ± 0.1°C Density: ± 0.0001 g cm ⁻³ Refractive index: read to 0.00005, rounded to 0.0001		
	Compositions: ± 0.1% REFERENCES:		
	REFERENCES;		
	REFERENCES :		
	REPERENCES :		
	REFERENCES :		

COMPONENTS:			ORIGINA	L MEASUREMENTS:	······································	
(1) 3-Methy	1-1-butanol (isopen	tanol,	Ginnings, P.M.; Baum R.			
isoamyl alcohol, isobutylcarbinol); C ₅ H ₁₂ 0; [123-51-3]				J. Am. Chem. Soc. <u>1937</u> , 59, 1111-3.		
(2) Water; H	2 ⁰ ; [7732-18-5]					
VARIABLES:			PREPARE	ED BY:		
Temperature:	20-30 [°] C		A. Mac	zynski; Z. Mac:	zynski	
EXPERIMENTAL V	ALUES:		L			
	Mutual solubi	lity of 3-met	hy1-1-t	outanol(l) and w	vater(2)	
t/°C	g(1)/100 (2)-rich phase		ase	$x_1(contract)$	ompiler) e (1)-rich phase	
20	2.85	90.53		0.00596	0.6614	
25	2.67	90.39		0.00557	0.6577	
30	2.53	90.24		0.00527	0.6539	
		Relati	ve dens	ity, d_4		
	t/ ^o c	Water-rich	phase	Alcohol-ri	ch phase	
	20	0.9941		0,8286		
	25	0.9932		0.8257	,	
	30	0.9921		0.8188		
· · - ···· -		AUXILIARY	INFORM	ATION		
METHOD /APPARA	TUS/PROCEDURE:		SOURCE	AND PURITY OF	MATERIALS:	
The volumetric method was used. Both components were introduced in known amounts into a two-bulb graduated and calibrated flask and shaken mechanically in a water-bath at constant temperature. After sufficient time the liquids were allowed to separate and the total volume was measured. Upon centrifugation, the phase separation line was read, and phase volumes were calculated. From the total weights of the components, the total volume individual phase volumes, and component concentrations in either phase were evaluated.			(2) ESTIMA Temp	anhydrous potas distilled from b.p. range 131 d_4^{25} 0.8071. not specified. ATED ERROR: erature: \pm 0.2 bility: bett	water, dried with ssium carbonate and metallic calcium; .5-131.7°C,	
			REFER	ENCES :		

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) 3-Methyl-l-butanol (isopentanol,	Mitsui, S; Sasaki, T.;
isoamyl alcohol, isobutylcarbinol);	J. Chem. Soc. Jpn, <u>1942</u> , 63, 1766-71.
С ₅ H ₁₂ 0; [123-51-3]	
(2) Water; H ₂ 0; [7732-18-5]	
VARIABLES:	PREPARED BY:
One temperature: 19 [°] C	N. Tsuchida
one temperature. 19 0	
EXPERIMENTAL VALUES:	
The solubility of (1) in (2) was estimated to	$h_{0} = 2.00 \pm 0.01 \text{ c(1)}/100 \text{ cm}^{3} \text{ cm} \text{ at } 19.16^{\circ}\text{ C}$
The solubility of (1) in (2) was estimated to	5 DE 3.00 ± 0.01 g(1)/100 cm sin at 19.14 0.
AUXILIARY	INFORMATION
METHOD /APPARATUS / PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
The solubility of butanol in the (1)-(2) system was determined experimentally. By	 Katayama, A.R.; boiled with aqueous KOH, washed with dilute phosphoric
means of the relation thus obtained, the	acid, dried with anhydrous K_2C0_3 and
solubility of (1) in (2) was determined by interpolation.	$CaSO_4$, distilled at $131^{\circ}C$.
	(2) not specified
The measurements were carried out by adding butanol to aqueous (1) containing ethanol	
until one drop produced a permanent	
turbidity; the ethanol increased the butanol solubility and permitted measure-	
ment over the saturation value.	NOTIMATED EDDOD.
	ESTIMATED ERROR: Temperature: ± 0.02°C
	Solubility: ± 0.01 g(1)/100g sln
	REFERENCES :

3-Methyl	I-1-butanol 14
COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) 3-Methyl-l-butanol (isopentanol,	Addison, C.C.;
isoamyl alcohol isobutylcarbinol);	J. Chem. Soc. <u>1945</u> , 98-106.
с ₅ н ₁₂ 0; [123-51-3]	
(2) Water; H ₂ 0; [7732-18-5]	
Ζ	
VARIABLES:	PREPARED BY:
One temperature: 20°C	S.H. Yalkowsky; S.C. Valvani; A.F.M. Barton
EXPERIMENTAL VALUES:	I <u></u>
The proportion of 3-methyl-1-butanol (1) in	the water-rich phase at equilibrium at
20° C was reported to be 2.66 g(1)/100g sln.	
The corresponding mole fraction solubility ca	alculated by the compiler is $x_1 = 0.00555$.
AIIXII.IARY	INFORMATION
METHOD /APPARATUS / PROCEDURE :	SOURCE AND PURITY OF MATERIALS:
A surface tension method was used. Suff-	
icient excess of (1) was added to 100 mL of	(1) impure alcohols were purified by fractional distillation, the middle
(2) in a stoppered flask to form a separate	fraction from a distillation being
lens on the surface. The mixture was	redistilled:
swirled gently, too Vigorous an agitation	
giving a semi-permanent emulsion and in-	b.p. $131.5^{\circ}c$ d_4^{20} 0.8127
correct readings. After settling, a small	$n_{\rm D}^{20}$ 1.4075
sample of the clear aqueous sln was with- drawn into a drop weight pipe and the surfac	5
tension determined. The swirling was con-	(2) not stated
tinued until a constant value was obtained.	
The surface tension-concentration curve was	
known, and only a slight extrapolation (logarithmic scale) was necessary to find	ESTIMATED ERROR:
the concentration corresponding to the	Solubility: ±0.5%

REFERENCES:

COMPONENTS:	ORIGINAL MEASUREMENTS:
COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) 2 M (1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1	Death II Cas Frances II F
(1) 3-Methyl-1-butanol (isopentanol, isocmyl alcohol); C ₅ H ₁₂ O; [123-51-3]	Booth, H.S.; Everson, H.E.
5 12 , 1	Ind. Eng. Chem. <u>1948</u> , 40, 1491-3.
(2) Water; H ₂ O; [7732-18-5]	
2	
VARIABLES:	PREPARED BY:
One temperature: 25 ⁰ C	S.H. Yalkowsky; S.C.Valvani; A.F.M.Barton
Sodium xylene sulfonate	tarianti, art.m.barton
EXPERIMENTAL VALUES:	
It was reported that the solubility of 3-meth	yl-l-butanol(l) in water(2) was
3.5 mL (1)/100 mL (2) at 25.0 ⁰ C.	
The corresponding value in 40% sodium xylene	sulfonate solution as solvent was
	Sufficience Sofucion as sofvent was
> 400 mL(1)/100 mL solvent.	
	INFORMATION
METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
A known volume of solvent (usually 50 mL) in	(1) not specified ("CP or highest grade
a tightly stoppered calibrated Babcock tube was thermostatted. Successive measured	commercial")
was thermostatted. Successive measured quantities of solute were added and equilib-	(2) "distilled"
rated until a slight excess of solute	
remained. The solution was centrifuged,	
returned to the thermostat bath for 10 min, and the volume of excess solute measured	
directly. This was a modification of the	
method described in ref 1.	
	ESTIMATED ERROR:
	Solubility: within 0.1 mL(1)/100 mL(2)
	REFERENCES :
	1. Hanslick, R.S. Dissertation, Columbia
	University, 1935.

COMPONENTS:	ORIGINAL MEASUREMENTS:		
<pre>(1) 3-Methyl-1-butanol (isopentanol,</pre>	Crittenden, E.D., Jr.; Hixon, A.N. Ind. Eng. Chem. <u>1954</u> , 46, 265-8.		
(2) Water; H ₂ O; [7732-18-5]			
VARIABLES:	PREPARED BY:		
One temperature: 25 ⁰ C	A. Maczynski		
EXPERIMENTAL VALUES:			
The solubility of 3-methyl-1-butanol in wate:	r at 25° C was reported to be $2.7g(1)/100g \text{ sln.}$		
The corresponding mole fraction, x_1 , calculated by the compiler is 0.0056.			
The solubility of water in 3-methyl-1-butano. sln.	l at 25 ⁰ C was reported to be 9.1 g(2)/100 g		
The corresponding mole fraction, $x_2^{}$, calculat	ted by the compiler is 0.33.		
AUXILIARY	INFORMATION		
METHOD / APPARATUS / PROCEDURE :	SOURCE AND PURITY OF MATERIALS:		
Presumably the titration method described	 source not specified; purified; 		
for ternary systems containing HCl was used. In this method the solubility was determined	purity not enocified		
by bringing 100-ml samples of (1) or (2) to a temperature $25^{\circ} \pm 0.10^{\circ}$ C and the second	(2) not specified.		
component was then added from a calibrated buret, with vigorous stirring, until the			
solution became permanently cloudy.			
	ESTIMATED ERROR:		
	Solubility: 2% (alcohol-rich)-10% (water- rich).		
	Temperature: ± 0.10°C		
	REFERENCES :		
	1		

COMPONENTS:	ORIGINAL MEASUREMENTS:
<pre>(1) 3-Methyl-1-butanol (isopentanol, isoamyl</pre>	Hyde, A.J.; Langbridge, D.M.; Lawrence, A.S.C. <i>Disc. Faraday Soc.</i> <u>1954</u> , <i>18</i> , 239-58.
(2) Water; H ₂ 0; [7732-18-5]	
VARIABLES:	PREPARED BY:
One temperature: 185,5 ⁰ C	A. Maczynski; A.F.M. Barton
EXPERIMENTAL VALUES:	
$(x_1 = 0.13, \text{ compiler}).$ The solubility of (1) in (2) was reported as	2.5%.
	INFORMATION
METHOD/APPARATUS/PROCEDURE: Not specified	<pre>SOURCE AND PURITY OF MATERIALS: (1) not specified (2) not specified</pre>
	ESTIMATED ERROR: Not specified REFERENCES:

COMPONENTS :	ORIGINAL MEASUREMENTS:
(1) 3-Methyl-1-butanol (isopentanol, isoamyl	Krupatkin, I.L.
alcohol, isobutylcarbinol); C5H ₁₂ 0;	Zh. Obshch. Khim. <u>1955</u> , 25, 1871-6;
[123-51-3]	*J. Gen. Chem. USSR <u>1955</u> , 25, 1815–9
(2) Water; H ₂ 0; [7732-18-5]	
VARIABLES:	PREPARED BY:
Temperature: 20 ⁰ C and 50 ⁰ C	S.H. Yalkowsky; S.C. Valvani; A.F.M. Barton
	,,,
EXPERIMENTAL VALUES:	
Mutual solubility of 3-methyl-1	-butanol (1) and water (2)
$t/^{o}$ C Water-rich phase	Alcohol-rich phase
$g(1)/100g sln x_1 g$	$x_{1}^{(1)/100g sln} x_{1}^{(1)}$
(compilers)	(compilers)
20 6.20 0.0133	85.46 0.546
50 4^a 0.009	82.02 0.483
AUXILIARY	INFORMATION
METHOD / APPARATUS / PROCEDURE :	SOURCE AND PURITY OF MATERIALS:
The data above formed part of the results of	(1) distilled;
a study of the ternary system including 2-methyl-2-butanol. The investigation used	b.p. 114 ^o C
the isothermal method, in ampoules with	(2) distilled twice
ground-glass stoppers in a water thermostat. Samples of one component at the specified	
constant temperature were titrated with the	
other component until turbidity developed.	
	ESTIMATED ERROR:
1	ESTIMATED ERROR: Not stated
	Not stated
	Not stated
	Not stated
	Not stated

	ORIGINAL MEASUREMENTS:
(1) 3-Methyl-l-butanol (isopentanol; isoamyl alcohol, isobutylcarbinol); C ₅ H ₁₂ 0; [123-51-3]	Weiser, R.B.; Geankopolis, C.J. Ind. Eng. Chem. <u>1955</u> , 47, 858-63.
(2) Water; H ₂ 0; [7732-18-5]	
VARIABLES:	PREPARED BY:
Temperature: 25 and 50 [°] C	A. Maczynski
EXPERIMENTAL VALUES:	
Mutual solubility of 3-me	methyl-l-butanol (1) and water (2)
t/ ^o C g(1)/100g sln (2)-rich phase (1)-rich ph	x _l (compiler) phase (2)-rich phase (1)-rich phase
25 2.48 90.2	25 0.00517 0.6541
49.5 2.53 88.5	5 0.00527 0.611
AUXILIARY	
	Y INFORMATION
METHOD/APPARATUS/PROCEDURE: Probably the titration method was used. No details were reported in the paper.	Y INFORMATION SOURCE AND PURITY OF MATERIALS: (1) CP reagent, source not specified; distilled; b.p. range 131.5-132.0 °C, n ¹⁵ 1.4085.
METHOD/APPARATUS/PROCEDURE: Probably the titration method was used.	SOURCE AND PURITY OF MATERIALS: (1) CP reagent, source not specified; distilled; b.p. range 131.5-132.0 °C,
METHOD/APPARATUS/PROCEDURE: Probably the titration method was used.	<pre>SOURCE AND PURITY OF MATERIALS: (1) CP reagent, source not specified; distilled; b.p. range 131.5-132.0 °C, n¹⁵ 1.4085. (2) not specified. ESTIMATED ERROR:</pre>
METHOD/APPARATUS/PROCEDURE: Probably the titration method was used.	 SOURCE AND PURITY OF MATERIALS: (1) CP reagent, source not specified; distilled; b.p. range 131.5-132.0 °C, n¹⁵ 1.4085. (2) not specified.

o-weary - buddon			
COMPONENTS :	ORIGINAL MEASUREMENTS:		
(1) 3-Methyl-1-butanol (isopentanol, isoamyl	Hayashi, M.; Sasaki, T.		
alcohol, isobutylcarbinol); C ₅ H ₁₂ 0;	Bull. Chem. Soc. Jpn. <u>1956</u> , 29, 857-9		
[123-51-3]			
(2) Water; H ₂ 0; [7732-18-5]			
VARIABLES:	PREPARED BY:		
One temperature: 30 ⁰ C	S.H. Yalkowsky; S.C. Valvani; A.F.M. Barton		
EXPERIMENTAL VALUES:			
2.587, 2.565, and 2.577 g(1)/100g sln.) The corresponding mole fraction solubility ca	. (This was the mean of three determinations: alculated by the compilers is $x_1 = 0.00536$.		
The solubility of the alcohol in dilute solut	tions of Tween 80, obtained by extrapolating		
to zero turbidity the linear relation between turbidity and solute concentration in the			
surfactant solution, was less than that in pure water but increased with increasing			
concentration of Tween 80.			

AUXILIARY INFORMATION		
The mixture was well shaken at a temperature below 30.1°C and then stood in the thermostat for 24h. After the excess solute particles cleared, a transparent saturated solution was obtained which was taken from the bottom of the vessel by a siphon. A known amount of this solution (about 20g) was titrated with Tween 80 solution. Concentration was determined by comparison of turbidity with that of standard samples. (The relation between the turbidity and the quantity of solute in the surfactant solution is linear, and the solubility limits are lower than the colubilities in pure water in the dilute	tated. ERROR: y: "possible error" 0.4%	

.

COMPONENTS :		ORIG	ORIGINAL MEASUREMENTS:	
(1) 3-Methyl-1-butanol (<i>isopentanol</i> ,		wl, Arn	old, V.W.; Washburn,	E.R.
isoamyl alcohol, isobutylcarbinol);		binol);	Phys. Chem. 1958, 62,	1088-90.
C ₅ H ₁₂ 0; [123-51-3]			<u></u> ,,	
(2) Water: H	2 ⁰ ; [7732-18-5]			
VARIABLES:		PREF	ARED BY:	
Temperature: 10-40 [°] C		Α.	A. Maczynski	
EXPERIMENTAL VAL	.UES:			
	Mutual solubili	ty of 3-methy1-	l-butanol (1) and wat	er (2)
t∕°c	g(1)/100g (2)-rich phase	sln (1)-rich phase	$x_1(\text{compine})$	
10	2.8	91.0	0.0059	0.674
25	2.4	90.2	0.0050	0.653
40	2.2	86.6	0.0046	0.569
		AUXILIARY INFO	RMATION	
METHOD/APPARATU	S/PROCEDURE:	SOU	RCE AND PURITY OF MAT	ERIALS:
	y of (1) in (2) was	determined	prepared from isob b.p. 131.9°C/760 m n_{L}^{25} 1.4048, d_{L}^{25} 0.4	n Hg;
tubes.	s method, ref 1, usin		not specified.	
determined by	y of (2) and (1) was analysing saturated e temperatures with nt.	solutions	·	
		EST	IMATED ERROR:	
			Not specified.	
			EDENCLO	
			ERENCES: Alexejeff, M.W. <i>B</i> : <i>38</i> , 145.	ull. soc. chim. <u>1882</u> ,

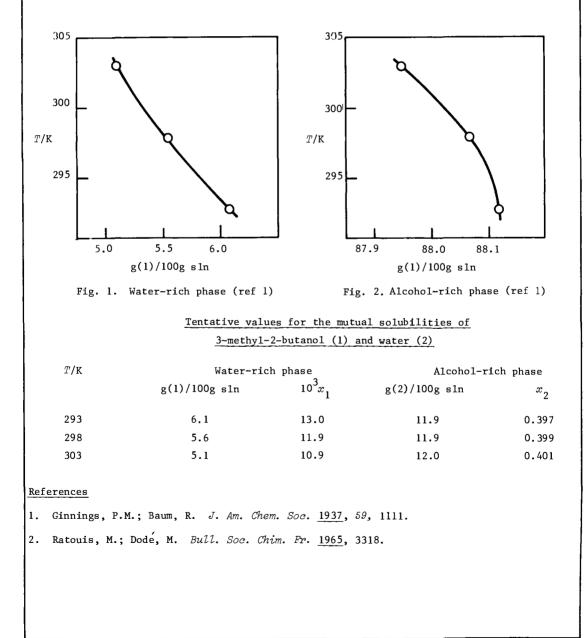
3-wietnyi-	1-butanoi is
COMPONENTS:	ORIGINAL MEASUREMENTS:
 (1) 3-Methyl-1-butanol (<i>isopentanol</i>, <i>isoamyl alcohol isobutylcarbinol</i>) C₅H₁₂0, [123-51-3] (2) Water; H₂0; [7732-18-5] 	Ratouis, M.; Dode; M. Bull. Soc. Chim. Fr. <u>1965</u> , 3318-22.
VARIABLES: One temperature: 30 ⁰ C Ringer solution also studied EXPERIMENTAL VALUES:	PREPARED BY: S.C. Valvani; S.H. Yalkowsky; A.F.M. Barton
30°C was reported to be 2.41 g(1)/100g sln. The corresponding mole fraction solubility, of The proportion of (1) in the water-rich phase equilibrium at 30°C was reported to be 2.38	e of a mixture with Ringer solution at
AUXILIARY	INFORMATION
METHOD/APPARATUS/PROCEDURE: In a round bottomed flask, 50 mL of water and a sufficient quantity of alcohol were introduced until two separate layers were formed. The flask assembly was equili- brated by agitation for a least 3 h in a constant temperature bath. Equilibrium solubility was attained by first supersat- urating at a slightly lower temperature (solubility of alcohols in water is inversely proportional to temperature) and then equilibrating at the desired tempera- ture. The aqueous layer was separated after an overnight storage in a bath. The alcohol content was determined by reacting the aqueous solution with potassium dichromate and titrating the excess dichromate with ferrous sulfate solution in the presence of phosphoric acid and diphenylamine barium sulfonate as an indicator.	<pre>SOURCE AND PURITY OF MATERIALS: (1) Prolabo, Paris; redistilled with 10:1 reflux ratio; b.p. 131.0-131.1°C/746 mm Hg n²⁵ 1.40608 (2) twice distilled from silica apparatus or ion-exchanged with Sagei A20.</pre> ESTIMATED ERROR: Solubility: relative error of 2 determina- tions less than 1%. Temperature: ±0.05°C REFERENCES:

COMPONENTS:	ORIGINAL MEASUREMENTS:		
 3-Methyl-l-butanol (isopentanol, isoamyl alcohol, isobutylcarbinol); C₅H₁₂0; [123-51-3] 			
(2) Water; H ₂ 0; [7732-18-5]			
VARIABLES:	PREPARED BY:		
Temperature: 40 and 60 ⁰ C	A. Maczynski		
EXPERIMENTAL VALUES:			
Mutual solubility of 3-methyl-l-butanol (1) and water (2)			
<pre>t/^oC g(1)/100g sln (2)-rich phase (1)-rich ph</pre>	x_1 (compiler) ase (2)-rich phase (1)-rich phase		
40 2.52 89.3	0.00525 0.630		
60 2.20 88.0	0.00457 0.600		
AUXILIARY	INFORMATION		
METHOD /APPARATUS / PROCEDURE :	SOURCE AND PURITY OF MATERIALS:		
The titration method was used. No details were reported in the paper.	(1) source not specified; distilled with heptane; purity 99.93 wt %; 0.07 wt % of water; n_D^{20} 1.4070 d_4^{20} 0.8112 b.p. 130.9°C. (2) not specified. ESTIMATED ERROR: Not specified. REFERENCES:		

COMPONENTS:	EVALUATOR:
(1) 3-Methyl-2-butanol	Z. Maczynska, Institute of Physical
(methylisopropylcarbinol); $C_5H_{12}O;$	Chemistry of the Polish Academy of Sciences,
[598-75-4]	Warsaw, Poland.
(2) Water; H ₂ 0; [7732-18-5]	November 1982

CRITICAL EVALUATION:

Solubilities in the system comprising 3-methyl-2-butanol (1) and water (2) have been reported in two publications. Ginnings and Baum (ref 1) carried out measurements of the mutual solubilities of the two components at 293, 298 and 303 K by the volumetric method (Figure 1). Ratouis and Dode (ref 2) determined the solubility of (1) in the water-rich phase at 303 K by an analytical method. Their value of 4.85 g(1)/100 g sln is in reasonable agreement with the value $5.10 \pm 0.1 \text{ g(1)}/100\text{ g sln}$ at 303 K of ref 1. The data are regarded as tentative, since comparison can be made at only one temperature and the other five points are derived from a single source.



COMPONENTS:	<u> </u>	C	ORIGINA	L MEASUREMENTS:	
<pre>(1) 3-Methy1-2-butanol (methylisopropylcarbinol); C₅H₁₂0, [598-75-4]</pre>		Ginnings, P.M.; Baum, R. J. Am. Chem. Soc. <u>1937</u> , 59, 1111-3.			
(2) Water; H	20; [7732-18-5]				
VARIABLES:	-	1	PREPARE		
Temperature:	20-30°C		A. Mac	zynski	
EXPERIMENTAL VA	LUES:	L			
	Mutual solub	ility of 3-me	thy1-2-	butanol(1) and wate	er(2)
t/ ^o c	g(1)/100	g sln		$x_1(\text{compi})$	ler)
	(2)-rich phase	(1)-rich pha	ase	1	(1)-rich phase
20	6.07	88.12		0.01303	0.6025
25	5.55	88.07		0.01186	0.6013
30	5.10	87.95		0.01086	0.5986
		Relat	ive den	sity d_4	
	t/ ^o c	Water-rich	phase	Alcohol -r ich j	phase
	20	0.9909		0.8390	
	25	0,9902		0.8352	
	30	0.9879		0.8348	
		AUXILIARY	INFORMA	TION	
METHOD /APPARAT	US/PROCEDURE:		SOURCE	AND PURITY OF MATE	RIALS:
Hill's volume Both componer amounts into calibrated fi a water-bath After suffic: allowed to se was measured phase separa volumes were weights of th individual pl	etric method was ad a two-bulb graduat lask and shaken mec at constant temper lent time the liqui eparate and the tot . Upon centrifuga tion line was read,	opted. in known ed and hanically in ature. ds were al volume tion, the and phase the total total volume, omponent	(1) (2) ESTIMA Tempe	Eastman best grade distilled from meta b.p. range 111.1-1 d_4^{25} 0.8134. not specified. TED ERROR: rature: \pm 0.1°C ility : better that (type of a	; allic calcium;

COMPONENTS :	ORIGINAL MEASUREMENTS:
 3-Methyl-2-butanol(methylisopropyl- carbinol) C₅H₁₂0; [598-75-4] 	Ratouis, M., Dodé, M. Bull. Soc. Chim. Fr. <u>1965</u> , 3318-22.
(2) Water; H_2^{0} ; [7732-18-5]	<i>babe</i> , <i>bbe</i> , <i>ontain</i> , <i>F1</i> , <u>1305</u> , 5516–22.
VARIABLES: One temperature: 30°C Ringer solution also studied EXPERIMENTAL VALUES: The proportion of 3-methyl-2-butanol (1) in t at 30°C was reported to be 4.85 g(1)/100g slr The corresponding mole fraction solubility of The proportion of (1) in the water-rich phase equilibrium at 30°C was reported to be 4.75 g	h. calculated by the compiler is $x_1 = 0.0103$. e of a mixture with Ringer solution at
AUXILIARY	INFORMATION
METHOD/APPARATUS/PROCEDURE: In a round bottomed flask, 50mL of water and a sufficient quantity of alcohol were intro- duced until two separate layers were formed. The flask assembly was equilibrated by agitation for a least 3 h in a constant temp bath. Equilibrium solubility was attained by first supersaturating at a slightly lower temperature (solubility of alcohols in water is inversely proportional to temperature) and then equilibrating at the desired temperature. The aqueous layer was separated after an overnight storage in a bath. The alcohol content was determined by reacting the aqueous solution with potassium dichromate and titrating the excess dichromate with ferrous sulfate solution in the presence of phos- phoric acid and diphenylamine barium sulfonate as an indicator.	<pre>redistilled with 10:1 reflux ratio, b.p. 112.4 - 112.5°C/766.7 mm Hg n²⁵ 1.40758. (2) twice distilled from silica apparatus or ion-exchanged with Sagei A20. ESTIMATED ERROR: Solubility: relative error of 2 determinations less than 1%.</pre>

Five-carbon Alcohols

2010 DUE 10	<u> </u>	LENIA LUATO		
COMPONENTS:	. 7	EVALUATO		ton Murdoch
(1) 1-Pentanol (n-pentyl alcohol, n-a		-	fter and A.F.M. Bar	
alcohol, n-butylcarbinol); C ₅ H ₁₂ O	;		ity, Perth, Western	AUSTIAIIA.
[71-41-0]		July, 1	305.	
(2) Water; H ₂ 0; [7732-18-5]				
CRITICAL EVALUATION:				
Solubilities in the system comprising	; 1-pent	anol (1)	and water (2) have	been reported in
the following publications:				
Reference	T/	'K	Phase	Method
Verschaffelt (ref 1)	279-3	309	alcohol-rich	synthetic
Herz (ref 2)	295		mutual	densimetric
Timmermans (ref 3)	Not o	compiled:	insufficient infor	mation
Fontein (ref 4)	Not o	compiled:	mixture of pentyl	alochols
Butler $et \ al.$ (ref 5)	298		water-rich	interferometric
Ginnings and Baum (ref 6)	293-3	303	mutual	volumetric
Jasper <i>et al.</i> (ref 7)	368		mutual	refractometric
Addison (ref 8)	293		water-rich	surface tension
Booth and Everson (ref 9)	298		water-rich	titration
Laddha and Smith (ref 10)	293		mutual	titration
Hansen <i>et al</i> .(ref 11)	298		water-rich	interferometric
Donahue and Bartell (ref 12)	298		mutual	analytical
Erichsen (ref 13)	273-4	455	mutual	synthetic
Erichsen (ref 14)	273-3	323	water-rich	synthetic
Crittenden and Hixon (ref 15)	298		mutua1	titration
Hyde $et \ all$. (ref 16)	457.5	5	u.c.s.t.	
Kinoshita <i>et al</i> .(ref 17)	298		water-rich	surface tension
Ratouis and Dode (ref 18)	303		water-rich	analytical
Ionin and Shanina (ref 19)	Not o	compiled:	unspecified pentyl wide b.p. range	alcohol with
Hanssens (ref 20)	298		mutual	interferometric
Krasnov and Gartseva (ref 21)	285,3	313	alcohol-rich	analytical
Zhuravleva and Zhuravlev (ref 22)	285-3	360	mutual	synthetic
Mullens $et \ al$ (ref 23)	298		water-rich	interferometric
Vochten and Petre (ref 24)	288		water-rich	surface tension
Korenman et al. (ref 25)	298		mutual	analytical
Lavrova and Lesteva (ref 26)	313,3	333	mutual	titration
Charykov <i>et al</i> . (ref 27)	293		alcohol-rich	analytical
Evans et al. (ref 28)	310		water-rich	analytical
Nishino and Nakamura (ref 29)	Not (compiled:	graphical informat	ion only
Singh and Haque (ref 30)	303		mutual	titration
Tokunaga $et \ al.$ (ref 31)	288-3	308	alcohol-rich	analytical

With the exception of those reports noted above (ref 3, 4, 19, 29) all original data are compiled in the data sheets immediately following this Critical Evaluation.

The data of Herz (ref 2), Booth and Everson (ref 9), Hanssens (ref 20), Mullens *et al*. (ref 23), Vochten and Petre (ref 24), Korenman (ref 25) and Evans *et al*. (ref 28) are given in weight/volume fractions without densities and so have been excluded from consideration in this Critical Evaluation. (continued next page)

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	1-Pe	ntanol	16
COMPONENTS	······································	EVALUATOR:	
(1) 1-Per	ntanol (n-pentyl alcohol, n-amyl	G.T. Hefter and A.F.M	. Barton, Murdoch
alcol	nol, n-butylcarbinol); C5H120:	University, Perth, We	stern Australia.
[71-4	+1-0]	July, 1983.	
(2) Water	; H ₂ 0; [7732-18-5]		
CRITICAL H	WALUATION (continued)	L	
In the wa	ater-rich phase the data of Jasper (et al. (ref 7), Laddha am	nd Smith (ref 10),
Hansen et	z al. (ref 11), Zhuravleva and Shura	avlev (ref 22), and Sing	h and Haque (ref 30)
disagree	markedly with all other studies and	l are rejected.	
with othe	Loohol-rich phase the datum of Jasp er studies (ref 13,22) and is also idered to refer to the same primary	rejected. The data of	
graphical "Best" va ed to the a convent The lette	c data are included in the Tables be l interpolation or extrapolation from alues have been obtained by simple e "best" values do not have statist ient representation of the spread of er (R) indicates "Recommended" data by reliable studies are in reasonable	om the data sheets are i averaging. The uncerta ical significance and sh f reported values and no . Data are "Recommende	ndicated by an asteris inty limits (σ _n) attac ould be regarded only t as error limits. d" if two or more
For conve	enience, further discussion of the t	vo phases is given separ	ately.
The solu	oility of 1-pentanol (1) in water (2)	
Surprisi	ngly little information is available	e except over the temper	ature range 293-303.
In this I	range agreement is excellent and the	e average values can be	recommended. Outside
this rang	ge only the data of Erichsen (ref l	3) are available and hen	ce must be considered
only as	tentative.		
	Recommended (R) and te	ntative solubilities	
	of 1-pentanol (1) i		
<i>т/</i> к		Solubility, g(1)/100g s	ln
	Reported values	"В	est" value (± σ_n)
273	3.05 (ref 13)		3.1
283	2.70 (ref 13)		2.7
293	2.36 (ref 6), 2.21 (ref 8), 2.35	(ref 13)	2.31 ± 0.07 (
298	2.208(ref 5), 2.19(ref 6), 2.21(ref 12), 2.22 [*] (ref 13), ref 15), 2.2 (ref 17)	2.20 ± 0.01 (

293	2.36 (ref 6), 2.21 (ref 8), 2.35 (ref 13)	2.31 ± 0.07 (R)
298	2.208(ref 5), 2.19(ref 6), 2.21(ref 12), 2.22 [*] (ref 13), 2.2 (ref 15), 2.2 (ref 17)	2.20 ± 0.01 (R)
303	2.03 (ref 6), 2.10 (ref 13), 2.00 (ref 18)	2.04 ± 0.04 (R)
313	1.90 (ref 13), 2.1 (ref 26)	2.0 ± 0.1
323	1.80 (ref 13)	1.8
333	1.80 (ref 13)	1.8
343	1.85 (ref 13)	1.9
353	1.90 (ref 13)	1.9
363	2.00 (ref 13)	2.0
373	2.25 (ref 13)	2.3
383	2.60 (ref 13)	2.6
393	3.00 (ref 13)	3.0
	(continued next page)	

COMPONEN	TS:	EVALUATOR:	
(1) 1-P	entanol (n-pentyl alcohol, n-amyl	G.T. Hefter and A.F.M. B	arton, Murdoch
	phol, n-butylcarbinol); C ₅ H ₁₂ 0:	University, Perth, Weste	-
_	-41-0]	July, 1983.	
(2) Wat	er; H ₂ 0; [7732-18-5]		
	EVALUATION (continued)	<u> </u>	
<i>Т</i> /К		Solubility, g(1)/100g sl	n
171	Reported value		est" value (±σ_)
			n'
403	3.55 (ref 13)		3.6
413	4.30 (ref 13)		4.3
423	5.35 (ref 13)		5.4
433	6.90 (ref 13)		6.9
443	9.55 (ref 13)		9.6
453	17.50 (ref 13)		17.5
The sol	ubility of water (2) in 1-pentanol (1	<u>)</u> .	
Agreeme	nt between the numerous studies is ex	tremely poor at almost all	temperatures
-	"best" values should be regarded as		-
	_	s system are clearly requir	-
possibl	e that the isomeric purity of the l-p	entanoi is a significant is	
possibl		of water (2) in 1-pentanol	
possibi T/K			. (1)
-		of water (2) in 1-pentanol Solubility, g(2)/100g s	. (1)
-	<u>Tentative solubilities</u>	of water (2) in 1-pentanol Solubility, g(2)/100g s	. (1) In
T/K	<u>Tentative solubilities</u> Reported val	of water (2) in 1-pentanol Solubility, g(2)/100g s ues "Be	. (1) ln est" value (± σ _n)
<i>Т/</i> К 273	<u>Tentative solubilities</u> Reported val 6.30 (ref 13) 8.92 [*] (ref 1), 6.80 (ref 13), 10.2 [*] 9.42 [*] (ref 1), 7.48(ref 6), 8.9(ref	of water (2) in 1-pentanol Solubility, g(2)/100g s ues "Be (ref 21) 10), 7.45(ref 13),	. (1) eln est" value (± σ _n) 6.3 8.6 ± 1.4
Т/к 273 283 293	<u>Tentative solubilities</u> Reported val 6.30 (ref 13) 8.92 [*] (ref 1), 6.80 (ref 13), 10.2 [*] 9.42 [*] (ref 1), 7.48(ref 6), 8.9(ref 9.1(ref	of water (2) in 1-pentanol Solubility, g(2)/100g s ues "Be (ref 21) 10), 7.45(ref 13), 27), 10.5(ref 31)	. (1) lln est" value (± σ _n) 6.3
Т/к 273 283	<u>Tentative solubilities</u> Reported val 6.30 (ref 13) 8.92 [*] (ref 1), 6.80 (ref 13), 10.2 [*] 9.42 [*] (ref 1), 7.48(ref 6), 8.9(ref 9.1(ref 9.67 [*] (ref 1),7.46(ref 6), 10.2(ref 7.5(ref 15), 9.8 [*] (ref	of water (2) in 1-pentanol Solubility, g(2)/100g s ues "Be (ref 21) 10), 7.45(ref 13), 27), 10.5(ref 31) 12), 7.78 [*] (ref 13), f 22), 10.6(ref 31)	. (1) eln est" value (± σ _n) 6.3 8.6 ± 1.4
T/K 273 283 293	<u>Tentative solubilities</u> Reported val 6.30 (ref 13) 8.92 [*] (ref 1), 6.80 (ref 13), 10.2 [*] 9.42 [*] (ref 1), 7.48(ref 6), 8.9(ref 9.1(ref 9.67 [*] (ref 1),7.46(ref 6), 10.2(ref 7.5(ref 15), 9.8 [*] (re 9.91 [*] (ref 1), 7.65(ref 6), 8.10(re	of water (2) in 1-pentanol Solubility, g(2)/100g s ues "Be (ref 21) 10), 7.45(ref 13), 27), 10.5(ref 31) 12), 7.78 [*] (ref 13), f 22), 10.6(ref 31) f 13), 10.0 [*] (ref 22),	$\frac{1}{1}$ (1) (1) (2) (3) (4) (5) (5) (5) (5) (5) (5) (5) (5
T/K 273 283 293 298 303	<u>Tentative solubilities</u> Reported val 6.30 (ref 13) 8.92 [*] (ref 1), 6.80 (ref 13), 10.2 [*] 9.42 [*] (ref 1), 7.48(ref 6), 8.9(ref 9.1(ref 9.67 [*] (ref 1), 7.46(ref 6), 10.2(ref 7.5(ref 15), 9.8 [*] (re 9.91 [*] (ref 1), 7.65(ref 6), 8.10(re 9.3 (re	of water (2) in 1-pentanol Solubility, g(2)/100g s ues "Be (ref 21) 10), 7.45(ref 13), 27), 10.5(ref 31) 12), 7.78 [*] (ref 13), f 22), 10.6(ref 31) f 13), 10.0 [*] (ref 22), f 30), 10.7 (ref 31)	$\frac{1}{10}$
T/K 273 283 293 298 303 313	Tentative solubilities Reported val 6.30 (ref 13) 8.92*(ref 1), 6.80 (ref 13), 10.2* 9.42*(ref 1), 7.48(ref 6), 8.9(ref 9.1(ref 9.67*(ref 1), 7.46(ref 6), 10.2(ref 7.5(ref 15), 9.8*(re 9.91*(ref 1), 7.65(ref 6), 8.10(re 9.3 (re 8.90 (ref 13), 10.48(ref 21), 10.6	of water (2) in 1-pentanol Solubility, g(2)/100g s ues "Be (ref 21) 10), 7.45(ref 13), 27), 10.5(ref 31) 12), 7.78 [*] (ref 13), f 22), 10.6(ref 31) f 13), 10.0 [*] (ref 22), f 30), 10.7 (ref 31)	$\frac{1}{10}$ (1) (1) (1) (2) (3) (4) (5) (5) (5) (5) (5) (5) (5) (5
T/K 273 283 293 298 303 313 323	Tentative solubilities Reported val 6.30 (ref 13) 8.92 [*] (ref 1), 6.80 (ref 13), 10.2 [*] 9.42 [*] (ref 1), 7.48(ref 6), 8.9(ref 9.1(ref 9.67 [*] (ref 1), 7.46(ref 6), 10.2(ref 7.5(ref 15), 9.8 [*] (re 9.91 [*] (ref 1), 7.65(ref 6), 8.10(re 9.3 (re 8.90 (ref 13), 10.48(ref 21), 10.6 9.75 (ref 13), 11.2 [*] (ref 22)	of water (2) in 1-pentanol Solubility, g(2)/100g s ues "Be (ref 21) 10), 7.45(ref 13), 27), 10.5(ref 31) 12), 7.78 [*] (ref 13), f 22), 10.6(ref 31) f 13), 10.0 [*] (ref 22), f 30), 10.7 (ref 31) *(ref 22), 10.5(ref 26)	$\frac{1}{10}$
T/K 273 283 293 298 303 313 323 333	Tentative solubilities Reported val 6.30 (ref 13) 8.92 [*] (ref 1), 6.80 (ref 13), 10.2 [*] 9.42 [*] (ref 1), 7.48(ref 6), 8.9(ref 9.1(ref 9.67 [*] (ref 1), 7.46(ref 6), 10.2(ref 7.5(ref 15), 9.8 [*] (ref 9.91 [*] (ref 1), 7.65(ref 6), 8.10(re 9.3 (re 8.90 (ref 13), 10.48(ref 21), 10.6 9.75 (ref 13), 11.2 [*] (ref 22) 10.65 (ref 13), 11.8 [*] (ref 22), 12.0	of water (2) in 1-pentanol Solubility, g(2)/100g s ues "Be (ref 21) 10), 7.45(ref 13), 27), 10.5(ref 31) 12), 7.78 [*] (ref 13), f 22), 10.6(ref 31) f 13), 10.0 [*] (ref 22), f 30), 10.7 (ref 31) *(ref 22), 10.5(ref 26)	$\frac{1}{10}$ (1) (1) (1) (2) (3) (3) (4) (5) (5) (5) (5) (5) (5) (5) (5
T/K 273 283 293 298 303 313 323 333 343	Tentative solubilities Reported val 6.30 (ref 13) 8.92*(ref 1), 6.80 (ref 13), 10.2* 9.42*(ref 1), 7.48(ref 6), 8.9(ref 9.1(ref 9.67*(ref 1), 7.46(ref 6), 10.2(ref 7.5(ref 15), 9.8*(re 9.91*(ref 1), 7.65(ref 6), 8.10(re 9.3 (re 8.90 (ref 13), 10.48(ref 21), 10.6 9.75 (ref 13), 11.2*(ref 22) 10.65 (ref 13), 11.8*(ref 22), 12.0 11.75 (ref 13), 12.7*(ref 22)	of water (2) in 1-pentanol Solubility, g(2)/100g s ues "Be (ref 21) 10), 7.45(ref 13), 27), 10.5(ref 31) 12), 7.78 [*] (ref 13), f 22), 10.6(ref 31) f 13), 10.0 [*] (ref 22), f 30), 10.7 (ref 31) *(ref 22), 10.5(ref 26)	$\frac{1}{11}$
T/K 273 283 293 298 303 313 323 333	Tentative solubilities Reported val 6.30 (ref 13) 8.92 [*] (ref 1), 6.80 (ref 13), 10.2 [*] 9.42 [*] (ref 1), 7.48(ref 6), 8.9(ref 9.1(ref 9.67 [*] (ref 1), 7.46(ref 6), 10.2(ref 7.5(ref 15), 9.8 [°] (re 9.91 [*] (ref 1), 7.65(ref 6), 8.10(re 9.3 (re 8.90 (ref 13), 10.48(ref 21), 10.6 9.75 (ref 13), 11.2 [*] (ref 22) 10.65 (ref 13), 11.8 [*] (ref 22), 12.0 11.75 (ref 13), 12.7 [*] (ref 22) 12.95 (ref 13), 13.7 [*] (ref 22)	of water (2) in 1-pentanol Solubility, g(2)/100g s ues "Be (ref 21) 10), 7.45(ref 13), 27), 10.5(ref 31) 12), 7.78 [*] (ref 13), f 22), 10.6(ref 31) f 13), 10.0 [*] (ref 22), f 30), 10.7 (ref 31) *(ref 22), 10.5(ref 26)	$\frac{1}{10}$ est" value $(\pm \sigma_n)$ 6.3 8.6 ± 1.4 8.8 ± 1.1 9.0 ± 1.3 9.3 ± 1.1 10.1 ± 0.7 10.5 ± 0.7 11.5 ± 0.6
T/K 273 283 293 298 303 313 323 333 343 353	Tentative solubilities Reported val 6.30 (ref 13) 8.92*(ref 1), 6.80 (ref 13), 10.2* 9.42*(ref 1), 7.48(ref 6), 8.9(ref 9.1(ref 9.67*(ref 1), 7.46(ref 6), 10.2(ref 7.5(ref 15), 9.8*(re 9.91*(ref 1), 7.65(ref 6), 8.10(re 9.3 (re 8.90 (ref 13), 10.48(ref 21), 10.6 9.75 (ref 13), 11.2*(ref 22) 10.65 (ref 13), 11.8*(ref 22), 12.0 11.75 (ref 13), 12.7*(ref 22) 12.95 (ref 13), 13.7*(ref 22) 14.35 (ref 13), 14.8*(ref 22)	of water (2) in 1-pentanol Solubility, g(2)/100g s ues "Be (ref 21) 10), 7.45(ref 13), 27), 10.5(ref 31) 12), 7.78 [*] (ref 13), f 22), 10.6(ref 31) f 13), 10.0 [*] (ref 22), f 30), 10.7 (ref 31) *(ref 22), 10.5(ref 26)	$\frac{1}{10}$
T/K 273 283 293 298 303 313 323 333 343 353 363 373	Tentative solubilities Reported val 6.30 (ref 13) 8.92*(ref 1), 6.80 (ref 13), 10.2* 9.42*(ref 1), 7.48(ref 6), 8.9(ref 9.1(ref 9.67*(ref 1), 7.46(ref 6), 10.2(ref 7.5(ref 15), 9.8*(re 9.91*(ref 1), 7.65(ref 6), 8.10(re 9.3 (re 8.90 (ref 13), 10.48(ref 21), 10.6 9.75 (ref 13), 11.2*(ref 22) 10.65 (ref 13), 11.8*(ref 22), 12.0 11.75 (ref 13), 12.7*(ref 22) 12.95 (ref 13), 13.7*(ref 22) 14.35 (ref 13), 14.8*(ref 22) 15.85 (ref 13)	of water (2) in 1-pentanol Solubility, g(2)/100g s ues "Be (ref 21) 10), 7.45(ref 13), 27), 10.5(ref 31) 12), 7.78 [*] (ref 13), f 22), 10.6(ref 31) f 13), 10.0 [*] (ref 22), f 30), 10.7 (ref 31) *(ref 22), 10.5(ref 26)	$\begin{array}{c} \frac{1}{1}\\ \frac{1}{$
T/K 273 283 293 298 303 313 323 333 343 353 363 373 383	Tentative solubilities Reported val 6.30 (ref 13) 8.92 [*] (ref 1), 6.80 (ref 13), 10.2 [*] 9.42 [*] (ref 1), 7.48(ref 6), 8.9(ref 9.1(ref 9.67 [*] (ref 1), 7.46(ref 6), 10.2(ref 7.5(ref 15), 9.8 [*] (re 9.91 [*] (ref 1), 7.65(ref 6), 8.10(re 9.3 (re 8.90 (ref 13), 10.48(ref 21), 10.6 9.75 (ref 13), 11.2 [*] (ref 22) 10.65 (ref 13), 11.8 [*] (ref 22), 12.0 11.75 (ref 13), 12.7 [*] (ref 22) 12.95 (ref 13), 13.7 [*] (ref 22) 14.35 (ref 13), 14.8 [*] (ref 22) 15.85 (ref 13) 17.60 (ref 13)	of water (2) in 1-pentanol Solubility, g(2)/100g s ues "Be (ref 21) 10), 7.45(ref 13), 27), 10.5(ref 31) 12), 7.78 [*] (ref 13), f 22), 10.6(ref 31) f 13), 10.0 [*] (ref 22), f 30), 10.7 (ref 31) *(ref 22), 10.5(ref 26)	$\frac{1}{1}$ (1) (1) (2) (3) (4) (5) (5) (5) (5) (5) (5) (5) (5
T/K 273 283 293 298 303 313 323 333 343 353 363 373 383 393	Tentative solubilities Reported val 6.30 (ref 13) 8.92*(ref 1), 6.80 (ref 13), 10.2* 9.42*(ref 1), 7.48(ref 6), 8.9(ref 9.1(ref 9.67*(ref 1), 7.46(ref 6), 10.2(ref 7.5(ref 15), 9.8*(re 9.91*(ref 1), 7.65(ref 6), 8.10(re 9.3 (re 8.90 (ref 13), 10.48(ref 21), 10.6 9.75 (ref 13), 11.2*(ref 22) 10.65 (ref 13), 11.8*(ref 22), 12.0 11.75 (ref 13), 12.7*(ref 22) 12.95 (ref 13), 13.7*(ref 22) 14.35 (ref 13), 14.8*(ref 22) 15.85 (ref 13) 17.60 (ref 13)	of water (2) in 1-pentanol Solubility, g(2)/100g s ues "Be (ref 21) 10), 7.45(ref 13), 27), 10.5(ref 31) 12), 7.78 [*] (ref 13), f 22), 10.6(ref 31) f 13), 10.0 [*] (ref 22), f 30), 10.7 (ref 31) *(ref 22), 10.5(ref 26)	$\frac{1}{10}$
T/K 273 283 293 298 303 313 323 333 343 353 363 373 383 393 403	Tentative solubilities Reported val 6.30 (ref 13) 8.92*(ref 1), 6.80 (ref 13), 10.2* 9.42*(ref 1), 7.48(ref 6), 8.9(ref 9.1(ref 9.67*(ref 1), 7.46(ref 6), 10.2(ref 7.5(ref 15), 9.8*(re 9.91*(ref 1), 7.65(ref 6), 8.10(re 9.3 (re 8.90 (ref 13), 10.48(ref 21), 10.6 9.75 (ref 13), 11.2*(ref 22) 10.65 (ref 13), 11.8*(ref 22), 12.0 11.75 (ref 13), 12.7*(ref 22) 12.95 (ref 13), 13.7*(ref 22) 14.35 (ref 13), 14.8*(ref 22) 15.85 (ref 13) 17.60 (ref 13) 19.60 (ref 13)	of water (2) in 1-pentanol Solubility, g(2)/100g s ues "Be (ref 21) 10), 7.45(ref 13), 27), 10.5(ref 31) 12), 7.78 [*] (ref 13), f 22), 10.6(ref 31) f 13), 10.0 [*] (ref 22), f 30), 10.7 (ref 31) *(ref 22), 10.5(ref 26)	$\begin{array}{c} \frac{1}{1}\\ \frac{1}{$
T/K 273 283 293 298 303 313 323 333 343 353 363 373 383 393 403 413	Tentative solubilities Reported val 6.30 (ref 13) 8.92 [*] (ref 1), 6.80 (ref 13), 10.2 [*] 9.42 [*] (ref 1), 7.48(ref 6), 8.9(ref 9.1(ref 9.67 [*] (ref 1), 7.46(ref 6), 10.2(ref 7.5(ref 15), 9.8 [*] (re 9.91 [*] (ref 1), 7.65(ref 6), 8.10(re 9.3 (re 8.90 (ref 13), 10.48(ref 21), 10.6 9.75 (ref 13), 11.2 [*] (ref 22) 10.65 (ref 13), 11.8 [*] (ref 22), 12.0 11.75 (ref 13), 12.7 [*] (ref 22) 12.95 (ref 13), 13.7 [*] (ref 22) 14.35 (ref 13), 14.8 [*] (ref 22) 15.85 (ref 13) 17.60 (ref 13) 19.60 (ref 13) 21.90 (ref 13) 24.65 (ref 13)	of water (2) in 1-pentanol Solubility, g(2)/100g s ues "Be (ref 21) 10), 7.45(ref 13), 27), 10.5(ref 31) 12), 7.78 [*] (ref 13), f 22), 10.6(ref 31) f 13), 10.0 [*] (ref 22), f 30), 10.7 (ref 31) *(ref 22), 10.5(ref 26)	$\begin{array}{c} (1) \\ \text{Pln} \\ \text{est" value } (\pm \sigma_n) \\ 6.3 \\ 8.6 \pm 1.4 \\ 8.8 \pm 1.1 \\ 9.0 \pm 1.3 \\ 9.3 \pm 1.1 \\ 10.1 \pm 0.7 \\ 10.5 \pm 0.7 \\ 11.5 \pm 0.6 \\ 12.2 \pm 0.5 \\ 13.3 \pm 0.4 \\ 14.6 \pm 0.2 \\ 15.9 \\ 17.6 \\ 19.6 \\ 21.9 \\ 24.7 \end{array}$
T/K 273 283 293 298 303 313 323 333 343 353 363 373 383 393 403 413 423	Tentative solubilities Reported val 6.30 (ref 13) 8.92*(ref 1), 6.80 (ref 13), 10.2* 9.42*(ref 1), 7.48(ref 6), 8.9(ref 9.1(ref 9.67*(ref 1), 7.46(ref 6), 10.2(ref 7.5(ref 15), 9.8*(re 9.91*(ref 1), 7.65(ref 6), 8.10(re 9.3 (re 8.90 (ref 13), 10.48(ref 21), 10.6 9.75 (ref 13), 11.2*(ref 22) 10.65 (ref 13), 11.8*(ref 22), 12.0 11.75 (ref 13), 12.7*(ref 22) 12.95 (ref 13), 13.7*(ref 22) 14.35 (ref 13), 14.8*(ref 22) 15.85 (ref 13) 17.60 (ref 13) 19.60 (ref 13) 21.90 (ref 13) 24.65 (ref 13)	of water (2) in 1-pentanol Solubility, g(2)/100g s ues "Be (ref 21) 10), 7.45(ref 13), 27), 10.5(ref 31) 12), 7.78 [*] (ref 13), f 22), 10.6(ref 31) f 13), 10.0 [*] (ref 22), f 30), 10.7 (ref 31) *(ref 22), 10.5(ref 26)	$\frac{1}{2} (1)$ 1. In est" value $(\pm \sigma_n)$ 6.3 8.6 \pm 1.4 8.8 \pm 1.1 9.0 \pm 1.3 9.3 \pm 1.1 10.1 \pm 0.7 10.5 \pm 0.7 11.5 \pm 0.6 12.2 \pm 0.5 13.3 \pm 0.4 14.6 \pm 0.2 15.9 17.6 19.6 21.9 24.7 28.0
T/K 273 283 293 298 303 313 323 333 343 353 363 373 383 393 403 413	Tentative solubilities Reported val 6.30 (ref 13) 8.92 [*] (ref 1), 6.80 (ref 13), 10.2 [*] 9.42 [*] (ref 1), 7.48(ref 6), 8.9(ref 9.1(ref 9.67 [*] (ref 1), 7.46(ref 6), 10.2(ref 7.5(ref 15), 9.8 [*] (re 9.91 [*] (ref 1), 7.65(ref 6), 8.10(re 9.3 (re 8.90 (ref 13), 10.48(ref 21), 10.6 9.75 (ref 13), 11.2 [*] (ref 22) 10.65 (ref 13), 11.8 [*] (ref 22), 12.0 11.75 (ref 13), 12.7 [*] (ref 22) 12.95 (ref 13), 13.7 [*] (ref 22) 14.35 (ref 13), 14.8 [*] (ref 22) 15.85 (ref 13) 17.60 (ref 13) 19.60 (ref 13) 21.90 (ref 13) 24.65 (ref 13)	of water (2) in 1-pentanol Solubility, g(2)/100g s ues "Be (ref 21) 10), 7.45(ref 13), 27), 10.5(ref 31) 12), 7.78 [*] (ref 13), f 22), 10.6(ref 31) f 13), 10.0 [*] (ref 22), f 30), 10.7 (ref 31) *(ref 22), 10.5(ref 26)	$\begin{array}{c} (1) \\ \text{Pln} \\ \text{est" value } (\pm \sigma_n) \\ 6.3 \\ 8.6 \pm 1.4 \\ 8.8 \pm 1.1 \\ 9.0 \pm 1.3 \\ 9.3 \pm 1.1 \\ 10.1 \pm 0.7 \\ 10.5 \pm 0.7 \\ 11.5 \pm 0.6 \\ 12.2 \pm 0.5 \\ 13.3 \pm 0.4 \\ 14.6 \pm 0.2 \\ 15.9 \\ 17.6 \\ 19.6 \\ 21.9 \\ 24.7 \end{array}$

COMPONENTS:	EVALUATOR:
<pre>(1) 1-Pentanol (n-pentyl alcohol, n-amyl alcohol, n-butylcarbinol); C₅H₁₂0; [71-41-0]</pre>	G.T. Hefter and A.F.M. Barton, Murdoch University, Perth, Western Australia, July, 1983.
(2) Water; H ₂ 0; [7732-18-5]	

CRITICAL EVALUATION (continued)

The upper critical solution temperature

The UCST has been reported as 457.6 K (184.4 $^{\circ}$ C) by Hyde *et al* (ref 16) which is in reasonable agreement with Erichsen's smoothed data (ref 13,14).

The dependence of the mutual solubility of 1-pentanol and water is illustrated in Figure 1. For ease of presentation only the data of Erichsen are plotted.

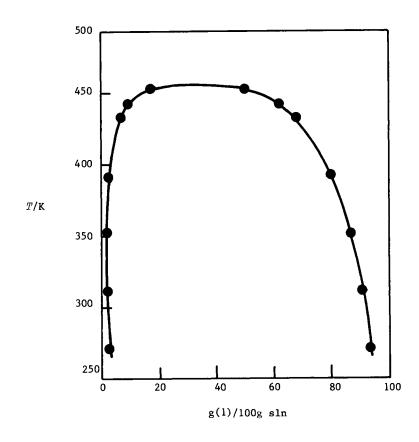


Fig. 1. Mutual solubility of (1) and (2) (data points from ref 13).

 (1) 1-Pentanol (n-pentyl aloohol, n-amyl aloohol, n-amyl aloohol, n-batylgaarbénal); Cyl120; (71-41-0] (2) Water; B_Q0; [7732-18-5] CRITICAL EVALUATION (continued) References Verschaffelt, J. Z. Phys. Chem. 1884, 15, 437. Herz, W. Ber. 1898, 31, 2669; Boll. Chim. Farm. 1915, 54, 37. Timmermans, J. Z. Phys. Chem. 1907, 58, 129. Fontein, F. Z. Phys. Chem. 1910, 75, 212. Butler, J.A.V.; Thomson, D.K.; Maclennan, W.H. J. Chem. Soc. 1933, 674. Ginnings, P.M.; Baum, R. J. Am. Chem. Soc. 1937, 59, 1111. Jasper, J.J.; Farrell, L.G.; Madoff, M. J. Chem. 1948, 40, 1491. Laddison, C.C. J. Chem. Soc. 1945, 98. Booth, H.S.; Everson, H.E. Ind. Eng. Chem. 1948, 40, 1491. Laddison, G.S.; Swith, J.M. Jud. Sng. Chem. 1952, 33, 166. Erichsen, L. von. Naturwhard. Chem. 1952, 33, 166. Erichsen, L. von. Naturwhard. Chem. 1952, 33, 166. Erichsen, L. von. Naturwhard. Chem. 1952, 34, 41. Crittenden, E.O., Jr.; Hixon, A.N. Ind. Eng. Chem. 1954, 46, 265. Hyde, K.; Ishikawa, H.; Shinoda, K. Bull. Chem. Soc. Jpn. 1958, 31, 1081. Batouis, M.; Dodé, M. & Will. Soc. Chem. File5, 318. Jonin, W.Y.; Shanina, P.I. Zh. Okehok. Khim. 1967, 37, 749; J. Gan. Chem. USSR 1975, 37, 703. Hanssens, I. Ascociatio van normale alcoholen on han affChiteit voor water en arganizable soluenism, Dectoraatsproefschrift, Leuven, 1971; Huyskens, P.; Mullens, J., Glomez, A.; Tau, Yyseh. Unhelm. Zawed, Khim. Khim. Tekhnol. 1970, 13, 952. Zhuravleva, I.K.; Thuravlev, E.F. Isu. Vyseh. Uchelm. Zawed, Khim. Khim. Tekhnol. 1970, 13, 480. Wathens, J.; Comez, A.; Tauk, J. Pull. Soc. Chem. Belg. 1975, 44, 46, 1810; 1972, 49, 1490; Fues. J. Pulle. Chem. 1974, 48, 1065; 1975, 49, 877. 	COMPONENTS:	EVALUATOR:		
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25. Korenman, I.M.; Gorokhov, A.A.; Polozenko, G.N. Zh. Fiz. Khim. <u>1974</u> , 48, 1810;			.;	
	24. Vochten, R.; Pet	stre, G. J. Colloid Interface Sci. <u>1973</u> , 42, 320.		
(continued next page)		(continued next page)		

сомро	NENTS:	EVALUATOR:
(1)	1-Pentanol (n-pentyl alcohol, n-amyl	G.T. Hefter and A.F.M. Barton, Murdoch
	alcohol, n-butylcarbinol); C ₅ H ₁₂ 0;	University, Perth, Western Australia.
	[71-41-0]	July, 1983
(2)	Water; H ₂ 0; [7732-18-5]	
CRITI	CAL EVALUATION (continued)	
26.	Lavrova, O.A.; Lesteva, T.M. Zh. Fiz. 1 3813-75.	Khim. <u>1976</u> , 50, 1617; Dep. Doc. VINITI
27.	Charykov, A.K.; Tikhomirov, V.I.; Potapo	ova, T.M. Zh. Obshch. Khim. <u>1978</u> , 48, 1916.
28.	Evans, B.K.; James, K.C.; Luscombe, D.K.	. J. Pharm. Sci. <u>1978</u> , 67, 277.
29.	Nishino, N.; Nakamura, M. Bull. Chem. S	Soc. Jpn. <u>1978</u> , 51, 1617; <u>1981</u> , 54, 545.
30.	30. Singh, R.P.; Haque, M.M. Indian J. Chem. <u>1979</u> , 17A, 449.	
31.	Tokunaga, S.; Manabe, M.; Koda, M. Niih Hen, (Memoirs Niihama Technical College	hama Kogyo Koto Semmon Gakko Kiyo, Rikogaku , Sci. and Eng.) <u>1980</u> , 16, 96.

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COMPONENTS :		ORIGINAL MEASUREMENTS:
	-77	
(1) 1-Pentanol (n-amyl alc n-butylcarbinol); C ₅ H ₁		Verschaffelt, J.
		Z. Phys. Chem. <u>1884</u> , 15, 437–57.
(2) Water; H ₂ 0; [7732-18-	۲C.	
VARIABLES:		PREPARED BY:
Temperature: 6-36 [°] C		A. Maczynski; Z. Maczynska; A Szafranski
Temperature: 6-36 C		A. Maczyliski, Z. Maczyliska, A Szarraliski
EXPERIMENTAL VALUES:		
	Solubility of wate	er (2) in 1-pentanol (1)
	0	
<i>t/</i>	⁰ C g(2)/100g	$\sin \omega_2$ (compiler)
6	8.72	0.319
	9.14	
25	9.67	0.344
32	10.00	0.352
36	10.20	0.357
	AUXILIARY	INFORMATION
METHOD/APPARATUS/PROCEDURE:		SOURCE AND PURITY OF MATERIALS:
The synthetic method was us	sed.	(1) not specified.
Weighed amounts of (1) and in an Eykmann's freezing po immersed in a water bath ar a calibrated thermometer. were measured.	oint apparatus nd equipped with	(2) not specified.
		ESTIMATED ERROR: Temperature: ± 0.5°C Solubility : ± 0.025 g(2)/100g sln (maximum error)

COMPONENTS:	ORIGINAL MEASUREMENTS:	
	ORIGINAL MEASUREMENTS:	
(1) 1-Pentanol (n-amyl alcohol,	Herz, W.	
n-butylcarbinol); C ₅ H ₁₂ 0; [71-41-0]	Ber. <u>1898</u> , <i>31</i> , 2669-72.	
(2) Water; H ₂ O; [7732-18-5]	Boll. chim. farm. 1915, 54, 37.	
2		
VARIABLES:	PREPARED BY:	
One temperature: 22 [°] C	A. Maczynski, Z. Maczynska; A. Szafranski; A.F.M. Barton	
EXPERIMENTAL VALUES:	· · · · · · · · · · · · · · · · · · ·	
The solubility of 1-pentanol in water at 22° C was reported to be 3.284 ml(1)/100 ml(2).		
The 1915 reference reported (without details) that the solubility of water in 1-pentanol at 22° C was 2.214 ml(2)/100 ml(1).		

AUXILIARY	INFORMATION
METHOD / APPARATUS / PROCEDURE :	SOURCE AND PURITY OF MATERIALS:
The densimetric method was used. The composition of the saturated solution was evaluated by extrapolation of calibrat- ion density measurements (carried out on a series of synthetic solutions) to the measured density of the saturated solution. The maximum difference between the actual and the synthetic densities was a few in the third decimal place.	 not specified. d²² 0.9980 g/cm³.
	ESTIMATED ERROR: Not specified.
	REFERENCES:

(1) 1-Pentanol (<i>n-amyl alcohol</i> , <i>n-butylcarbinol</i>); $C_5H_{12}O$; [71-41-0] (2) Water; H_2O ; [7732-18-5] VARIABLES: One temperature: $25^{\circ}C$ EXPERIMENTAL VALUES: The proportion of 1-pentanol (1) in the water-r reported to be 2.208 g(1)/100g sln, the mean of (2.209, 2.203, 2.207, 2.212, 2.211 g(1)/100g sl was reported as $x_1 = 0.00460$. An approximate determination of the mole fracti phase gave $x_1 = 0.71$. METHOD/APPARATUS/PROCEDURE: An analytical method was used, with a U-tube apparatus having two internal stoppers. Suitable quantities of (1) and (2) were placed in one of the connected vessels and shaken in the thermostat for some hours. The liquid was allowed to separate into two layers, the heavier aqueous layer being separated by raising the stoppers and allow- ing part of the liquid to run into the	
(1) 1-Pentanol (<i>n-cmyl alcohol</i> , <i>n-butylcarbinol</i>); $C_{5}H_{12}O;$ [71-41-0] (2) Water; $H_{2}O;$ [7732-18-5] VARIABLES: One temperature: $25^{\circ}C$ EXPERIMENTAL VALUES: The proportion of 1-pentanol (1) in the water-r reported to be 2.208 g(1)/100g sln, the mean of (2.209, 2.203, 2.207, 2.212, 2.211 g(1)/100g sl was reported as $x_{1} = 0.00460$. An approximate determination of the mole fracti phase gave $x_{1} = 0.71$. METHOD/APPARATUS/PROCEDURE: An analytical method was used, with a U-tube apparatus having two internal stoppers. Suitable quantities of (1) and (2) were placed in one of the connected vessels and shaken in the thermostat for some hours. The liquid was allowed to separate into two layers, the heavier aqueous layer being separated by raising the stoppers and allow- ing part of the liquid to run into the connected vessel. A weighed portion of the separated sln was diluted with about an equal quantity of (2) and the resulting sln	IGINAL MEASUREMENTS:
$n-butylcarbinol); C_{5}H_{12}0; [71-41-0] M$ $(2) Water; H_{2}0; [7732-18-5]$ VARIABLES: One temperature: 25°C EXPERIMENTAL VALUES: The proportion of 1-pentanol (1) in the water-r reported to be 2.208 g(1)/100g sln, the mean of (2.209, 2.203, 2.207, 2.212, 2.211 g(1)/100g sl was reported as $x_1 = 0.00460$. An approximate determination of the mole fracti phase gave $x_1 = 0.71$. METHOD APPARATUS/PROCEDURE: An analytical method was used, with a U-tube apparatus having two internal stoppers. Suitable quantities of (1) and (2) were placed in one of the connected vessels and shaken in the thermostat for some hours. The liquid was allowed to separate into two layers, the heavier aqueous layer being separated sln was diluted with about an equal quantity of (2) and the resulting sln	utler, J.A.V.; Thomson, D.W.;
(2) Water; H_2^0 ; $[7732-18-5]$ VARIABLES: One temperature: $25^{\circ}C$ EXPERIMENTAL VALUES: The proportion of 1-pentanol (1) in the water-r reported to be 2.208 g(1)/100g sln, the mean of (2.209, 2.203, 2.207, 2.212, 2.211 g(1)/100g sl was reported as $x_1 = 0.00460$. An approximate determination of the mole fractic phase gave $x_1 = 0.71$. METHOD APPARATUS/PROCEDURE: An analytical method was used, with a U-tube apparatus having two internal stoppers. Suitable quantities of (1) and (2) were placed in one of the connected vessels and shaken in the thermostat for some hours. The liquid was allowed to separate into two layers, the heavier aqueous layer being separated by raising the stoppers and allow- ing part of the liquid to run into the connected vessel. A weighed portion of the separated sln was diluted with about an equal quantity of (2) and the resulting sln	aclennan, W.H.
(2) water; n_2^{0} ; $[1/32-10-3]$ VARIABLES: One temperature: $25^{\circ}C$ EXPERIMENTAL VALUES: The proportion of 1-pentanol (1) in the water-r reported to be 2.208 g(1)/100g sln, the mean of (2.209, 2.203, 2.207, 2.212, 2.211 g(1)/100g sl was reported as $x_1 = 0.00460$. An approximate determination of the mole fracti phase gave $x_1 = 0.71$. METHOD APPARATUS/PROCEDURE: An analytical method was used, with a U-tube apparatus having two internal stoppers. Suitable quantities of (1) and (2) were placed in one of the connected vessels and shaken in the thermostat for some hours. The liquid was allowed to separate into two layers, the heavier aqueous layer being separated by raising the stoppers and allow- ing part of the liquid to run into the connected vessel. A weighed portion of the separated sln was diluted with about an equal quantity of (2) and the resulting sln	. Chem. Soc. 1933, 674-80.
One temperature: 25° C S EXPERIMENTAL VALUES: The proportion of 1-pentanol (1) in the water-r reported to be 2.208 g(1)/100g sln, the mean of (2.209, 2.203, 2.207, 2.212, 2.211 g(1)/100g sl was reported as $x_1 = 0.00460$. An approximate determination of the mole fractic phase gave $x_1 = 0.71$. Auxiliary interval of the mole fractic phase gave $x_1 = 0.71$. METHOD/APPARATUS/PROCEDURE: An analytical method was used, with a U-tube apparatus having two internal stoppers. Suitable quantities of (1) and (2) were placed in one of the connected vessels and shaken in the thermostat for some hours. The liquid was allowed to separate into two layers, the heavier aqueous layer being separated by raising the stoppers and allow- ing part of the liquid to run into the connected vessel. A weighed portion of the separated sln was diluted with about an equal quantity of (2) and the resulting sln	
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METHOD APPARATUS/PROCEDURE: An analytical method was used, with a U-tube apparatus having two internal stoppers. Suitable quantities of (1) and (2) were placed in one of the connected vessels and shaken in the thermostat for some hours. The liquid was allowed to separate into two layers, the heavier aqueous layer being separated by raising the stoppers and allow- ing part of the liquid to run into the connected vessel. A weighed portion of the separated sln was diluted with about an equal quantity of (2) and the resulting sln	FORMATION
An analytical method was used, with a U-tube apparatus having two internal stoppers. Suitable quantities of (1) and (2) were placed in one of the connected vessels and shaken in the thermostat for some hours. The liquid was allowed to separate into two layers, the heavier aqueous layer being separated by raising the stoppers and allow- ing part of the liquid to run into the connected vessel. A weighed portion of the (separated sln was diluted with about an equal quantity of (2) and the resulting sln	URCE AND PURITY OF MATERIALS:
ferometer. To avoid the possibility of reading the position of the wrong fringe 2 cells (1 cm and 5 cm) were used. The method was unsuitable for analysis of alcohol-rich slns as no stoppered inter-	 B.D.H.; repeatedly fractionated under 30 cm Hempel column in all-glas apparatus, middle fraction dried with Ca and fractionated; b.p. 137.60 - 137.70°C (corr.) d²⁵₄ 0.81146 n²⁰_D 1.41043 not stated and stated STIMATED ERROR: olubility: the result is the mean of five eterminations. emperature: not stated (but in related <u>xperiments it was ± 0.03°C).</u>

 (1) 1-Pentanol (n-cmyl alcohol, n-chutyloxrbinol); C₃B₁₂O₅ (71-41-0] (2) Water; H₂O; [7732-18-5] VARIABLES: Temperature: 20-30°C A. Maczynski and Z. Maczynska EXPERIMENTAL VALUES: Mutual solubility of 1-pentanol(1) and water(2) t/°C g(1)/100g sin x1(compiler) (2)-rich phase (1)-rich phase (2)-rich phase (1)-rich phase 20 2.36 92.52 0.00491 0.7165 25 2.19 92.54 0.00455 0.7171 30 2.03 92.35 0.00421 0.7115 Relative density, d₄ t/°C Water-rich phase Alcohol-rich phase 20 0.9939 0.6317 25 0.9930 0.2327 30 0.9919 0.8233 MUTULIARY INFORMATION METHOD/APPARATUS/PROCEDURE: Hill's volumetric method was adopted. auter-bat a constant temperature, and phase volumes ware accurated, prom the total volume ware measured. Upon centrifugation, the phase separations in elither phase were evaluated. STIMATED ERKOR: Temperature: ± 0.1°C Solubility: batter than 0.1 wt% (type of error not specified) REFERENCLS: 	COMPONENTS:		ORIGINAL MEASUREMENTS:
VARIABLES: Temperature: $20-30^{\circ}C$ PREPARED BY: A. Maczynski and Z. MaczynskaEXPERIMENTAL VALUES:Mutual solubility of 1-pentanol(1) and water(2) t/°C $x/^{\circ}C$ $t/^{\circ}C$ $g(1)/100g$ sln $x_1(compiler)$ $(2)-rich phase(2)-rich phase(1)-rich phase(2)-rich phase202.3692.520.00491202.3692.520.00491202.3692.520.00491202.3692.520.00491202.350.004210.7115302.0392.350.00421200.99390.8317250.99300.8287300.99190.8253METHOD/APPARATUS/PROCEDURE:10Hill's volumetric method was adopted.Both components were introduced in knownamounts into a two-bub graduated andcalibrated flask and shaken mechanically ina water-bath at constant temperature.After sufficient time the liquids wereallowed to separate and the total volume wasmeasured.9000000000000000000000000000000000000$	<i>n-butylcarbinol);</i> C ₅ H ₁₂ 0; [71-41-0]		
Temperature: $20-30^{\circ}C$ A. Maczynski and Z. MaczynskaEXPERIMENTAL VALUES:Hutual solubility of 1-pentanol(1) and water(2) $t/^{\circ}C$ $g(1)/100g$ sln $x_1(compiler)$ (2) -rich phase (1) -rich phase (2) -rich phase (1) -rich phase 20 2.36 92.52 0.00491 0.7165 25 2.19 92.54 0.00455 0.7171 30 2.03 92.35 0.00421 0.7115 Relative density, d_4 $t/^{\circ}C$ Water-rich phase 20 0.9939 0.8317 25 0.9930 0.8287 30 0.9919 0.8253 SOURCE AND PURITY OF MATERIALS:Hill's volumetric method was adopted.Both components were introduced in known amounts into a two-bulb graduated and calibrate flask and shaken mechanically in a water-bath at constant temperature. After sufficient time the liquid were allowed to separate and the total volume was measured.ESTINATED ERROR: Temperature: to $1.0^{\circ}C$ Solubility: better than 0.1 wt% (type of error not specified)			
EXPERIMENTAL VALUES: Hutual solubility of 1-pentanol(1) and water(2) $t/^{\circ}C$ g(1)/100g sln x1(compiler) (2)-rich phase (1)-rich phase (2)-rich phase (1)-rich phase 20 2.36 92.52 0.000491 0.7165 25 2.19 92.54 0.00455 0.7171 30 2.03 92.35 0.00421 0.7115 Relative density, d_4 $t/^{\circ}C$ Water-rich phase Alcohol-rich phase 20 0.9939 0.8317 25 0.9930 0.8287 30 0.9919 0.8253 METHOD APPARATUS/PROCEDURE: Hill's volumetric method was adopted. Both components were introduced in known amounts into a two-bub graduated and calibrated flask and shaken mechanically in a water-bath at constant temperature. After sufficient time the liquids were allowed to separate and the total volume was nessured. Upon centrifugation, the phase separation line was read, and phase volumes were calculated. From the total weights of the components, the total volume same read, and phase volumes individual phase volumes, and component concentrations in either phase were evaluated. ESTIMATED ERBOR: Temperature: $t 0.1^{\circ}C$ Solubility: better than 0.1 wt% (type of error not specified)	VARIABLES:		PREPARED BY:
Mutual solubility of 1-pentanol(1) and water(2) $t/^{0}C$ g(1)/100g sln $x_{1}(compiler)$ (2)-rich phase(1)-rich phase(2)-rich phase(1)-rich phase202.3692.520.004910.7165252.1992.540.004550.7171302.0392.350.004210.7115Relative density, d_{4} $t/^{0}C$ Water-rich phase200.99390.8317250.99300.8287300.99190.8253SOURCE AND PURITY OF MATERIALS:Hill's volumetric method was adopted.Both components were introduced in known amounts into a two-bulb graduated and calibrated flask and shaken mechanically in a water-bath at constant temperature.After sufficient time the liquids were allowed to separate and the total volume was measured. Upon centrifugation, the phase ware separation line was read, and phase volumes were calculated. From the total weights of the components, the total volume, individual phase volumes, and component concentrations in either phase were evaluated.ESTIMATED ERROR: Temperature: $\pm 0.1^{0}C$ Solubility: better than 0.1 wt% (type of error not specified)	Temperature: 20-30 ⁰ C		A. Maczynski and Z. Maczynska
$\frac{t/^{0}c}{2} \qquad g(1)/100g sln} \qquad x_1(compiler)$ $(2)-rich phase (1)-rich phase (2)-rich phase (1)-rich phase (2)-rich phase (1)-rich phase (2)-rich phase (1)-rich phase (2)-rich phase $	EXPERIMENTAL VALUES:		
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(2)-rich phase(1)-rich phase(2)-rich phase(1)-rich phase202.3692.520.004910.7165252.1992.540.004550.7171302.0392.350.004210.7115Relative density, d_4 $t/^{\circ}C$ Water-rich phaseAlcohol-rich phase200.99390.8317250.99300.8287300.99190.8253SOURCE AND PURITY OF MATERIALS:Hill's volumetric method was adopted.Both components were introduced in known amounts into a two-bulb graduated and calibrated flask and shake mechanically in a water-bath at constant temperature; After sufficient time the liquids were allowed to separate and the total volume was measured. Upon centrifugation, the phase separation line was read, and phase volumes were calculated. From the total volume, individual phase volumes, and component concentrations in either phase were evaluated.ESTIMATED ERROR: Temperature: $\pm 0.1^{\circ}C$ Solubility: better than 0.1 wtz (type of error not specified)	$t/^{o}C$ g(2)	l)/100g sln	x_1 (compiler)
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$\begin{array}{c c c c c c c c c c c c c c c c c c c $	20 2.36	92.52	2 0.00491 0.7165
Relative density, d_4 $t/^{\circ}C$ Water-rich phaseAlcohol-rich phase200.99390.8317250.99300.8287300.99190.8253300.99190.8253SOURCE AND FURITY OF MATERIALS:Hill's volumetric method was adopted.Both components were introduced in known amounts into a two-bulb graduated and calibrated flask and shaken mechanically in a water-bath at constant temperature. After sufficient time the liquids were allowed to separate and the total volume was measured. Upon centrifugation, the phase separation line was read, and phase volumes were calculated. From the total volume, individual phase volumes, and component concentrations in either phase were evaluated.Source AND FURITY OF MATERIALS: (1) Eastman best grade; distilled from metallic calcium; b.p. range 137.6-138.3°C, d_4^{25} 0.8110.(2) not specified.(2) not specified.ESTIMATED ERROR: Temperature: \pm 0.1°C Solubility: better than 0.1 wt% 	25 2.19	92.54	4 0.00455 0.7171
$t/^{\circ}C$ Water-rich phaseAlcohol-rich phase200.99390.8317250.99300.8287300.99190.8253300.99190.8253METHOD/APPARATUS/PROCEDURE:Hill's volumetric method was adopted.Both components were introduced in known amounts into a two-bulb graduated and calibrated flask and shake mechanically in a water-bath at constant temperature. After sufficient time the liquids were allowed to separate and the total volume vas measured. Upon centrifugation, the phase separation line was read, and phase volumes were calculated.SOURCE AND PURITY OF MATERIALS: (1) Eastman best grade; distilled from metallic calcium; b.p. range 137.6-138.3°C, d_4^{25} 0.8110. (2) not specified.(2) not specified.(2) not specified.ESTIMATED ERROR: rundvidual phase volumes, individual phase volumes, individual phase volumes, and component concentrations in either phase were evaluated.ESTIMATED ERROR: Temperature: $\pm 0.1^{\circ}C$ Solubility: better than 0.1 wt%	30 2.03	92.35	5 0.00421 0.7115
$t/^{\circ}C$ Water-rich phaseAlcohol-rich phase200.99390.8317250.99300.8287300.99190.8253300.99190.8253METHOD/APPARATUS/PROCEDURE:Hill's volumetric method was adopted.Both components were introduced in known amounts into a two-bulb graduated and calibrated flask and shake mechanically in a water-bath at constant temperature. After sufficient time the liquids were allowed to separate and the total volume was measured. Upon centrifugation, the phase separation line was read, and phase volumes were calculated.SOURCE AND PURITY OF MATERIALS: (1) Eastman best grade; distilled from metallic calcium; b.p. range 137.6-138.3°C, d_4^{25} 0.8110. (2) not specified.(2) not specified.(2) not specified.ESTIMATED ERROR: rundvidual phase volumes, individual phase volumes, individual phase volumes, and component concentrations in either phase were evaluated.ESTIMATED ERROR: Temperature: $\pm 0.1^{\circ}C$ Solubility: better than 0.1 wt%		Relative	e density, d.
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AUXILIARY INFORMATION METHOD/APPARATUS/PROCEDURE: Hill's volumetric method was adopted. Both components were introduced in known amounts into a two-bulb graduated and calibrated flask and shaken mechanically in a water-bath at constant temperature. After sufficient time the liquids were allowed to separate and the total volume was measured. Upon centrifugation, the phase separation line was read, and phase volumes were calculated. From the total weights of the components, the total volume, individual phase volumes, and component concentrations in either phase were evaluated. (1) Eastman best grade; distilled from metallic calcium; b.p. range 137.6-138.3°C, d2 ²⁵ 0.8110. (2) not specified. (2) not specified. (2) not specified. (2) not specified.			
METHOD/APPARATUS/PROCEDURE:SOURCE AND PURITY OF MATERIALS:Hill's volumetric method was adopted.(1) Eastman best grade; distilled from metallic calcium; b.p. range 137.6-138.3°C, d_2^{25} 0.8110.Both components were introduced in known amounts into a two-bulb graduated and calibrated flask and shaken mechanically in a water-bath at constant temperature. After sufficient time the liquids were allowed to separate and the total volume was measured. Upon centrifugation, the phase separation line was read, and phase volumes were calculated. From the total weights of the components, the total volume, individual phase volumes, and component concentrations in either phase were evaluated.SOURCE AND PURITY OF MATERIALS: (1) Eastman best grade; distilled from metallic calcium; b.p. range 137.6-138.3°C, d_2^{25} 0.8110.(2) not specified.(2) not specified.(2) not specified.(2) not specified.			
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	Hill's volumetric method were intra- amounts into a two-bulb g calibrated flask and shak a water-bath at constant After sufficient time the allowed to separate and ti measured. Upon centrifu separation line was read, were calculated. From ti of the components, the to individual phase volumes, concentrations in either	was adopted. oduced in known raduated and en mechanically in temperature. liquids were he total volume was gation, the phase and phase volumes he total weights tal volume, and component	 (1) Eastman best grade; distilled from metallic calcium; b.p. range 137.6-138.3°C, d²⁵₄ 0.8110. (2) not specified. s ESTIMATED ERROR: Temperature: ± 0.1°C Solubility: better than 0.1 wt% (type of error not specified)

COMPONENTS:	ORIGINAL MEASUREMENTS:	
(1) 1-Pentanol (n-amyl alcohol, n-butyl	Jasper, J.J.; Farrell, L.G.; Madoff, M.	
carbinol); C ₅ H ₁₂ 0; [71-41-0]	J. Chem. Educ. <u>1944</u> , 21, 536-8.	
(2) Water; H ₂ 0; [7732-18-5]		
VARIABLES:	PREPARED BY:	
One temperature: 95.3 ⁰ C	A.F.M. Barton	
The mole fractions of 1-pentanol (1) at equilibrium at the 1 atm boiling point (95.3 ^o C) of the binary mixture with water (2) were $x_1 = 0.024$ in the water-rich phase and $x_1 = 0.481$ in the alcohol-rich phase.		
of the binary mixture with water (2) were		
of the binary mixture with water (2) were $x_1 = 0.481$ in the alcohol-rich phase.	$x_1 = 0.024$ in the water-rich phase and ties, calculated by the compilers, are 10.7	

AUXILIARY METHOD/APPARATUS/PROCEDURE: The vapor-liquid temperature-composition diagram was determined by the method previously described in ref 1. Samples of distillate and residue from distillation with both excess water and excess 1-pentanol were analyzed by refractive index. Ethanol was added to the samples to ensure homogeneity during analysis, and compositions were determined from a calibration curve. The results reported were obtained while two layers remained in the distillation flask.	ESTIMATED ERROR: Not stated.
	REFERENCES: (1) Jasper, J.J.; Campbell, C.J.; Marshall, D.E. J. Chem. Educ. <u>1941</u> , 18, 540-2.

	ORIGINAL MEASUREMENTS:
(1) 1-Pentanol (n-cmyl alcohol,	Addison, C.C.
<i>n-butylcarbinol);</i> C ₅ H ₁₂ O; [71-41-0]	J. Chem. Soc. <u>1945</u> , 98-106.
<i>•</i>	
(2) Water; H ₂ 0; [7732-18-5]	
VARIABLES:	PREPARED BY:
One temperature: 20 ⁰ C	S.H. Yalkowsky; S.C. Valvani; A.F.M. Barton
	S.n. laikowsky, S.C. Valvani, A.F.M. Balton
EXPERIMENTAL VALUES:	
The proportion of 1-pentanol (1) in the wate	r-rich phase at equilibrium at 20 ⁰ C was
reported to be 2.21 g(1)/100g sln.	Then phase at equilibrium at 10 0 was
The corresponding mole fraction solubility ca	alculated by the compilers is $x_1 = 0.00460$.
	I
	INFORMATION
METHOD / APPARATUS / PROCEDURE :	SOURCE AND PURITY OF MATERIALS:
METHOD/APPARATUS/PROCEDURE: A surface tension method was used.	SOURCE AND PURITY OF MATERIALS: (1) impure alcohols were purified by
METHOD/APPARATUS/PROCEDURE: A surface tension method was used. Sufficient excess of (1) was added to 100 m of (2) in a stoppered flask to form a	SOURCE AND PURITY OF MATERIALS: (1) impure alcohols were purified by fractional distillation, the middle fraction from a distillation being
METHOD/APPARATUS/PROCEDURE: A surface tension method was used. Sufficient excess of (1) was added to 100 m of (2) in a stoppered flask to form a separate lens on the surface. The mixture	SOURCE AND PURITY OF MATERIALS: (1) impure alcohols were purified by fractional distillation, the middle fraction from a distillation being redistilled;
METHOD/APPARATUS/PROCEDURE: A surface tension method was used. Sufficient excess of (1) was added to 100 m of (2) in a stoppered flask to form a separate lens on the surface. The mixture was swirled gently, too vigorous an	SOURCE AND PURITY OF MATERIALS: (1) impure alcohols were purified by fractional distillation, the middle fraction from a distillation being
METHOD/APPARATUS/PROCEDURE: A surface tension method was used. Sufficient excess of (1) was added to 100 m of (2) in a stoppered flask to form a separate lens on the surface. The mixture was swirled gently, too vigorous an agitation giving a semi-permanent emulsion and incorrect readings. After settling,	SOURCE AND PURITY OF MATERIALS: (1) impure alcohols were purified by fractional distillation, the middle fraction from a distillation being redistilled;
METHOD/APPARATUS/PROCEDURE: A surface tension method was used. Sufficient excess of (1) was added to 100 m of (2) in a stoppered flask to form a separate lens on the surface. The mixture was swirled gently, too vigorous an agitation giving a semi-permanent emulsion and incorrect readings. After settling, a small sample of the clear aqueous sln was withdrawn into a drop weight pipet and the	SOURCE AND PURITY OF MATERIALS: (1) impure alcohols were purified by fractional distillation, the middle fraction from a distillation being redistilled; b.p. 138.0°C d_4^{20} 0.8154 n_D^{20} 1.4102
METHOD/APPARATUS/PROCEDURE: A surface tension method was used. Sufficient excess of (1) was added to 100 m of (2) in a stoppered flask to form a separate lens on the surface. The mixture was swirled gently, too vigorous an agitation giving a semi-permanent emulsion and incorrect readings. After settling, a small sample of the clear aqueous sln was withdrawn into a drop weight pipet and the surface tension determined. The swirling	SOURCE AND PURITY OF MATERIALS: (1) impure alcohols were purified by fractional distillation, the middle fraction from a distillation being redistilled; b.p. 138.0°C d_4^{20} 0.8154
METHOD/APPARATUS/PROCEDURE: A surface tension method was used. Sufficient excess of (1) was added to 100 m of (2) in a stoppered flask to form a separate lens on the surface. The mixture was swirled gently, too vigorous an agitation giving a semi-permanent emulsion and incorrect readings. After settling, a small sample of the clear aqueous sln was withdrawn into a drop weight pipet and the surface tension determined. The swirling was continued until a constant value was obtained. The surface tension-concen-	SOURCE AND PURITY OF MATERIALS: (1) impure alcohols were purified by fractional distillation, the middle fraction from a distillation being redistilled; b.p. 138.0°C d_4^{20} 0.8154 n_D^{20} 1.4102
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METHOD/APPARATUS/PROCEDURE: A surface tension method was used. Sufficient excess of (1) was added to 100 m of (2) in a stoppered flask to form a separate lens on the surface. The mixture was swirled gently, too vigorous an agitation giving a semi-permanent emulsion and incorrect readings. After settling, a small sample of the clear aqueous sln was withdrawn into a drop weight pipet and the surface tension determined. The swirling was continued until a constant value was obtained. The surface tension-concen- tration curve was known, and only a slight extrapolation (logarithmic scale) was nec- essary to find the concentration	SOURCE AND PURITY OF MATERIALS: (1) impure alcohols were purified by fractional distillation, the middle fraction from a distillation being redistilled; b.p. 138.0°C d_4^{20} 0.8154 n_D^{20} 1.4102 (2) not stated
METHOD/APPARATUS/PROCEDURE: A surface tension method was used. Sufficient excess of (1) was added to 100 m of (2) in a stoppered flask to form a separate lens on the surface. The mixture was swirled gently, too vigorous an agitation giving a semi-permanent emulsion and incorrect readings. After settling, a small sample of the clear aqueous sln was withdrawn into a drop weight pipet and the surface tension determined. The swirling was continued until a constant value was obtained. The surface tension-concen- tration curve was known, and only a slight extrapolation (logarithmic scale) was nec-	SOURCE AND PURITY OF MATERIALS: (1) impure alcohols were purified by fractional distillation, the middle fraction from a distillation being redistilled; b.p. 138.0°C d_4^{20} 0.8154 n_D^{20} 1.4102 (2) not stated ESTIMATED ERROR:
METHOD/APPARATUS/PROCEDURE: A surface tension method was used. Sufficient excess of (1) was added to 100 m of (2) in a stoppered flask to form a separate lens on the surface. The mixture was swirled gently, too vigorous an agitation giving a semi-permanent emulsion and incorrect readings. After settling, a small sample of the clear aqueous sln was withdrawn into a drop weight pipet and the surface tension determined. The swirling was continued until a constant value was obtained. The surface tension-concen- tration curve was known, and only a slight extrapolation (logarithmic scale) was nec- essary to find the concentration	<pre>SOURCE AND PURITY OF MATERIALS: (1) impure alcohols were purified by fractional distillation, the middle fraction from a distillation being redistilled; b.p. 138.0°C d₄²⁰ 0.8154 n_D²⁰ 1.4102 (2) not stated ESTIMATED ERROR: Solubility: ± 0.5%</pre>
METHOD/APPARATUS/PROCEDURE: A surface tension method was used. Sufficient excess of (1) was added to 100 m of (2) in a stoppered flask to form a separate lens on the surface. The mixture was swirled gently, too vigorous an agitation giving a semi-permanent emulsion and incorrect readings. After settling, a small sample of the clear aqueous sln was withdrawn into a drop weight pipet and the surface tension determined. The swirling was continued until a constant value was obtained. The surface tension-concen- tration curve was known, and only a slight extrapolation (logarithmic scale) was nec- essary to find the concentration	SOURCE AND PURITY OF MATERIALS: (1) impure alcohols were purified by fractional distillation, the middle fraction from a distillation being redistilled; b.p. 138.0°C d_4^{20} 0.8154 n_D^{20} 1.4102 (2) not stated ESTIMATED ERROR:
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METHOD/APPARATUS/PROCEDURE: A surface tension method was used. Sufficient excess of (1) was added to 100 m of (2) in a stoppered flask to form a separate lens on the surface. The mixture was swirled gently, too vigorous an agitation giving a semi-permanent emulsion and incorrect readings. After settling, a small sample of the clear aqueous sln was withdrawn into a drop weight pipet and the surface tension determined. The swirling was continued until a constant value was obtained. The surface tension-concen- tration curve was known, and only a slight extrapolation (logarithmic scale) was nec- essary to find the concentration	<pre>SOURCE AND PURITY OF MATERIALS: (1) impure alcohols were purified by fractional distillation, the middle fraction from a distillation being redistilled; b.p. 138.0°C d₄²⁰ 0.8154 n_D²⁰ 1.4102 (2) not stated ESTIMATED ERROR: Solubility: ± 0.5%</pre>
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METHOD/APPARATUS/PROCEDURE: A surface tension method was used. Sufficient excess of (1) was added to 100 m of (2) in a stoppered flask to form a separate lens on the surface. The mixture was swirled gently, too vigorous an agitation giving a semi-permanent emulsion and incorrect readings. After settling, a small sample of the clear aqueous sln was withdrawn into a drop weight pipet and the surface tension determined. The swirling was continued until a constant value was obtained. The surface tension-concen- tration curve was known, and only a slight extrapolation (logarithmic scale) was nec- essary to find the concentration	<pre>SOURCE AND PURITY OF MATERIALS: (1) impure alcohols were purified by fractional distillation, the middle fraction from a distillation being redistilled; b.p. 138.0°C d₄²⁰ 0.8154 n_D²⁰ 1.4102 (2) not stated ESTIMATED ERROR: Solubility: ± 0.5%</pre>

COMPONENTS :	ORIGINAL MEASUREMENTS:
(1) 1-Pentanol (<i>n-amyl alcohol</i> ;	Booth, H.S.; Everson, H.E.
n-butylcarbinol); C ₅ H ₁₂ 0; [71-41-0]	Ind. Eng. Chem. <u>1948</u> , 40, 1491-3.
(2) Water; H ₂ 0; [7732-18-5]	
VARIABLES:	
One temperature: 25 [°] C	PREPARED BY: S.H. Yalkowsky; S.C. Valvani; A.F.M. Barton
-	Sin larkowsky, S.C. Valvani, Allin Barton
Sodium xylene sulfonate	
EXPERIMENTAL VALUES:	
at 25.0 ⁰ C.	anol (1) in water (2) was $3.4 \text{ mL}(1)/100\text{mL}$ (2)
The corresponding value in 40% sodium xylene	suironate solution as solvent was
>400 mL/(1)/100mL solvent.	
	1
AUXILIARY	INFORMATION
METHOD / APPARATUS / PROCEDURE :	SOURCE AND PURITY OF MATERIALS:
	(1) "CP or highest grade commercial".
A known volume of (2) or aqueous solvent (usually 50mL) in a tightly stoppered	(1) of of highest grade commercial.
calibrated Babcock tube was thermostatted.	(2) "distilled"
Successive measured quantities (1) were	
added and equilibrated until a slight excess of solute remained. The solution was	
centrifuged, returned to the thermostat	
bath for 10 min. and the volume of excess	
solute measured directly. This was a modification of the method described in	
ref 1.	
	ESTIMATED ERROR:
	Solubility: within 0.1 mL(1)/100mL (2)
	REFERENCES:
	1. Henslick, R.S. Dissertation, Columbia
]	University, 1935.
	UNIVEISILY, 1955.

COMPONENTS:	ORIGINAL MEASUREMENTS:
	1
(1) 1-Pentanol (<i>n-amyl alcohol</i> ,	Laddha, G.S.; Smith, J.M.
n-butylcarbinol); C ₅ H ₁₂ 0; [71-41-0]	Ind. Eng. Chem., <u>1943</u> , 40, 494–6.
(2) Water; H ₂ 0; [7732-18-5]	
-	
	PREPARED BY:
One temperature: 20 ⁰ C	A. Maczynski
EXPERIMENTAL VALUES:	
The solubility of 1-pentanol in water at 20 $^{ m o}$	C was reported to be 1.5 $g(1)/100g \ sln$.
The corresponding mole fraction, $x_1^{}$, calcula	ted by compiler is 0.0031.
The corresponding were, "1,	
The solubility of water in 1-pentanol at 20 ⁰	C was reported to be 8.9 g(2)/100g sln.
The corresponding mole fraction, $x_2^{}$, calcula	ted by compiler is 0.32.
AUXILIARY	INFORMATION
METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
The titration method was used.	 Mallinckrodt Chemical Co., reagent grade;
One component was placed in a 20 [°] C constant-	b.p. range 134-137°C, but nearly all
temperature bath for 1 h . Then titration	distilled at 137°C;
was carried out in several steps, in order	d^{20} 0.817.
that the mixture could be frequently returned to the constant-temperature bath	(2) distilled.
to ensure maintenance of the 20°C temperat-	
ure. The end point was taken when turbidity appeared over the entire solution.	
·	
	ESTIMATED ERROR:
	Not specified.
	REFERENCES :
	ALL LALIGED.
	1

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(1) 1-Pentanol (<i>n-amyl alcohol</i> ,				
-	COMPONENTS: (1) $1-Pertonal (n-amul alashal)$		ORIGINAL MEASUREMENTS: Donahue, D.J.; Bartell, F.E.	
	71 61 07		<u>1952</u> , <i>56</i> , 480-4.	
n-butylcarbinol); C ₅ H ₁₂ 0;[/1-41-0]	J. Fuys. Chem.	<u>1952</u> , 00, 480-4.	
(2) Water; H ₂ 0; [7732-18-5]				
VARIABLES: One temperature: 25 ⁰ C		PREPARED BY: A.F.M. Barton.		
one temperature. 25 C		A.F.M. Darton.		
EXPERIMENTAL VALUES:				
	Density		Mutual solubilities	
1	g mL ⁻¹	x_1	g(1)/100g sln (compiler)	
		-	<u></u>	
Alcohol-rich phase (0.8325	0.643	89.8	
Water-rich phase (0.9935	0.00459 ^a	2.21	
a From ref 1 and 2				
From ref 1 and 2				
.				
	AUXILIARY	INFORMATION	<u>.</u>	
METHOD / APPARATUS / PROCEDURE :		SOURCE AND PURI	ITY OF MATERIALS:	
Mixtures were placed in glass st	oppered	SOURCE AND PURI (1) "best rea	gent grade",	
Mixtures were placed in glass st flasks and were shaken intermitt least 3 days in a water bath.	oppered ently for at The organic	SOURCE AND PURI (1) "best rea		
Mixtures were placed in glass st flasks and were shaken intermitt least 3 days in a water bath. phase was analyzed for water con	oppered ently for at The organic tent by the	SOURCE AND PURI (1) "best rea	gent grade", al distillation.	
Mixtures were placed in glass st flasks and were shaken intermitt least 3 days in a water bath. phase was analyzed for water con Karl Fischer method and the aque	oppered ently for at The organic tent by the ous phase	SOURCE AND PUR (1) "best rea fraction	gent grade", al distillation.	
Mixtures were placed in glass st flasks and were shaken intermitt least 3 days in a water bath. phase was analyzed for water con Karl Fischer method and the aque was analyzed interferometrically. solubility measurements formed p	oppered ently for at The organic tent by the ous phase The art of a	SOURCE AND PUR (1) "best rea fraction	gent grade", al distillation.	
Mixtures were placed in glass st flasks and were shaken intermitt least 3 days in a water bath. phase was analyzed for water con Karl Fischer method and the aque was analyzed interferometrically. solubility measurements formed p study of water-organic liquid in	oppered ently for at The organic tent by the ous phase The art of a	SOURCE AND PUR (1) "best rea fraction	gent grade", al distillation.	
Mixtures were placed in glass st flasks and were shaken intermitt least 3 days in a water bath. phase was analyzed for water con Karl Fischer method and the aque was analyzed interferometrically. solubility measurements formed p	oppered ently for at The organic tent by the ous phase The art of a	SOURCE AND PUR (1) "best rea fraction	gent grade", al distillation.	
Mixtures were placed in glass st flasks and were shaken intermitt least 3 days in a water bath. phase was analyzed for water con Karl Fischer method and the aque was analyzed interferometrically. solubility measurements formed p study of water-organic liquid in	oppered ently for at The organic tent by the ous phase The art of a	SOURCE AND PUR (1) "best rea fraction	gent grade", al distillation.	
Mixtures were placed in glass st flasks and were shaken intermitt least 3 days in a water bath. phase was analyzed for water con Karl Fischer method and the aque was analyzed interferometrically. solubility measurements formed p study of water-organic liquid in	oppered ently for at The organic tent by the ous phase The art of a	SOURCE AND PURI (1) "best rea fraction (2) "purified	gent grade", al distillation. "	
Mixtures were placed in glass st flasks and were shaken intermitt least 3 days in a water bath. phase was analyzed for water con Karl Fischer method and the aque was analyzed interferometrically. solubility measurements formed p study of water-organic liquid in	oppered ently for at The organic tent by the ous phase The art of a	SOURCE AND PURI (1) "best rea fraction (2) "purified ESTIMATED ERRO	gent grade", al distillation. " R:	
Mixtures were placed in glass st flasks and were shaken intermitt least 3 days in a water bath. phase was analyzed for water con Karl Fischer method and the aque was analyzed interferometrically. solubility measurements formed p study of water-organic liquid in	oppered ently for at The organic tent by the ous phase The art of a	SOURCE AND PURI (1) "best rea fraction (2) "purified	gent grade", al distillation. " R:	
Mixtures were placed in glass st flasks and were shaken intermitt least 3 days in a water bath. phase was analyzed for water con Karl Fischer method and the aque was analyzed interferometrically. solubility measurements formed p study of water-organic liquid in	oppered ently for at The organic tent by the ous phase The art of a	SOURCE AND PURI (1) "best rea fraction (2) "purified ESTIMATED ERRO	gent grade", al distillation. " R:	
Mixtures were placed in glass st flasks and were shaken intermitt least 3 days in a water bath. phase was analyzed for water con Karl Fischer method and the aque was analyzed interferometrically. solubility measurements formed p study of water-organic liquid in	oppered ently for at The organic tent by the ous phase The art of a	SOURCE AND PURI (1) "best rea fraction (2) "purified ESTIMATED ERRO	gent grade", al distillation. " R:	
Mixtures were placed in glass st flasks and were shaken intermitt least 3 days in a water bath. phase was analyzed for water con Karl Fischer method and the aque was analyzed interferometrically. solubility measurements formed p study of water-organic liquid in	oppered ently for at The organic tent by the ous phase The art of a	SOURCE AND PUR (1) "best rea fraction (2) "purified ESTIMATED ERRO Temperature: REFERENCES: 1. Butler, J.A	gent grade", al distillation. " R: ± 0.1 ⁰ C V.; Thomson, D.W.; Maclennan,	
Mixtures were placed in glass st flasks and were shaken intermitt least 3 days in a water bath. phase was analyzed for water con Karl Fischer method and the aque was analyzed interferometrically. solubility measurements formed p study of water-organic liquid in	oppered ently for at The organic tent by the ous phase The art of a	SOURCE AND PURI (1) "best rea fraction (2) "purified ESTIMATED ERRO Temperature: REFERENCES: 1. Butler, J.A W.H. J. Ch	gent grade", al distillation. " R: ± 0.1 ⁰ C 	
Mixtures were placed in glass st flasks and were shaken intermitt least 3 days in a water bath. phase was analyzed for water con Karl Fischer method and the aque was analyzed interferometrically. solubility measurements formed p study of water-organic liquid in	oppered ently for at The organic tent by the ous phase The art of a	SOURCE AND PURI (1) "best rea fraction (2) "purified ESTIMATED ERRO Temperature: REFERENCES: 1. Butler, J.A W.H. J. Ch 2. Hansen, R.S	gent grade", al distillation. " R: ± 0.1 ⁰ C 	
Mixtures were placed in glass st flasks and were shaken intermitt least 3 days in a water bath. phase was analyzed for water con Karl Fischer method and the aque was analyzed interferometrically. solubility measurements formed p study of water-organic liquid in	oppered ently for at The organic tent by the ous phase The art of a	SOURCE AND PURI (1) "best rea fraction (2) "purified ESTIMATED ERRO Temperature: REFERENCES: 1. Butler, J.A W.H. J. Ch 2. Hansen, R.S	gent grade", al distillation. " R: ± 0.1 ⁰ C 	

COMPONENTS:		ORIGINAL MEASUREMENTS:	
(1) 1-Pentanol (<i>n-amyl alc</i>		Erichsen, L. von	
n-butylcarbinol); C ₅	H ₁₂ 0; [71-41-0]	Brennst. Chem. <u>1952</u> , 3	3, 166-72.
(2) Water; H ₂ 0; [7732-18	-5]		
2			
VARIABLES:	······································	PREPARED BY:	
Temperature: 0-180 ⁰ C		S.H. Yalkowsky and Z.	Maczynska
		····	
EXPERIMENTAL VALUES:	al solubility of 1	-pentanol and water	
	-	-	
T/ ^O C (2)-r g(1)/100g s1r	rich phase •	(1)-rich p g(1)/100g sln	x_1
0 3.05	0.0064	93.70	0.7526
10 2.70	0.0055	93.20	0.7370
20 2.35	0.0049	92.55	0.7175
30 2.10 40 1.90	0.0044 0.0039	91.90 91.10	0.6988 0.6767
50 1.80	0.0036	90.25	0.6543
60 1.80	0.0036	89.35	0.6317
70 1.85	0.0038	88.25	0.6057
80 1.90	0.0039	87.05	0.5788
90 2.00	0.0041	85.65	0.5497
100 2.25 110 2.60	0.0047 0.0054	84.15 82.40	0.5205 0.4890
120 3.00	0.0063	80.40	0.4561
130 3.55	0.0075	78.10	0.4217
140 4.30	0.0092	75.35	0.3846
150 5.35	0.0114	72.05	0.3451
160 6.90	0.0149	68.00	0.3029
170 9.55 180 17.50	0.0211 0.0416	62.45 50.30	0.2548 0.1714
AUXILIARY		INFORMATION	
METHOD/APPARATUS/PROCEDURE:		SOURCE AND PURITY OF M	IATERIALS:
The synthetic method was u	used.	(1) Merck, or Ciba,	or industrial products;
			nemically free from
The measurements were carr glass ampules placed in an		isomers; b.p. 137.8-137.9	0°C (757 mm Ha)
equipped with two glass wi			, c (/)/ nun ng)
points were measured with		$n_{\rm D}^{20}$ 1.4098.	
	Each measurement	(2) not specified.	
was repeated twice.			
		ESTIMATED ERROR:	
		Not specified.	
		REFERENCES :	
1			

			ORIGINAL MEASUREMENTS:
(1) 1-Pentanol (n-a	myl alcohol,		Erichsen, L. von
n-butylcarbinol); C ₅ H ₁₂ 0;	[71-41-0]	Naturwissenschaften <u>1952</u> , 39, 41-2.
(2) Water; H ₂ 0; [7	732-18-5]		
VARIABLES:			PREPARED BY:
Temperature: 0-50 [°] C			A. Maczynski; Z Maczynska
EXPERIMENTAL VALUES:			
	Solubi	lity of 1-	pentanol in water
	t∕°c	x_1	g(1)/100g sln
		T	(compiler)
	0	0.0064	3.1
	10	0.0055	2.6
	20	0.0049	2.4
	30	0.0044	2.1
	40	0.0039	1.9
	50	0.0036	1.7
		AUXILIARY	INFORMATION
METHOD/APPARATUS/PROCE	EDURE:		SOURCE AND PURITY OF MATERIALS:
The synthetic method	was used.		(1) not specified.
No details were repo	rted in the p	aper.	(2) not specified.
			ESTIMATED ERROR:
			Not specified.
			REFERENCES:

COMPONENTS :	ORIGINAL MEASUREMENTS:
(1) 1-Pentanol (<i>n-amyl alcohol</i> ,	Crittenden, E.D., Jr.; Hixon, A.N.
n-butylcarbinol); C ₅ H ₁₀ 0; [71-41-0]	Ind. Eng. Chem. <u>1954</u> , 46, 265-8.
(2) Water; H ₂ 0; [7732-18-5]	
VARIABLES:	PREPARED BY:
One temperature: 25 ⁰ C	A. Maczynski
EXPERIMENTAL VALUES:	· · · · · · · · · · · · · · · · · · ·
The solubility of 1-pentanol in water at 25 ⁰	C was reported to be $2.2g(1)/100g$ sin
The corresponding mole fraction, $x_1^{}$, calcula	ted by the compiler is 0.0046.
The solubility of water in 1-pentanol at 25 ^C	C was reported to be 7.5g(2)/100g sln.
The corresponding mole fraction, x_{γ} , calcula	ted by the compiler is 0.28.
corresponding more traction, w ₂ , calcula	,
AUXILIARY	INFORMATION
METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
Presumably the titration method described for ternary systems containing LCl was used.	<pre>(1) source not specified; purified;</pre>
In this method the solubility was determined	
by bringing 100-ml samples of (1) or (2) to a temperature $25 \pm 0.10^{\circ}$ C and the second	(2) not specified.
component was then added from a calibrated	
buret, with vigorous stirring, until the solution became permanently cloudy.	
	ESTIMATED ERROR:
	Solubility: 2% (alcohol-rich)- 10%
	(water-rich)
	Temperature: ± 0.10°C. REFERENCES:
	REFERENCES:

COMPONENTS:	ORIGINAL MEASUREMENTS:
 1-Pentanol (<i>n-amyl alcohol</i>, <i>n-butylcarbinol</i>); C₅H₁₂0; [71-41-0] Water; H₂0; [7732-18-5] 	Hyde, A.J.; Langbridge, D.M.; Lawrence, A.S.C. Disc. Faraday Soc., <u>1954</u> , 18, 239-58.
_	
VARIABLES:	PREPARED BY:
One temperature: 184.4 ⁰ C	A. Maczynski; A.F.M. Barton
EXPERIMENTAL VALUES:	L
$(x_1 = 0.134, \text{ compiler}).$	reported to be 184.4° C at $43.0 \text{ g}(1)/100 \text{g sln}$
The room temperature solubility of (1) and (2) was reported as 2.0%
	INFORMATION
METHOD /APPARATUS / PROCEDURE :	SOURCE AND PURITY OF MATERIALS:
Not specified.	(1) not specified.
	(2) not specified.
	ESTIMATED ERROR:
	Not specified.
	REFERENCES :

COMPONENTS:	ORIGINAL MEASUREMENTS:
 (1) 1-Pentanol (n-amyl alcohol; n-butylcarbinol); C₅H₁₂0; [71-41-0] (2) Water; H₂0; [7732-18-5] 	Kinoshita, K; Ishikawa, H; Shinoda, K; Bull. Chem. Soc. Jpn. <u>1958</u> ,31, 1081-4.
VARIABLES:	PREPARED BY:
One temperature: 25 [°] C	S.H. Yalkowsky; S.C. Valvani; A.F.M. Barton

EXPERIMENTAL VALUES:

The concentration of 1-pentanol (1) in the water-rich phase at equilibrium at 25.0° C was reported to be 0.25 mol(1) L⁻¹. The weight percentage solubility was reported as 2.2 g(1)/100g sln, and the corresponding mole fraction solubility, calculated by the compilers, is $x_1 = 0.0046$.

AUXILIARY INFORMATION		
METHOD/APPARATUS/PROCEDURE: The surface tension in aqueous solutions of alcohols monotonically decreases up to their saturation concentration and remains con- stant in the heterogeneous region of (ref 1-4). Surface tension was measured by the drop weight method, using a tip 6 mm in diameter, the measurements being carried out in a water thermostat. From the (surface tension) - (logarithm of concentra- tion) curves the saturation points were determined as the intersections of the curves with the horizontal straight lines passing through the lowest experimental points.	<pre>SOURCE AND PURITY OF MATERIALS: (1) purified by vacuum distillation through 50-100 cm column; b.p. 138°C (2) not stated</pre>	
	ESTIMATED ERROR: Temperature: 0.05°C Solubility: within 4% REFERENCES: 1. Motylewski, S. Z.Anorg.Chem. <u>1904</u> , 38, 410. 2. Taubamann, A. Z. Physik. Chem <u>1932</u> , A161, 141. 3. Zimmerman, H.K.,Jr. Chem. Rev. <u>1952</u> , 51, 25. 4. Shinodo, K.; Yamanaka, T.; Kinoshita, K. J.Phys. Chem. <u>1959</u> , 63, 648.	

1 1	ORIGINAL MEASUREMENTS: Ratouis, M.; Dode, M.;
(1) l-Pentanol (<i>n-amyl alcohol</i> ,	
n-butylcarbinol); C ₅ H ₁₂ 0;	Bull. Soc. Chim. Fr. <u>1965</u> , 3318-22.
[71-41-0]	
(2) Water; H ₂ 0; [7732-18-5]	
2,2	
WADTADI DO.	
	PREPARED BY:
One temperature: 30°C	S.C. Valvani; S.H. Yalkowsky; A.F.M. Barton
Ringer solution also studied	
EXPERIMENTAL VALUES:	
The proportion of l-pentanol (1) in the water-	-rich phase at equilibrium at 30°C
was reported to be 2.00 $g(1)/100g \ sln$.	F
The corresponding mole fraction solubility, ca	alculated by the compilers, is
$x_1 = 0.00415.$	
The proportion of (1) in the water-rich phase	of a mixture with Ringer solution at
equilibrium at 30° C was reported to be 1.92 g	(1)/100g sln.
AUXILIARY	INFORMATION
METHOD/APPARATUS/PROCEDURE:	CONDOR AND DUDITY OF MATERIALC.
	SOURCE AND PURITY OF MATERIALS:
In a round bottomed flask, 50 mL of water	(1) Prolabo, Paris;
and a sufficient quantity of alcohol were introduced until two separate layers were	redistilled with 10:1 reflux ratio;
formed. The flask assembly was equilibrated	b.p. 138.6-138.7/763 mm Hg
by agitation for at least 3 h in a constant	$n_{\rm p}^{25} = 1.40800$
temperature bath. Equilibrium solubility was attained by first supersaturating at a	
slightly lower temperature (solubility of	(2) twice distilled from silica apparatus
alcohols in water decreases with increasing	or ion-exchanged with Sagei A20
temperature) and the equilibrating at the desired temperature. The aqueous layer	
was separated after an overnight storage in	
a bath. The alcohol content was determined	
by reacting the aqueous solution with potassium dichromate and titrating the	Solubility: relative error of 2 determina- tions less than 1%
excess dichromate with ferrous sulfate	Temperature: ± 0.05°C
solution in the presence of phosphoric acid	
and diphenylamine barium sulfonate as an indicator.	REFERENCES :
Indicator,	
•	

ORIGINAL MEASUREMENTS:
Hanssens, I. Associatie van normalle alcoholen en hun affiniteit voor water en organische solventen Doctoraatsproefschrift, Leuven, 1969.
PREPARED BY:
M.C. Haulait-Pirson; A.F.M. Barton

EXPERIMENTAL VALUES:

The concentration of 1-pentanol (1) in the water-rich phase was reported as 0.2405 mol(1)/L sln, and the concentration of water (2) in the alcohol-rich phase was reported as 8.290 mol(2)/L sln.

The corresponding solubilities on a mass/volume basis, calculated by the compilers, are 21.2 g(1)/L sln, and 149.4 g(2)/L sln respectively.

(The temperature was unspecified in the Thesis, but reported as 298 K for related investigations in ref 2.)

AUXILIARY INFORMATION		
METHOD/APPARATUS/PROCEDURE: (1) and (2) were equilibrated using a cell described in ref 1. The Rayleigh M75 interference refractometer with the cell M160 for liquids was used for the determina- tion of the concentrations. Cell thick- nesses were 1, 3 and 10 cm depending on the concentration range. Standard solutions	SOURCE AND PURITY OF MATERIALS; (1) Merck p.a. (2) distilled	
covering the whole range of concentrations investigated were used for the calibration.	ESTIMATED ERROR: Solubility: ± 0.00036 - 0.05 mol(1) depending on concentration.	
	 REFERENCES: (1) Meeussen, E.; Huyskens, P. J.Chim. Phys. <u>1966</u>, 63, 845. (2) Huyskens, P; Mullens, J.; Gomez, A.; Tack, J. Bull. Soc. Chim. Belg. <u>1975</u>, 84, 253-62. 	

	DETOTIAL ACTACUED MONTO
COMPONENTS :	DRIGINAL MEASUREMENTS:
(1) 1-Pentanol (n-amyl alcohol,	Krasnov, K.S.; Gartseva, L.A.
<i>n-butylcarbinol</i>); $C_5H_{12}O;$ [71-41-0]	Izv. Vyssh. Ucheb. Zaved. Khim. Khim. Tekhnol. <u>1970</u> , 13(7), 952-6.
(2) Water; H ₂ 0; [7732-18-5]	
VARIABLES:	PREPARED BY:
Temperature: 12 and 40 [°] C	A. Maczynski and Z. Maczynska
EXPERIMENTAL VALUES:	
	water (2) in l-pentanol (1)
t/ ^o C g(2)/1	00g sln x_2 (compiler)
12 10	.20 0.357
	.48 0.364
40 10	+00.00
AUXILIARY	INFORMATION
METHOD /APPARATUS / PROCEDURE :	SOURCE AND PURITY OF MATERIALS:
The analytical method was used. A saturated mixture of (1) and (2) was	<pre>(1) source not specified; CP reagent; distilled;</pre>
placed in a thermostat and the phases allowed to separate. Then (2) was determined in	no isomers by GLC;
the organic layer by the Karl Fischer analysis.	4
	(2) not specified.
	ESTIMATED ERROR:
	ESTIMATED ERROR: Temperature: ± 0.05 [°] C Solubility: ± 0.05 wt % (not specified)
	Temperature: ± 0.05 ⁰ C
	Temperature: ± 0.05 ⁰ C Solubility: ± 0.05 wt % (not specified)
	Temperature: ± 0.05 ⁰ C Solubility: ± 0.05 wt % (not specified)
	Temperature: ± 0.05 ⁰ C Solubility: ± 0.05 wt % (not specified)

COMPONENTS:	ORIGINAL MEASUREMENTS:	
(1) 1-Pentanol (n-amyl alcohol,	Zhuravleva, I.K.; Zhuravlev, E.F.	
<i>n-butylcarbinol); E</i> ₅ H ₁₂ O; [71-41-0]		
(2) Water; H ₂ 0; [7732-18-5]	Izv. Vyssh. Ucheb. Zaved. Khim. Khim. Tekhnol. <u>1970</u> , 13, 480-5.	
(2) Haller, "20," [7752-10-5]		
VARIABLES:	PREPARED BY:	
Temperature: 12-94 [°] C	Z. Maczynska	
Temperature. 12-94 6	2. Maczyliska	
EXPERIMENTAL VALUES:		
Solubility of 1-pentanol (1) in water (2)		
t/ ^o C g(1)/100g	sln $x_1(\text{compiler})$	
12.0 2.0	0.0042	
63.0 1.6	0.0033	
94.0 2.0	0.0042	
Solubility of water (2) in 1-pentanol (1)		
t/ ⁰ C g(2)/100g	sln $x_2(\text{compiler})$	
29.0 10.0	0.352	
41.5 10.7	0.370	
56.0 11.5	0.389	
66.0 12.4	0.409	
73.5 13.0	0.422	
86.5 14.4	0.452	
AUXI LI A	ARY INFORMATION	
METHOD / APPARATUS / PROCEDURE :	SOURCE AND PURITY OF MATERIALS:	
Alekseev's method (ref 1) was used.	(1) source not specified;	
No details were reported in the paper.	freshly distilled; purity not specified.	
no details were reported in the paper.	(2) twice distilled.	
	ESTIMATED ERROR:	
	Not specified.	
	REFERENCES :	
	1. Alekseev, V.F. Zh. russk. Khim., o-va,	
	1. Alesseev, v.r. $2n$. russk. $Rnim., o-va, 1876, 8, 249.$	

1-Pentanol		18
<pre>OMPONENTS: (1) 1-Pentanol (n-amyl alcohol; n-butylcarbinol); C₅H₁₂0; [71-41-0] (2) Water; H₂0; [7732-18-5] VARIABLES: One temperature: 25°C EXPERIMENTAL VALUES: At equilibrium at 25°C the concentration of J was reported as 0.241 mol(1)/L sln, and the alcohol-rich phase was reported as 8.290 mol(The corresponding solubilities on a mass/volu are 21.24 g(1)/L sln, and 149.4 g(2)/L sln, n</pre>	concentration of water (2) in the (2)/L sln. me basis, calculated by the compilers,	
	INFORMATION	
METHOD/APPARATUS/PROCEDURE: The partition of the two components was made using a cell described in ref 1. The Rayleigh Interference Refractometer M154 was used for the determination of the concentrations. Standard solutions covering the whole range of concentration investigated were used for the calibration.	SOURCE AND PURITY OF MATERIALS: (1) Merck (p.a.). (2) distilled	

ESTIMATED ERROR: Solubility: ± 0.001 mol(1)/L sln.

REFERENCES :

Meeussen, E.; Huyskens, P.
 J. Chim. Phys. <u>1966</u>, 63, 845

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) 1-Pentanol (n-amyl alcohol,	Vochten, R.; Petre, G.;
n-butylcarbinol); C ₅ H ₁₂ 0; [71-41-0]	J. Colloid Interface Sci. <u>1973</u> , 42, 320-7.
(2) Water; H ₂ O; [7732-18-5]	
VARIABLES:	PREPARED BY:
One temperature: 15 [°] C	S.H. Yalkowsky; S.C. Valvani; A.F.M. Barton
EXPERIMENTAL VALUES:	
The concentration of 1-pentanol (1) in the wa	ater-rich phase at equilibrium at 150
was reported to be 0.26 mol(1)/L sln.	ater-rich phase at equilibrium at 15 C
was reported to be 0.20 mor(1)/2 sin.	
The corresponding mass/volume solubility, ca	culated by the compilers, is
22.9 g(1)/L sln.	
AUXILIARY	INFORMATION
METHOD / APPARATUS / PROCEDURE :	SOURCE AND PURITY OF MATERIALS:
The solubility was obtained from the	(1) purified by distillation and preparative
surface tension of saturated solvents	gas chromatography;
measured by the staticmethod of Wilhelmy (platinum plate). The apparatus consisted	b.p. 127.8 ⁰ C/760 mm Hg
of an electrobalance (R.G. Cahn) connected	(2) triply distilled from permanganate
with a high impedance null detector (FLUKE type 845 AR). An all-Pyrex vessel was	solution.
used.	
	ESTIMATED ERROR:
	Temperature: $\pm 0.1^{\circ}$ C
	Solubility: ± 0.01 mol(1)/L sln.
	(probably standard deviation)
	REFERENCES :
1	1

COMPONENTS:	ORIGINAL MEASUREMENTS:
 (1) 1-Pentanol (<i>n-amyl alcohol</i>, <i>n-butylcarbinol</i>); C₅H₁₂O; [71-41-0] (2) Water; H₂O; [7732-18-5] 	Korenman, I.M.; Gorokhov, A.A.; Polozenko G.N. Zhur. Fiz. Khim. <u>1974</u> , 48, 1810-2; *Russ. J. Phys. Chem. <u>1974</u> , 48, 1065-7; Zhur. Fiz. Khim. <u>1975</u> , 49, 1490-3; *Russ. J. Phys. Chem. <u>1975</u> , 49, 877-8.
VARIABLES:	PREPARED BY:
One temperature: 25 [°] C	A.F.M. Barton
reported to be 0.27 mol $(1)/L$ sln, and the rich phase was reported to be 4.37 mol $(2)/L$	
reported to be 0.27 mol $(1)/L$ sln, and the rich phase was reported to be 4.37 mol $(2)/L$	ne concentration of water (2) in the alcohol- /L sln. volume basis, calculated by the compiler, are

AUXILIARY INFORMATION		
METHOD/APPARATUS/PROCEDURE: The two liquids were shaken in a closed vessel at 25.0 \pm 0.1°C until equilibrium was established. The soly of the alcohol in the aqueous phase was determined on a Tsvet- l chromatograph with a flame-ionization detector. The sorbent was a polyethylene glycol adipate deposited on Polychrom-1 (10% of the mass of the carrier). The column had an internal diameter 4 mm, its temp. was 140°C, and the flow of the carrier gas (nitrogen) was 50 mL min ⁻¹ , The soly of water in the alcohol was determined on a UKh-2 universal chromatograph under isothermal conditions (150°C) with a heat- conductivity detector. The 1 m by 6 mm column was filled with Polysorb1The carrier gas was helium (50 mL min ⁻¹). The study formed part of an investigation of salting-out by alkali halides of higher alcohol-water systems.	SOURCE AND PURITY OF MATERIALS: Not stated. ESTIMATED ERROR: Temperature: ±0.1°C Solubility: not stated; the results report- ed are the arithmetic means from four sets of experiments. REFERENCES:	

	ORIGINAL	MEASUREMENTS:]
binol); C ₅ H ₁₂ 0; [71-	-41-0] Zh. Fiz	s. Khim., <u>1976</u> , 50,	
	PREPARED	BY:	
0 and 60 [°] C	A. Macz	zynski	
UES:	1	······································	
Mutual solubi	lity of 1-pentanc	ol and water	
		T	
2.1	89.5	0.0044	0.635
2.0	87.95	0.0041	0.5986
		100	
ethod was used.	(1) s		;
	<pre>>; [7732-18-5] 40 and 60[°]C UES: Mutual solubi. g(1)/100g si (2)-rich phase (1) 2.1 2.0</pre>	AL (n-amyl alcohol, obinol); C ₅ H ₁₂ 0; [71-41-0] Lavrova abinol); C ₅ H ₁₂ 0; [71-41-0] Zh. Fiz b; [7732-18-5] PREPARED ao and 60°C A. Macz UES: Mutual solubility of 1-pentanc g(1)/100g sln (2)-rich phase (2)-rich phase (1)-rich phase 2.0 87.95 2.0 87.95	Abinol); C ₅ H ₁₂ 0; [71-41-0] Zh. Fiz. Khim., <u>1976</u> , 50, VINITI 3813-75. 20; [7732-18-5] PREPARED BY: 40 and 60°C A. Maczynski UES: Mutual solubility of 1-pentanol and water g(1)/100g sln x ₁ (compile (2)-rich phase (1)-rich phase 2.1 89.5 0.0044 2.0 87.95 0.0041

COMPONENTS -	ODICINAL ACTIONNES
COMPONENTS :	ORIGINAL MEASUREMENTS:
<pre>(1) 1-Pentanol (n-amyl alcohol, n-butylcarbinol); C₅H₁₂0: [71-41-0]</pre>	Charykov, A.K.; Tikhomirov, V.I.; Potapova, T.M.
(2) Water; H ₂ 0; [7732-18-5]	Zh. Obshch. Khim. <u>1978</u> , 48, 1916-21.
VARIABLES:	PREPARED BY:
One temperature: 20 ⁰ C	A. Maczynski
0	
EXPERIMENTAL VALUES:	
The solubility of water in 1-propanol at 20	^o C was reported to be $x_2 = 0.33$.
The corresponding mass per cent value calcu	lated by the compiler is 9.1 g(2)/100 sln.
	INFORMATION
METHOD /APPARATUS / PROCEDURE :	SOURCE AND PURITY OF MATERIALS:
The analytical method was used.	(1) not specified.
The solubility of (2) in (1) was determined by Karl Fischer reagent method. Three determinations were made.	(2) not specified.
	ESTIMATED ERROR:
	Not specified.
	REFERENCES :

COMPONENTS:	ORIGINAL MEASUREMENTS:
 1-Pentanol (n-amyl alcohol, n-butylcarbinol); C₅H₁₂0; [71-41-0] 	Evans, B.K.; James, K.C.; Luscombe, D.K. J. Pharm. Sci. <u>1978</u> , 67, 277-8.
(2) Water; H ₂ 0; [7732-18-5]	
VARIABLES:	PREPARED BY:
One temperature: 37 ⁰ C	S.H. Yalkowsky; S.C. Valvani; A.F.M. Barton
EXPERIMENTAL VALUES:	······································

The concentration of 1-pentanol (1) in the water-rich phase at equilibrium at 37° C was reported to be 0.213 mol(1) L⁻¹ sln.

The corresponding solubility on a mass/volume basis, calculated by the compilers is 18.8 g(1) $\rm L^{-1}$ sln.

AUXILIARY INFORMATION		
METHOD/APPARATUS/PROCEDURE: This determination is one of a large number in the paper reported only briefly; the following is the procedure assumed by the compiler to have been used. A moderate excess of solute was stirred continuously with water for up to 10h in a sealed conical flask immersed in a water thermostat bath, and allowed to stand overnight in the bath. After separation, analysis was by g.l.c. using a hydrogen flame-ionization detection system. Two columns were used for the range of solutes, one consisting of 10% Apiezon L on 80-100 mesh Chromosorb W, and the other of Poropak Q polymer beads. The columns were conditioned before use for 48h at 210-220°C with a nitrogen flow rate of 60 mL min ⁻¹ .	SOURCE AND PURITY OF MATERIALS: (1) "purest product commercially available" no further purification (2) not stated. ESTIMATED ERROR: not stated REFERENCES:	

1-Pentanol		
COMPONENTS: (1) 1-Pentanol (<i>n-amyl alcohol</i> , <i>n-butylcarbinol</i>); C ₅ H ₁₂ 0; [71-41-0] (2) Water; H ₂ 0; [7732-18-5]	ORIGINAL MEASUREMENTS: Nishino, N.; Nakamura, M. Bull. Chem. Soc. Japan <u>1978</u> , 51, 1617-20; <u>1981</u> , 54, 545-8.	
VARIABLES: Temperature: 275-360 K	PREPARED BY: G.T. Hefter	
EXPERIMENTAL VALUES:		
The mutual solubility of (1) and (2) in mole fractions are reported over the temperature range in graphical form. Graphical data are also presented for the heat of evaporation of (1).		
	Y INFORMATION	
METHOD/APPARATUS/PROCEDURE: The turbidimetric method was used. Twenty to thirty glass ampoules containing aqueous solutions of ca . 5 cm of various concentra- tions near the solubility at room tempera- ture were immersed in a water thermostat. The distinction between clear and turbid ampoules was made after equilibrium was established (ca . 2h). The smooth curve drawn to separate the clear and turbid regions was regarded as the solubility curve	 given); dried over calcium oxide; kept in ampoules over magnesium powder. (2) Deionized, refluxed for 15h with potassium permanganate then distilled. 	
	Not stated.	

REFERENCES:

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) 1-Pentanol (n-amyl alcohol,	Singh, R.P.; Haque, M.M.
<i>n-butylcarbinol</i>); C ₅ H ₁₂ 0; [71-41-0]	Indian J. Chem. <u>1979</u> , 17A, 449-51.
(2) Water; H ₂ O; [7732-18-5]	
2	
VARIABLES:	
One temperature: 30°C	PREPARED BY:
one temperature: 50 C	A.F.M. Barton
EXPERIMENTAL VALUES:	
Mutual solubility of 1-pent	
mol(2)/mol(1)	$g(1)/100g \ sln$ x_1 (compiler)
	-
-	662 90.7
Water-rich phase 291.30 0.0	0342 1.65
AUXILIARY	INFORMATION
METHOD / AP PARATUS / PROCEDURE :	SOURCE AND PURITY OF MATERIALS:
Titrations of one component with the other (ref 1) were carried out in well-stoppered	<pre>(1) BDH AR; purified;</pre>
volumetric flasks. The shaking after each addition was done ultrasonically for at	density and refractive index checked
least 30 minutes. These results form part	(2) conductivity water from all-glass still
of a study of the ternary system 1-pentanol/ methanol/water.	
	ESTIMATED ERROR: Temperature: ± 0.1 ⁰ C
	Solubility: each titration was repeated at
	least three times
	REFERENCES;
	(1) Simonsen, D.R.; Washburn, E.R.
	J. Am. Chem. Soc. <u>1946</u> , 68, 235.
l	

COMPONENTS:		ORIGINAL MEAS	ORIGINAL MEASUREMENTS:			
(1) 1-Pentanol (n-amyl alcohol,		Tokunaga, S.	; Manabe, M.; Koda, M.;			
n-butylcar	binol); C ₅ H ₁₂ 0; [71-41-0]] Niihama Kogya	Niihama Kogyo Koto Semmon Gakko Kiyo,			
(2) Water; H ₂ 0; [7732-18-5] VARIABLES:		Rikogaku Her	Rikogaku Hen (Memoirs Niihama Technical College, Sci. and Eng.) <u>1980</u> , 16, 96-101. PREPARED BY:			
		College, Sci				
		PREPARED BY:				
Temperature:	15 – 35 [°] C	A.F.M. Bart	on			
	LUES: Solubility of water		-rich phase			
XPERIMENTAL VA		(2) in the alcohol x_2	-rich phase mol (1)/mol (2)			
	Solubility of water		-			
t∕°c	Solubility of water g(2)/100g sln	<i>x</i> ₂	mol (1)/mol (2)			
<i>t/^oC</i> 15	Solubility of water g(2)/100g sln 10.4	x ₂ 0.362	mol (1)/mol (2) 1.77			
15 20	Solubility of water g(2)/100g sln 10.4 10.5	^x 2 0.362 0.365	mol (1)/mol (2) 1.77 1.74			

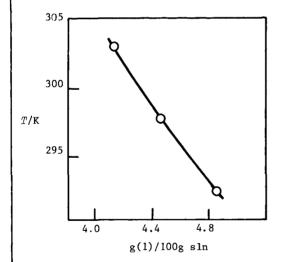
AUXILIARY INFORMATION				
METHOD/APPARATUS/PROCEDURE: The mixtures of 1-pentanol (~5 mL) and	SOURCE AND PURITY OF MATERIALS:			
water (~10 mL) were stirred magnetically in a stoppered vessel and allowed to stand for 10-12 h in a water thermostat. The alcohol phase was analyzed for water by Karl Fischer titration.	no impurities detectable by gas chromatography. (2) deionized;			
	distilled prior to use.			
	ESTIMATED ERROR:			
	Temperature: ± 0.1°C			
	Solubility: each result is the mean of three determinations.			
	REFERENCES :			

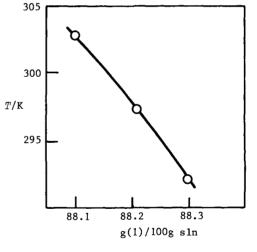
COMPONENTS:	EVALUATOR:		
 (1) 2-Pentanol (methyl-n-propylcarbinol); C₅H₁₂0; [6032-29-7] (2) Water; H₂0; [7732-18-5] 	A. Maczynski, Institute of Physical Chemistry of the Polish Academy of Sciences, Warsaw, Poland. November 1982		

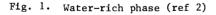
CRITICAL EVALUATION:

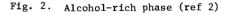
Solubilities in the system comprising 2-pentanol (1) and water (2) have been reported in six publications. Clough and Johns (ref 1) determined the mutual solubilities of the two components at 293 K, but neither the method nor the estimated reliability was reported. Ginnings and Baum (ref 2) measured mutual solubilities at 293, 298 and 303 K by the volumetric method (Figures 1 and 2). Ratouis and Dode (ref 3) determined the solubility of (1) in (2) at one temperature (303 K) by an analytical method. Mullens (ref 4) also determined the solubility in the water-rich phase at one temperature (298 K). Nishino and Nakamura provided graphical information only of the solubility of (1) in (2) (ref 5) and of (2) in (1) (ref 6).

The value 4.09 g(1)/100g sln at 303 K of Ratouis and Dode (ref 3) is in excellent agreement with that of 4.13 \pm 0.1 g(1)/100g sln of ref 2. The data given in ref 1 and 4 are both lower than these, but the values from ref 2 and 3 are considered more reliable, only these sources providing an estimated error. Since the comparison is possible for only one point, and since the other five points are from a single report, the data are regarded as tentative.









Tentative	values	for t	he m	utual	solub	ilities
of 2-	-pentano	51 (1)	and	water	c (2)	

T/K	Water-rich phase		Alcohol-rich phase		
	g(1)/100g sln	$10^{3}x_{1}$	g(2)/100g sln	<i>x</i> 2	
293	4.9	10.3	11.7	0.393	
298	4.5	9.4	11.8	0.395	
303	4.1	8.7	11.9	0.398	
			(continued new	kt page)	

COMPONENTS:	EVALUATOR:		
 (1) 2-Pentanol (methyl-n-propylcarbinol); C₅H₁₀0; [6032-29-7] (2) Water; H₂0; [7732-18-5] 	A. Maczynski, Institute of Physical Chemistry of the Polish Academy of Sciences, Warsaw, Poland. November 1982		
CRITICAL EVALUATION (continued)			
References			

- 1. Clough, W.W.; Johns, C.O. Ind. Eng. Chem. <u>1923</u>, 15, 1030.
- 2. Ginnings, P.M.; Baum, R. J. Am. Chem. Soc. 1937, 59, 1111.
- 3. Ratouis, M.; Dode, M. Bull. Soc. Chim. Fr. 1965, 3318.
- Mullens, J. Alcoholassociaten, doctoraatsproefschrift, Leuven, <u>1971</u>; Huyskens, P.; Mullens, J.; Gomez, A.; Tack, J. Bull. Soc. Chim. Belg. <u>1975</u>, 84, 253.
- 5. Nishino, N.; Nakamura, M. Bull. Chem. Soc. Japan 1978, 51, 1617.
- 6. Nishino, N.; Nakamura, M. Bull. Chem. Soc. Japan <u>1981</u>, 54, 545.

COMPONENTS:	ORIGINAL MEASUREMENTS:			
(1) 2-Pentanol (methyl-n-j	Clough, W.W.; Johns, C.O.			
C ₅ H ₁₂ 0; [6032-29-7]	Ind. Eng. Chem. <u>1923</u> , 15, 1030-2.			
(2) Water; H ₂ 0; [7732-18-	-5]			
VARIABLES:		PREPARED BY	<:	
One temperature: 20 ⁰ C		S.H. Yalko	wsky; S.C. Valva	ni; A.F.M. Barton
EXPERIMENTAL VALUES:		••••••••••••••••••••••••••••••••••••••		
	Mutual solubility	of 2-pentan	ol (1) and water	(2) at 20°C
	g(1)/100g(2) g	(2)/100g(1)	g(1)/100g sln	x_1
			(compiler)	(compiler)
Alcohol-rich phase	4.2	-	4.0	0.0085
Water-rich phase	-	11.2	89.9	0.644
	AUXILIARY	INFORMATION	1	
ME THOD / AP PARATUS / PROCEDURE	SOURCE AND	PURITY OF MATER		
	•			IALS:
Not stated		(1) fract		
			119.2°C/760 mm H	g
		d ₄ ²⁰ 0	.8088	
		ESTIMATED	ERROR:	
		Not state	ed	
		REFERENCES	3 ·	
		KET EKENOEC	· ·	
				l
				l
L		1		

COMPONENTS:		ORIGINAL MEASUREMENTS:			
 2-Pentanol (methyl-n-propylcarbinol); C₅H₁₂0; [6032-19-7] Water; H₂0; [7732-18-5] 		Ginnings, P.M.; Baum, R. J. Am. Chem. Soc. <u>1937</u> , 59, 1111-3.			
VARIABLES:			PREPA	RED BY:	
Temperature: 2	0-30°C		A. M	aczynski and Z. Maczy	vnska
EXPERIMENTAL VALU	JES:				
	Mutual solub:	ility of 2-p	entano	1(1) and water(2)	
t/°c	g(1)/10	Og sin		x_1 (comp	piler)
			phase	(2)-rich phase	(1)-rich phase
20	4.86	88	.30	0.01032	0.6066
25	4.46	88	.21	0.00944	0.6045
30	4.13	88	.10	0.00872	0.6020
		Relative	densi	ty, d_4	
	t/ ^o c W	ater-rich pha	ase	Alcohol-rich phase	
	20	0.9914		0,8317	
	25	0,9909		0.8280	
	30	0.9898		0.8243	
		AUXILIARY	INFOR	MATION	
METHOD / APPARATUS	/PROCEDURE:		SOUR	E AND PURITY OF MATE	RIALS:
The volumetric method was used. Both components were introduced in known amounts into a two-bulb graduated and calibrated flask and shaken mechanically in a water-bath at constant temperature. After sufficient time the liquids were allowed to separate and the total volume was measured. Upon centrifugation, the phase separation line was read, and phase volumes were calculated. From the total weights of the components, the total volume, individual phase volumes, and component concentrations in either phase were evaluated.		ESTI Temp Solu	distilled from meta b.p. range 119.2-2. d_4^{25} 0.8056. not specified. MATED ERROR: errature: $\pm 0.1^{\circ}$ C bbility: better tha	119.7 [°] C,	

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) 2-Pentanol (methyl-n-propylcarbinol);	Ratouis, M.; Dode, M.;
C ₅ H ₁₂ 0; [6032-29-7]	Bull. Soc. Chim. Fr. 1965, 3318-22.
	, · · · · · · · · · · · · · · · · ·
(2) Water; H ₂ 0; [7732-18-5]	
:	
VARIABLES:	PREPARED BY:
One temperature: 30°C	S.C. Valvani; S.H. Yalkowsky; A.F.M. Barton
Ringer solution also studied	o.c. valvani, o.n. laikowsky, A.F.M. Barton
EXPERIMENTAL VALUES:	
The proportion of 2-pentanol (1) in the water	-rich phase at equilibrium at 30 [°] C
was reported to be $4.09 \text{ g}(1)/100 \text{g sln}$.	
The corresponding mole fraction solubility, c	alculated by the compilers, is
$x_1 = 0.00864.$	
1	
The proportion of (1) in the water-rich phase	of a mixture with Ringer solution
at equilibrium at 30 ⁰ C was reported to be 3.9	3 g(1)/100g sln.
AUXILIARY	INFORMATION
METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
In a round bottomed flask, 50 mL of water and a sufficient quantity of alcohol were	(1) Fluke A.G. Buchs S.G.;
introduced until two separate layers were	redistilled with 10:1 reflux ratio; b.p. 119 ⁰ C/760 mm Hg
formed. The flask assembly was equilibrate by agitation for at least 3 h in a constant	$n_{\rm p}^{25} = 1.40454$
temperature bath. Equilibrium solubility	$n_{\rm D} = 1.40454$
was attained by first supersaturating at a	(2) twice distilled from silica apparatus
slightly lower temperature (solubility of alcohols in water decreases with increasing	or ion-exchanged with Sagei A20
temperature) and then equilibrating at the	
desired temperature. The aqueous layer was separated after an overnight storage in	
a bath. The alcohol content was determined	
by reacting the aqueous solution with potassium dichromate and titrating the	Solubility: relative error of 2 determina- tions less than 1%.
excess dichromate with ferrous sulfate	Temperature: $\pm 0.05^{\circ}C$
solution in the presence of phosphoric acid and diphenylamine barium sulfonate as an	
indicator.	REFERENCES:

COMPONENTS:	ORIGINAL MEASUREMENTS:
 (1) 2-Pentanol (methyl-n-propylcarbinol); C₅H₁₂0; [6032-29-7] (2) Water; H₂0; [7732-18-5] 	<pre>*Mullens, J. Alcoholassociaten, doctoraatsproefschrift, Leuven, <u>1971</u> Huyskens, P.; Mullens, J.; Gomez, A.; Tack, J.; Bull. Soc. Chim. Belg. <u>1975</u>, 84, 253-62.</pre>
VARIABLES: One temperature: 25 ⁰ C	PREPARED BY: M.C. Haulait-Pirson; A.F.M. Barton

EXPERIMENTAL VALUES:

At equilibrium at $25^{\circ}C$ the concentration of 2-pentanol (2) in the water-rich phase was reported as 0.478 mol(1) L^{-1} sln, and the concentration of water (2) in the alcohol-rich phase was reported as 8.369 mol(2) L^{-1} sln.

The corresponding solubilities on a mass/volume basis calculated by the compilers are 42.1 g(1) L^{-1} sln and 150.8 g(2) L^{-1} sln, respectively.

AUXILIARY	INFORMATION
METHOD/APPARATUS/PROCEDURE: The partition of the two components was made using a cell described in ref 1. The Rayleigh Interference Refractometer M154 was used for the determination of the concentrations. Standard solutions covering the whole range of concentration investigated were used for the calibration.	SOURCE AND PURITY OF MATERIALS: (1) Merck (p.a.) (2) distilled
	ESTIMATED ERROR: Solubility: ± 0.001 mol(1) L ⁻¹ sln
	REFERENCES: (1) Meeussen, E.; Huyskens, P. J. Chim. Phys. <u>1966</u> , 63, 845.

COMPONENTS:	ORIGINAL MEASUREMENTS:
 (1) 2-Pentanol (methyl-n-propylcarbinol); C₅H₁₂0; [6032-29-7] (2) Water; H₂0; [7732-18-5] 	Nishino, N.; Nakamura, M. Bull. Chem. Soc. Jpn. <u>1978,</u> 51, 1617-20; <u>1981</u> , 54, 545-8.
VARIABLES:	PREPARED BY:
Temperature; 275-360 K	G.T. Hefter
EXPERIMENTAL VALUES:	· · · · · · · · · · · · · · · · · · ·

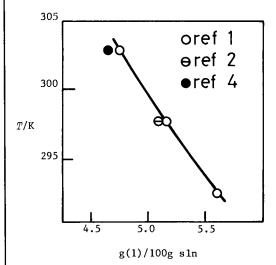
The mutual solubility of (1) and (2) in mole fractions are reported over the temperature range in graphical form. Graphical data are also presented for the heat of evaporation of (1).

AUXILIARY	INFORMATION
METHOD/APPARATUS/PROCEDURE: The turbidimetric method was used. Twenty to thirty glass ampoules containing aqueous solutions of ca . 5 cm of various concentra- tions near the solubility at room tempera- ture were immersed in a water thermostat. The distinction between clear and turbid ampoules was made after equilibrium was established (ca . 2h). The smooth curve drawn to separate the clear and turbid regions was regarded as the solubility curve.	 SOURCE AND PURITY OF MATERIALS: (1) G.R. grade (various commercial sources given); dried over calcium oxide; kept in ampoules over magnesium powder. (2) Deionized, refluxed for 15h with potassium permanganate then distilled.
	ESTIMATED ERROR: Not stated.
	REFERENCES:

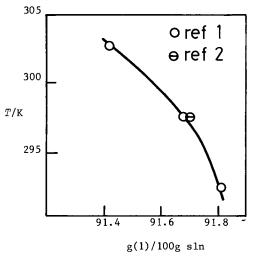
COMPONENTS:	EVALUATOR:
(1) 3-Pentanol (<i>diethylcarbinol</i>); C ₅ H ₁₂ 0;	A. Maczynski, Institute of Physical
[584-02-1]	Chemistry of the Polish Academy of Sciences,
(2) Water; H ₂ 0; [7732-18-5]	Warsaw, Poland.
	November 1982

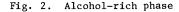
Solubilities in the system comprising 3-pentanol (1) and water (2) have been reported in six publications. Ginnings and Baum (ref 1) carried out measurements of the mutual solubilities of the two components at 293, 298 and 303 K by the volumetric method. Crittenden and Hixon determined mutual solubilities at one temperature (298 K) presumably by titration method. Hyde *et al.* (ref 3) reported the upper critical point and a "room temperature" solubility and Ratouis and Dodé (ref 4) measured the solubility of (1) in (2) at one temperature (303 K) by an analytical method. Nishino and Nakamura provided graphical information only of the solubility of (1) in (2) (ref 5) and of (2) in (1) (ref 6).

For the water-rich phase, values 5.1 g(1)/100 g sln at 298 K (ref 2), and 4.65 g(1)/100 g sln at 303 K (ref 4) are in good agreement with the values of ref 1 (5.15 and 4.75 g(1)/100 g sln, respectively) (Figure 1). Accordingly, the water-rich phase solubility data of ref 1 are recommended. For the alcohol-rich phase, the value 91.7 g(1)/100 g sln of ref 2 at 298 K is in very good agreement with the value 91.68 g(1)/100 g sln of ref 1, (Figure 2) so these data of ref 1 are also recommended. The upper critical solution temperature given in ref 3 is regarded as tentative, as there are no supporting data.









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COMPONENTS :		EVALUATOR:	
 (1) 3-Pentanol (<i>diethylcarbinol</i>); C₅H₁₂O; [584-02-1] (2) Water; H₂O; [7732-18-5] 		A. Maczynski, Institute of Phys: Chemistry of the Polish Academy Warsaw, Poland. November 1982	
CRITICAL EVALUA	TION: (continued)		<u> </u>
		entative values for the mutual 3-pentanol (1) and water (2)	
T/K	Water-rich phase	Alcohol-rich ph	ase
	g(1)/100g s1n x ₁	g(2)/100g sln	<i>x</i> ₂
293	5.6 (tentative) 0.0	120 8.2 (tentative) 0.304
298	5.2 (recommended) 0.0	110 8.3 (recommended)) 0.308
303	4.8 (recommended) 0.0	101 8.6 (tentative) 0.315
489.4	upper critical solution	n temperature (tentative)	
References		- 0. 1027 50 1111	
	P.M.; Baum, R.J. J. Am. Che		
	n, E.D., Jr.; Hixon, A.N. Inc		
		e, A.S.C. Disc. Faraday Soc. <u>1954</u> ,	18, 239.
4. Ratouis, M.; Dode, M. Bull. Soc. Chim. Fr. <u>1965</u> , 3318.			
5. Nishino, N.; Nakamura, M. Bull. Chem. Soc. Jpn. <u>1978</u> , 51, 1617.			
6. Nishino,	N.; Nakamura, M. Bull. Chem.	. Soc. Jpn. <u>1981</u> , 54, 545.	

(1) 3-Pentanol (disthylocrybinol); C ₃ H ₁₂ O; [584-02-1] (2) Water; H ₂ O; [7732-18-5] Cinnings, P.M.; Baum, R. J. Am. Chem. Soc. <u>1937</u> , 59, 1111-3. ARIABLES: Temperature: 20-30 [°] C A. Maczynski and Z. Maczynska (2)-rich phase (1)-rich phase (2)-rich phase (2)-rich phase (1)-rich phase (2)-rich phase (3) (2)-rich phase (3) (3) (3) (3) (4)-75 (3) (4)-75 (3) (4)-8330 (3) (5)-9914 (4)-8330 (3) (5)-9914 (5)-8330 (3) (5)-9914 (6)-8368 (2) (6)-8368 (2) (6)-8368 (2) (6)-8368 (2) (6)-8368 (2) (6)-8368 (2) (6)-8368 (2) (6)-8368 (2) (7)-903 (8)-830 (3) (3) (3) (4)-8330 (3) (5)-9914 (6)-8306 (6)-8324 (5)-9914 (6)-8306 (6)-8324 (5)-9914 (6)-8306 (6)-8324 (5)-9914 (6)-8306 (6)-8324 (5)-9914 (6)-8306 (6)-8324 (5)-9914 (6)-8306 (6)-8324 (6)-8306 (7)-903 (6)-8324 (7)-903 (6)-8324 (7)-903 (6)-8324 (7)-903 (7)-903 (7)-903 (8)-804 <	OMPONENTS:			ORIGINAL M	EASUREMENTS:	
ARIABLES: PREPARED BY: Temperature: $20-30^{\circ}$ C A. Maczynski and Z. Maczynska XPERIMENTAL VALUES: Mutual solubility of 3-pentanol(1) and water(2) $t/^{\circ}$ C $(2)-rich phase (2)-rich phase $	[584-02-1	ן); c ₅ H ₁₂ 0;			
Mutual solubility of 3-pentanol(1) and water(2) $t/^{\circ}C$ g(1)/100g sln x_1 (compiler) $t/^{\circ}C$ (2)-rich phase(1)-rich phase(2)-rich phase(1)-rich phase205.6191.810.012000.6961255.1591.660.010970.6924304.7591.420.010080.6852Relative density, d_4 $t/^{\circ}C$ Water-rich phaseAlcohol-rich phase200.99200.836825200.99200.8368250.99140.8330300.99030.8294AUXILIARY INFORMATIONAUXILIARY INFORMATIONAUXILIARY INFORMATIONCullist and shaken mechanically in a water-bat at constant temperature. After sufficient time the liquids were allowed to separate and the total volume was measured. Upon centrifugation, the phase separation line was read, and phase volumes, individual phase volumes, and component concentrations in either phase 	VARIABLES:					
$\frac{g(1)/100g \ sln}{(2)-rich \ phase} (1)-rich \ phase} (2)-rich \ phase (1)-rich \ phase (2)-rich \ phase \$	XPERIMENTAL VA	LUES:	I		<u> </u>	
$\frac{t}{^{\circ}C}$ (2)-rich phase (1)-rich phase (2)-rich phase (1)-rich phase 20 5.61 91.81 0.01200 0.6961 25 5.15 91.68 0.01097 0.6924 30 4.75 91.42 0.01008 0.6852 Relative density, d_4 $t/^{\circ}C$ Water-rich phase Alcohol-rich phase 20 0.9920 0.8368 25 0.9914 0.8330 30 0.9903 0.8294 $\frac{ETHOD/APPARATUS/PROCEDURE:}{E}$ Hill's volumetric method was adopted. Both components were introduced in known amounts into a two-bulb graduated and calibrated flask and shaken mechanically in a water-bath at constant temperature. After sufficient time the liquids were allowed to separate and the total volume was measured. Upon centrifugation, the phase separation line was read, and phase volumes were calculated. From the total wolume, individual phase volumes, and component concentrations in either phase were evaluated. ESTIMATED ERROR: Coublic trip the total volume, individual phase volumes, and component concentrations in either phase were evaluated. ESTIMATED ERROR: Coublic trip the total volume, individual phase volumes, and component concentrations in either phase were evaluated. ESTIMATED ERROR: Coublic trip the total volume, individual phase volumes, and component concentrations in either phase Were evaluated. ESTIMATED ERROR: Coublic trip the constant temperature: $\pm 0.1^{\circ}C$ Soublic trip the constant temperature. ESTIMATED ERROR: Coublic trip the constan		Mutual solub	oility of 3-p	entanol(1)	and water(2)	
(2)-rich phase (1)-rich phase (2)-rich phase (1)-rich phase 20 5.61 91.81 0.01200 0.6961 25 5.15 91.68 0.01097 0.6924 30 4.75 91.42 0.01008 0.6852 Relative density, d_4 $t/^{\circ}C$ Water-rich phase Alcohol-rich phase 20 0.9920 0.8368 25 0.9914 0.8330 30 0.9903 0.8294 AUXILIARY INFORMATION AUXILIARY INFORMATION AUXILIARY INFORMATION AUXILIARY INFORMATION AUXILIARY INFORMATION AUXILIARY INFORMATION	± 1 ⁰ c	g(1)/100g	sln		x_1 (cor	mpiler)
$\begin{array}{c ccccccccccccccccccccccccccccccccccc$		(2)-rich phase	(1)-rich pha	ase (2)	-rich phase	(1)-rich phase
30 4.75 91.42 0.0108 0.6852 Relative density, d_4 $t/^{\circ}C$ Water-rich phase Alcohol-rich phase 20 0.9920 0.8368 25 0.9914 0.8330 30 0.9903 0.8294 MUXILIARY INFORMATION ETHOD/APPARATUS/PROCEDURE: Hill's volumetric method was adopted. Both components were introduced in known amounts into a two-bulb graduated and calibrated flask and shaken mechanically in a water-bulb graduated and calibrated flask and shaken mechanically in was measured. Upon centrifugation, the total volume, individual phase volumes, and component concentrations in either phase were evaluated. With the ter than 0.1 wt % (type of error not specified)	20	5.61	91.81		0.01200	0.6961
Relative density, d_4 $t/^{\circ}C$ Water-rich phaseAlcohol-rich phase200.99200.8368250.99140.8330300.99030.8294AUXILIARY INFORMATIONMETHOD/APPARATUS/PROCEDURE:Hill's volumetric method was adopted.Both components were introduced in known amounts into a two-bulb graduated and calibrated flask and shaken mechanically in a water-bath at constant temperature.SOURCE AND PURITY OF MATERIALS:(1) Eastman best grade; distilled from metallic calcium; b.p. range 115.4-115.9°C, d_4^2 0.8195.(2) not specified.(2) not specified.ESTIMATED ERROR: Component concentrations in either phase were evaluated.ESTIMATED ERROR: Temperature: $\pm 0.1^{\circ}C$ Solubility: better than 0.1 wt χ (type of error not specified)	25	5.15	91.68		0.01097	0.6924
t/°C Water-rich phase Alcohol-rich phase 20 0.9920 0.8368 25 0.9914 0.8330 30 0.9903 0.8294 AUXILIARY INFORMATION AUXILIARY INFORMATION AUXILIARY INFORMATION 	30	4.75	91.42		0.01008	0.6852
20 0.9920 0.8368 25 0.9914 0.8330 30 0.9903 0.8294 AUXILIARY INFORMATION AUXILIARY INFORMATION AUXILIARY I			Relat	ive densit	y, d ₄	
25 0.9914 0.8330 30 0.9903 0.8294 AUXILIARY INFORMATION AUXILIARY INFORMATION AUXILIARY INFORMATION SOURCE AND PURITY OF MATERIALS: AUXILIARY INFORMATION SOURCE AND PURITY OF MATERIALS: AUXILIARY INFORMATION AUXILIARY INFORMATION AUXILIARY INFORMATION AUXILIARY INFORMATION AUXILIARY INFORMATION AU		t/ ^o c	Water-ric	h phase	Alcohol-ric	h phase
30 0.9903 0.8294 AUXILIARY INFORMATION AUXILIARY INFORMATION AUXILIARY INFORMATION AUXILIARY INFORMATION AUXILIARY INFORMATION ACTHOD/APPARATUS/PROCEDURE: Hill's volumetric method was adopted. Both components were introduced in known amounts into a two-bulb graduated and calibrated flask and shaken mechanically in a water-bath at constant temperature. After sufficient time the liquids were allowed to separate and the total volume was measured. Upon centrifugation, the phase separation line was read, and phase volumes, individual phase volumes, and component concentrations in either phase were evaluated. From the total volume, individual phase volumes, and component concentrations in either phase were evaluated.		20	0.99	20	0.8368	
AUXILIARY INFORMATION METHOD/APPARATUS/PROCEDURE: Hill's volumetric method was adopted. Both components were introduced in known amounts into a two-bulb graduated and calibrated flask and shaken mechanically in a water-bath at constant temperature. After sufficient time the liquids were allowed to separate and the total volume was measured. Upon centrifugation, the phase separation line was read, and phase volume, individual phase volumes, and component concentrations in either phase were evaluated. AUXILIARY INFORMATION SOURCE AND PURITY OF MATERIALS: (1) Eastman best grade; distilled from metallic calcium; b.p. range l15.4-115.9°C, d ²⁵ 0.8195. (2) not specified. ESTIMATED ERROR: Temperature: $\pm 0.1^{\circ}C$ Solubility: better than 0.1 wt % (type of error not specified.		25	0.99	14	0.8330	
<pre>METHOD/APPARATUS/PROCEDURE: Hill's volumetric method was adopted. Both components were introduced in known amounts into a two-bulb graduated and calibrated flask and shaken mechanically in a water-bath at constant temperature. After sufficient time the liquids were allowed to separate and the total volume was measured. Upon centrifugation, the phase separation line was read, and phase volumes were calculated. From the total weights of the components, the total volume, individual phase volumes, and component concentrations in either phase were evaluated.</pre> SOURCE AND PURITY OF MATERIALS: (1) Eastman best grade; distilled from metallic calcium; b.p. range 115.4-115.9°C, d ²⁵ 0.8195. (2) not specified. (2) not specified. ESTIMATED ERROR: Temperature: ± 0.1°C Solubility: better than 0.1 wt % (type of error not specified)						
<pre>METHOD/APPARATUS/PROCEDURE: Hill's volumetric method was adopted. Both components were introduced in known amounts into a two-bulb graduated and calibrated flask and shaken mechanically in a water-bath at constant temperature. After sufficient time the liquids were allowed to separate and the total volume was measured. Upon centrifugation, the phase separation line was read, and phase volumes were calculated. From the total weights of the components, the total volume, individual phase volumes, and component concentrations in either phase were evaluated.</pre> SOURCE AND PURITY OF MATERIALS: (1) Eastman best grade; distilled from metallic calcium; b.p. range 115.4-115.9°C, d ²⁵ 0.8195. (2) not specified. (2) not specified. ESTIMATED ERROR: Temperature: ± 0.1°C Solubility: better than 0.1 wt % (type of error not specified.				TNEODWATTO		
 Hill's volumetric method was adopted. Both components were introduced in known amounts into a two-bulb graduated and calibrated flask and shaken mechanically in a water-bath at constant temperature. After sufficient time the liquids were allowed to separate and the total volume was measured. Upon centrifugation, the phase separation line was read, and phase volumes were calculated. From the total weights of the components, the total volume, individual phase volumes, and component concentrations in either phase were evaluated. (1) Eastman best grade; distilled from metallic calcium; b.p. range 115.4-115.9°C, d²⁵ 0.8195. (2) not specified. (2) not specified. (2) not specified. (3) ESTIMATED ERROR: Temperature: ± 0.1°C Solubility: better than 0.1 wt % (type of error not specified. 		IC (DDOCEDURE.	AUXILIARY	,		
	Hill's volum Both component amounts into calibrated f a water-bath After suffic: allowed to se was measured phase separation volumes were weights of the volume, indi- component contents	etric method was ad nts were introduced a two-bulb graduat lask and shaken med at constant temper ient time the liqui eparate and the tot . Upon centrifuga tion line was read calculated. From ne components, the vidual phase volume acentrations in eit	in known ted and chanically in rature. ids were cal volume ation, the , and phase n the total total es, and	<pre>(1) East dist b.p. (2) not</pre>	ERROR: ELTROR:	de; etallic calcium; -115.9°C, d ²⁵ 0.8195. 4

COMPONENTS:	ORIGINAL MEASUREMENTS:
 3-Pentanol (<i>diethylcarbinol</i>); C₅H₁₂0; [584-02-1] Water; H₂0; [7732-18-5] 	Crittenden, E.D., Jr.; Hixon, A.N.; Ind. Eng. Chem., <u>1954</u> , 46, 265-8.
VARIABLES:	PREPARED BY:
One temperature: 25 [°] C	A. Maczynski
EXPERIMENTAL VALUES:	
The solubility of 3-pentanol in water at 25	$^{\circ}$ C was reported to be 5.1 g(1)/100g sln.
The corresponding mole fraction, $x_1^{}$, calcul	ated by the compiler is 0.011.
The solubility of water in 3-pentanol at 25	^o C was reported to be 8.3 g(2)/100g sln-
The corresponding mole fraction, x_{γ} , calcul	ated by the compiler is 0.31.
	INFORMATION
METHOD/APPARATUS/PROCEDURE: Presumably the titration method described for ternary systems containing HCl was used. In this method the solubility was determined by bringing 100-mL samples of (1) or (2) to a temperature 25.0 ± 0.1°C and the second component was then added from a calibrated buret, with vigorous stirring, until the solution became permanently cloudy.	purity not specified.
	ESTIMATED ERROR: Solubility: 2% (alcohol-rich) - 10% water- rich) Temperature: ± 0.10 [°] C. REFERENCES:

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) 3-Pentanol (<i>diethylcarbinol</i>); C ₅ H ₁₂ 0; [584-01-1]	Hyde, A.J.; Langbridge, D.M.; Lawrence, A.S.C Disc. Faraday Soc. <u>1954</u> , 18, 239-58.
(2) Water; H ₂ O; [7732-18-5]	
VARIABLES :	PREPARED BY:
One temperature: 216 ⁰ C	A. Maczynski, and A.F.M. Barton
EXPERIMENTAL VALUES:	
The upper critical solution temperature was : $(x_1 = 0.133, \text{ compiler}).$ The solubility of (1) in (2) was reported as	
AUXILIARY	INFORMATION
METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
Not specified	(1) not specified.
	(2) not specified.
	ESTIMATED ERROR:
	Not specified.
	REFERENCES:

COMPONENTS :	ORIGINAL MEASUREMENTS:
(1) 3-Pentanol (<i>diethylcarbinol</i>);	Ratouis, M.; Dode, M.;
C ₅ H ₁₂ 0; [584-02-1]	Bull. Soc. Chim. Fr. <u>1965;</u> 3318-22.
5 12	
(2) Water; H ₂ O; [7732-18-5]	
VARIABLES:	PREPARED BY:
One temperature: 30°C	S.C. Valvani; S.H. Yalkowsky; A.F.M. Barton
Ringer solution also studied	
EXPERIMENTAL VALUES:	
The proportion of 3-pentanol (1) in the water	-rich phase at equilibrium at 30 ⁰ C
was reported to be $4.65 \text{ g}(1)/100 \text{g sln}$.	
The corresponding mole fraction solubility, c	alculated by the compilers, is
$x_1 = 0.00987.$	
The proportion of (1) in the water-rich phase	
equilibrium at 30° C was reported to be 4.36 g	(1)/100g sln.
AUXILIARY	INFORMATION
METHOD / APPARATUS / PROCEDURE :	SOURCE AND PURITY OF MATERIALS:
In a round bottomed flask, 50 mL of water and a sufficient quantity of alcohol were	(1) Fluka A.G. Buchs S.G.; redistilled with 10:1 reflux ratio
introduced until two separate layers were	$h = 115 7^{\circ} C/759.6 mm Hc$
formed. The flask assembly was equilibrated by agitation for at least 3 h in a constant	$n_{\rm D}^{25} = 1.40842$
temperature bath. Equilibrium solubility was attained by first supersaturating at a	2 (2) twice distilled from silica apparatus
slightly lower temperature (solubility of	or ion-exchanged with Sagei A20
alcohols in water decreases with increasing temperature) and then equilibrating at the	
desired temperature. The aqueous layer	
was separated after an overnight storage in a bath. The alcohol content was deter-	ESTIMATED ERROR:
mined by reacting the aqueous solution with potassium dichromate and titrating the	Solubility: relative error of 2 determina-
excess dichromate with ferrous sulfate	tions less than 1%.
solution in the presence of phosphoric acid and diphenylamine barium sulfonate as an	Temperature: ± 0.05°C
indicator.	REFERENCES :

COMPONENTS :	ORIGINAL MEASUREMENTS:
 (1) 3-Pentanol (<i>diethylcarbinol</i>); C₅H₁₂0; [584-02-1] (2) Water; H₂0; [7732-18-5] 	Nishino, N.; Nakamura, M. Bull. Chem. Soc. Jpn. <u>1978</u> , 51, 1617-20; <u>1981</u> , 54, 545-8.
VARIABLES: Temperature: 275-360 K	PREPARED BY: G.T. Hefter

EXPERIMENTAL VALUES:

The mutual solubility of (1) and (2) in mole fractions are reported over the temperature range in graphical form. Graphical data are also presented for the heat of evaporation of (1).

AUXILIARY	INFORMATION
METHOD / APPARATUS / PROCEDURE :	SOURCE AND PURITY OF MATERIALS:
The turbidimetric method was used. Twenty to thirty glass ampoules containing aqueous solutions of ca . 5 cm of various concentra- tions near the solubility at room tempera- ture were immersed in a water thermostat. The distinction between clear and turbid ampoules was made after equilibrium was established (ca . 2h). The smooth curve drawn to separate the clear and turbid regions was regarded as the solubility curve.	 G.R. grade (various commercial sources given); dried over calcium oxide; kept in ampoules over magnesium powder. Deionized, refluxed for 15h with potassium permanganate then distilled. ESTIMATED ERROR:
	Not stated.
	REFERENCES:

COMPONENTS: (1) Cyclohexanol; C ₆ H ₁₂ O; [108-93-0] (2) Water; H ₂ O; [7732-18-5]		er and A.F.M. Ba 7, Perth, Weste: 3.	
CRITICAL EVALUATION:			
Solubilities in the system comprising	g cyclohexanol (1) a	and water (2) h	ave been reported
in the following publications:			
Reference	T/K	Phase	Method
Forcrand (ref 1)	284	mutual	analytical
Sidgwick and Sutton (ref 2)	258-459	mutual	synthetic
Booth and Everson (ref 3,4)	298,333	(1) in (2)	titration
Hansen et al. (ref 5)	298	(1) in (2)	interferometric
Zil'berman (ref 6)	273-457	mutual	synthetic
Skrzec and Murphy (ref 7)	300	mutual	titration
Tettamanti et al. (ref 8)	293	mutual	titration
Lavrova and Lesteva (ref 9)	313, 333	mutual	titration

The original data are compiled in the data sheets immediately following this Critical Evaluation.

In preparing this Critical Evaluation the data of Booth and Everson (ref 3,4) in volume/ volume fractions were excluded as no density data were included in the original references.

In both the water-rich and alcohol-rich phases the data of Forcrand (ref 1), Skrzec and Murphy (ref 7) and Tettamanti *et al.* (ref 8) disagree markedly with other studies (ref 2,5,6) and are rejected. All other data are included in the tables below. Values obtained by the Evaluators by graphical interpolation or extrapolation from the data sheets are indicated by an asterisk (*). "Best" values have been obtained by simple averaging. The uncertainty limits (σ_n) attached to the "best" values do not have statistical significance and should be regarded only as a convenient representation of the spread of reported values and not as error limits. The letter (*R*) designates "Recommended" data. Data are "Recommended" if two or more apparently reliable studies are in reasonable agreement ($\leq \pm 5\%$).

For convenience further discussion for the two phases will be given separately.

Solubility of cyclohexanol (1) in water (2)

Excluding the data already rejected (see above) the reported solubilities for the waterrich phase are in good agreement except at very high temperatures (>423 K).

COMPONEN	TS:	EVALUATOR:
(1) Cyclohexanol; C ₆ H ₁₂ 0; [108-93-0]		G.T. Hefter and A.F.M. Barton, Murdoch
(2) Water; H ₂ 0; [7732-18-5]		University, Perth, Western Australia.
(2) wale	2, [7752-10-5]	June, 1983.
CRITICAL	EVALUATION (continued)	-
	Tentative and Recommende	ed (R) values for the solubility
	of cyclohexanol	(1) in water (2).
Т/К		Solubility, g(1)/100g sln
	Reported valu	
273	5.34 (ref 6)	n 5.3
273	4.66 [*] (ref 2), 4.57 (ref 6)	$4.62 \pm 0.05 (R)$
293	3.95 [*] (ref 2), 4.00 (ref 6)	$3.97 \pm 0.03 (R)$
298	3.70 [*] (ref 2), 3.92 (ref 5)	3.8 ± 0.1 (R)
303	3.50 [*] (ref 2), 3.60 (ref 6)	$3.55 \pm 0.05 (R)$
313	3.23 [*] (ref 2), 3.33 (ref 6), 3.33	(ref 9) 3.30 ± 0.05 (R)
323	3.14 (ref 6)	3.1
333	3.1 [*] (ref 6)	3.1
343	3.19 (ref 6)	3.2
353	3.41 (ref 6)	3.4
363	3.65 (ref 6)	3.7
373	3.93 (ref 6)	3.9
383	4.28 (ref 6)	4.3
393	5.0 [*] (ref 2), 4.7 (ref 6)	4.9 ± 0.2 (R)
403	5.8 [*] (ref 2), 5.3 (ref 6)	5.6 ± 0.3 (R)
413	6.6 [*] (ref 2), 6.1 (ref 6)	6.4 ± 0.3 (R)
423	8.2 [*] (ref 2), 7.2 (ref 6)	7.7 ± 0.5
433	9.8 [*] (ref 2), 8.8 (ref 6)	9.3 ± 0.5
443	13.0 [*] (ref 2), 11.5 (ref 6)	12.3 ± 0.8
453	20.0 [*] (ref 2), 17.8 (ref 6)	19 ± 1
1		

Solubility of water (2) in cyclohexanol (1)

The existence of two extensive sets of data in reasonable (although not fully satisfactory) agreement enables values to be recommended over a wide range of temperatures. Insufficient data are available below 313 K to enable a realistic assessment of their reliability to be made.

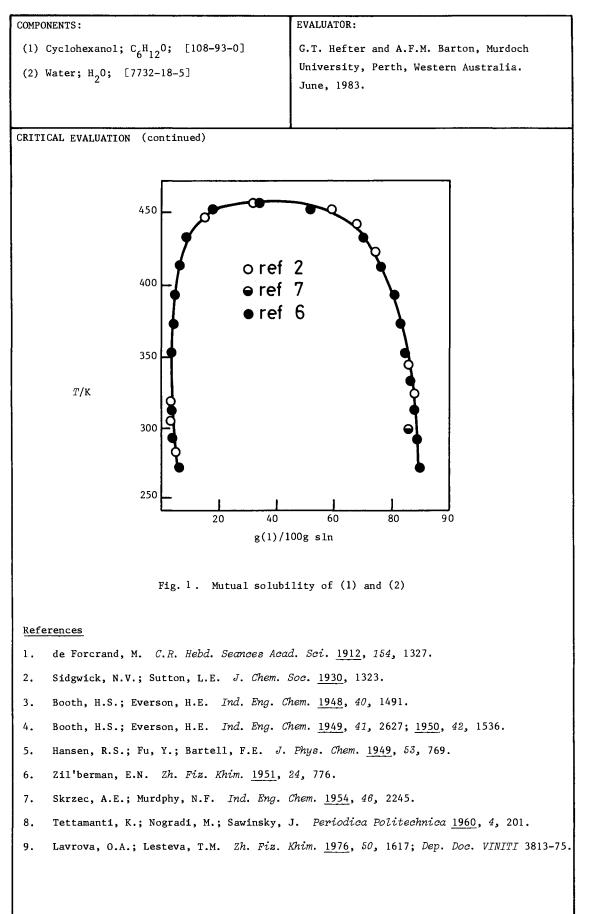
COMPONENTS	<u>.</u>	EVALUATOR:				
(1) Cyclohexanol; C ₆ H ₁₂ 0; [108-93-0] (2) Water; H ₀ ; [7732-18-5] 2		G.T. Hefter and A.F.M. Barton, Murdoch University, Perth, Western Australia. June, 1983				
CRITICAL E	CRITICAL EVALUATION (continued)					
	Tentative and Recommended	(R) values for the solubility				
	of water (2) in	cyclohexanol (1)				
Т/К		Solubility, g(1)/100g sln				
	Reported Valu	"Best" value $\begin{pmatrix} \pm \sigma \\ n \end{pmatrix}$				
273	10.13 (ref 6)	10.1				
283	10.53 (ref 6)	10.5				
293	11.07 (ref 6)	11.1				
298	11.35 [*] (ref 6)	11.4				
303	11.63 (ref 6)	11.6				
313	12.23 (ref 6), 12.21 (ref 9)	12.2 (R)				
323	12.00 [*] (ref 2), 12.89 (ref 6)	12.4 ± 0.5 (R)				
333	12.7 [*] (ref 2), 13.6 (ref 6), 13.52	(ref 9) 13.3 ± 0.4 (R)				
343	13.3 [*] (ref 2), 14.34 (ref 6)	13.8 ± 0.5 (R)				
353	14.0 [*] (ref 2), 15.17 (ref 6)	14.6 ± 0.6 (R)				
363	14.5 [*] (ref 2), 16.07 (ref 6)	15.3 ± 0.8				
373	15.4 [*] (ref 2), 17.04 (ref 6)	16.2 ± 0.8				
383	16.5 [*] (ref 2), 18.1 (ref 6)	17.3 ± 0.8 (R)				
393	18.0 [*] (ref 2), 19.3 (ref 6)	18.7 ± 0.7 (R)				
403	19.5 [*] (ref 2), 20.7 (ref 6)	20.1 ± 0.6 (R)				
413	22.0 [*] (ref 2), 23.6 (ref 6)	22.8 ± 0.8 (R)				
423	25.0 [*] (ref 2), 25.3 (ref 6)	25.2 ± 0.2 (R)				
433	28.5 [*] (ref 2), 29.5 (ref 6)	29.0 ± 0.5 (R)				
443	32.5 [*] (ref 2), 36.2 (ref 6)	34 ± 2				
453	41.0 [*] (ref 2), 47.7 (ref 6)	44 ± 3				

Upper critical solution temperature

The UCST has been reported as 457 K ($184^{\circ}C$) at 33.9 g(1)/100g sln (ref 6).

Representative data for the mutual solubilities of cyclohexanol and water are plotted in Figure 1.

(continued next page)



COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Cyclohexanol; C ₆ H ₁₂ O; [108-93-0]	de Forcrand, M.
(2) Water; H ₂ 0; [7732-18-5]	C.R. Hebd. Seances Acad. Sci. 1912, 154,
(2) mater, 20, (102 10 5)	1327-30.
VARIABLES:	PREPARED BY:
Temperature: 11 [°] C	A. Maczynski
EXPERIMENTAL VALUES:	
The solubility of cyclohexanol in water at ll	$^{\circ}$ C was reported to be 5.67 g(1)/100g (2).
The corresponding mass percent and mole fract	ion, x_1 , calculated by the compiler are
5.37 g(1)/100g sln and 0.0101.	1
The solubility of water in cyclohexanol at 11	C was reported to be 11.27 g(2)/100g (1).
The corresponding mass percent and mole fract	ion, $x_2^{}$, calculated by the compiler are
10.13 g(2)/100g sln and 0.3853.	
-	
AUXILIARY	INFORMATION
METHOD / APPARATUS / PROCEDURE :	SOURCE AND PURITY OF MATERIALS:
An analytical method was used.	(1) Laboratoire de catalyse de Toulouse;
	recrystallized;
No details were reported in the paper.	b.p. 160.9° C (766 mm Hg) m.p. 22.45°C, $\frac{22.5}{d_{4}}$ 0.9471.
	(2) not specified.
	LOTINATED EDDOD.
	ESTIMATED ERROR:
	Not specified.
	REFERENCES :

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Cyclohexanol, C ₆ H ₁₂ O; [108-93-0]	Sidgwick, N.V.; Sutton, L.E.
(2) Materia II 0 [7722 19 5]	J. Chem. Soc. <u>1930</u> , 1323-6.
(2) Water, H ₂ 0 [7732-18-5]	
VARIABLES:	PREPARED BY:
Temperature: (-15) - 185 [°] C	A. Maczynski and Z. Maczynska
EXPERIMENTAL VALUES:	
The Ic	e Line
t/ ⁰ C g(1)/100g sln	$x_1(\text{compiler})$
-15.4 93.0	0.705
-10.2 92.3	0.683
- 7.6 91.2	0.652
- 4.9 90.45	0.630
- 4.1 90.08	0.620
- 2.0 89.0	0.593
- 1.2 88.3	0.579
- 1.1 88.45	0.579
- 0.9 5.00	0.0093
- 0.6 3.33	0.00616
- 0.32 1.67	0.00304
- 0.3 1.67	0.00304
	(continued next page)
METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
The usual synthetic method was used.	(1) British Drug Houses Ltd.; fractionally distilled at about 10 mm
At the higher temperatures sealed glass tubes were used. At large proportions,	Hg; 99.85 wt % purity (if 23.6°C is taken
the turbidity appearance temperature of (1)	as the true m.p.)
rose with successive heatings (decomposit- ion ?) and the first reading was taken.	(2) not specified.
Upward of 87.9% of (1) the curve was too	
steep and turbidity too faint to take reliable temperature measurements.	
	1
	ESTIMATED ERROR:
	Not specified.
	-
	REFERENCES :

COMPONENTS: ORIGINAL MEASUREMENTS: (1) Cyclohexanol; C₆H₁₂0; [108-93-0] Sidgwick, N.V.; Sutton, L.E. J. Chem. Soc. 1930, 1323-6. (2) Water; H₂0; [7732-18-5] EXPERIMENTAL VALUES: (continued) The Liquid-Liquid Curve $t/^{\circ}c$ x_1 (compiler) g(1)/100g s1n (2)-rich phase (1)-rich phase (2)-rich phase (1)-rich phase 7.2 5.00 0.00938 _ 0.00894 9.4 4.78 _ _ 4.58 0.00856 9.7 11.2 4.41 0.00823 12.0 4.55 0.00850 _ ---0.00788 14.2 4.23 _ 0.00800 15.2 4.29 _ 4.09 0.00762 16.3 _ 20.6 3.95 0.00734 _ 20.8 3.82 0.00709 _ 24.6 3.75 0.00696 27.55 3.52 _ 0.00652 28.7 3.57 0.00661 _ _ 31.85 3.37 0.00623 _ _ 33.6 3.41 _ 0.00631 _ 0.00602 40.4 3.26 0.00587 _ 40.45 3.18 ---0.00589 45.8 3.19 _ _ 87.9 0.5664 51.55 _ 71.5 86.75 _ 0.5407 -0.5219 85.95 72.75 _ _ 93.63 85.3 _ 0.5106 _ 0.00965 121.95 5.14 _ _ 0.4214 80.2 130.9 -_ 74.6 0.3456 150.35 -_ 156.9 9.22 -0.01793 -70.1 0.2965 163.03 _ _ 0.2811 68.5 168.64 _ _ 68.0 0.2764 169.7 _ _ 174.3 15.00 -0.0307 _ 179.4 19.2 _ 0.0410 _ 59.4 0.2083 180.1 _ _ 52.3 _ 0.1647 183.66 _ 0.0793 184.72 32.4 _ -

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Cyclohexanol; C ₆ H ₁₂ O; [108-93-0]	Booth, H.S.; Everson, H.E.
(1) 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1,	Ind. Eng. Chem. <u>1948</u> , 40, 1491-3.
(2) Water; H ₂ 0; [7732-18-5]	,,,,
VARIABLES:	PREPARED BY:
One temperature: 25°C	S.H. Yalkowsky; S.C. Valvani; A.F.M. Barton
Sodium xylene sulfonate	
EXPERIMENTAL VALUES:	
It was reported that the solubility of cycloh	exanol (1) in water (2) was $3.4 \text{ mL}(1)/100 \text{mL}$
(2) at 25.0° C.	
The corresponding value in 40% sodium xylene	sulfonate solution as solvent was >400 $mL(1)/$
100mL solvent.	
	INFORMATION
METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
A known volume of solvent (usually 50mL) in a tightly stoppered Babcock tube was	(1) "CP or highest grade commercial".
thermostatted. Successive measured	(2) distilled.
quantities of solute were added and equilibrated until a slight excess of solute	
remained. The solution was centrifuged,	
returned to the thermostat bath for 10 min, and the volume of excess solute measured	
directly. This was a modification of the	
method described in ref 1.	
	ESTIMATED ERROR:
	Solubility: within 0.1 mL(1)/100mL (2)
	REFERENCES:
	(1) Hanslick, R.S. Dissertation, Columbia
	University, 1935.

COMPONENTS:					ORIGINAL MEASUREMENTS:						
(1) Cyclohexanol; C ₆ H ₁₂ 0; [108-93-0]					Booth, H.S.; Everson, H.E.						
(2) Water; H ₂ 0; [7732-18-5]					Ind. Eng. Chem. <u>1949</u> , 41, 2627-8; <u>1950</u> ,						
				42,	1536-7						
VARIABLES: Temperature: 25 [°] C and 60	1 ⁰ C					ARED B		C Val	vani• 4	А.F.M. В	arton
Hydrotropic solutes (sodi		vlsulf	onates`		5.11	• 14160	wsky, s		vuni, i		di con
			onaces,	<u></u>							
EXPERIMENTAL VALUES: It was reported that the	soluh	ilitie	sofo	vclc	hex	anol (1) in wa	ter (2)	at 25.	0°C and	[
60 [°] C were 3.40 mL(1)/100										units qu	
for the table of data in										-	
agreed with ref 1 and with										s in aqu	ieous
solutions of hydrotropic							-				
			S	0111	oili	ty. mL((1)/100-	nL solve	ent for	•	
								itions		-	
Arylsulfonate		5.0	8.0	10.	.0	15.0	20.0	22.0	25.0	34.6	40.0
Sodium benzenesulfonate	25 ⁰ C	4.08	_	4.	.43	_	14.1	28.8	>400	_	-
	60 [°] C		-		.05	_	13.8	27.0	>400	-	-
Sodium p -cymenesulfonate	25 ⁰ C	13.6	30.1	_	_	54.2	76.7	_	_	145	_
Sodium <i>p</i> -cymenesuiionale	23 С 60 [°] С	11.0	25.9	43.		61.6	70.6	_	_	119.4	_
											100
Sodium toluenesulfonate	25 [°] C		-	8.6		54.1	>400		-	-	>400
		4.13	-	8.6	62	61.8	365	-	-	-	>400
Sodium xylenesulfonate	25 [°] C		-	17	.3	131	>400	-	-	-	>400
	60 ⁰ C	5.03	-	20	.2	127	>400	-	-	-	>400
Sodium <i>o</i> -xylenesulfonate			-	17	• 5	-	210	-	-	-	-
	60 ⁰ С	4.57	-	15	.9	-	200	- (conti	- Lnued no	- ext page	- 2)
		4	UXILIA	RY	INFO	RMATIO	N				
METHOD / APPARATUS / PROCEDUR	E ·							ΟΕ ΜΑΤ	FRIALS		
A known volume of solven	t (usu			;	SOURCE AND PURITY OF MATERIALS: (1) "CP or highest grate commercial"						
in a tightly stoppered v atted. Successive meas					(2) dist	illed.				
solute were added and eq	uilibr	ated u	ntil a			3.4		metost	Unondo	tto Chor	nicola
slight excess of solute the previous study (ref			Unlike ures		50			ichigan		tte Chem	licars
were not centrifuged, bu rotation of the solubili	t sepa	rated	by gen		Sodium <i>p</i> -xylenesulfonate: prepared from						
were immersed in the the	rmosta	t bath	n, in	.y	30						n Kodak)
order to maintain the sa temperature. The volum	mples e of e	at cor xcess	nstant solute		ļ						
was measured directly.											
				ESTIMATED ERROR:							
					No	t state	ed.				
					REF	ERENCE	S:				
								Everso	n, H.E.		
								em. <u>194</u>		1491.	

COMPONENTS: (1) Cyclohexanol; C ₆ H ₁₂ O; [108-93-0] (2) Water; H ₂ O; [7732-18-5]				Boot Ind.	h, H.S.	Chem. <u>19</u>	son, H.H		B; <u>195(</u>	<u>)</u> ,
EXPERIMENTAL VALUES (cont	inued)			lubilit various	•••	• •				
		5.0	8.0	10.0	15.0	20.0	22.0	25.0	34.6	40.0
Sodium <i>m</i> -xylenesulfonate				19.5 17.8	-	196 197	-	- -	-	>400 >400
Sodium p-xylenesulfonate				19.0 17.0		-	-	-	-	- -

COMPONENTS:	ORIGINAL MEASUREMENTS:
 (1) Cyclohexanol; C₆H₁₂O; [108-93-0] (2) Water; H₂O; [7732-18-5] 	Hansen, R.S.,; Fu, Y.; Bartell, F.E. J. Phys. Chem. <u>1949</u> , 53, 769-85.
VARIABLES:	PREPARED BY:
One temperature: 25 [°] C	A. Maczynski and Z. Maczynska
EXPERIMENTAL VALUES:	
The solubility of cyclohexanol in water at 2	$^{\circ}$ C was reported to be 3.92 g(1)/100g sln.
The corresponding mole fraction, x_1 , calculat	ed by the compilers is 7.28 x 10 ⁻³ .
AUXILIARY	INFORMATION
METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS;
The interferometer method was used. An excess of (1) was added to (2) in a mercury-sealed flask which was shaken mechanically for 48 h in an air chamber thermostatted at $25.0 \pm 1^{\circ}$. The flask was then allowed to stand for 3 h in an air bath, after which a portion of the water- rich phase was removed by means of a hypodermic syringe and compared inter- ferometrically with the most concentrated solution of (2) that could be prepared.	 (1) source not specified; reagent grade; distilled and redistilled; b.p. 158°C (730 mm Hg). (2) distilled from alkaline permanganate solution. ESTIMATED ERROR: Temperature: ± 0.1°C Solubility: ± 0.01 wt % (mean from three determinations) REFERENCES:

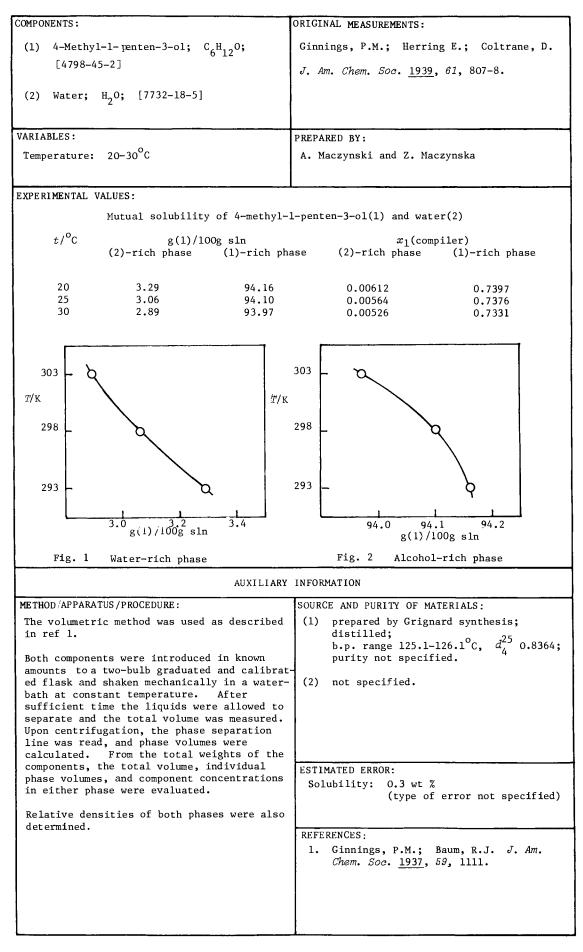
COMPONENTS:	ORIGINAL MEASUREMENTS:		
(1) Cyclohexanol; $C_{6}H_{12}^{0}$ [108-93-0]	Zil'berman, E.N.		
(2) Water, H ₂ 0; [7732-18-5]	Zh. Fiz. Khim. <u>1951</u> , 24, 776–8.		
(2) water, ¹² 0, [7752 10 5]			
VARIABLES:	PREPARED BY:		
Temperature: 0-184 [°] C	A. Maczynski and Z. Maczynska		
Temperature. 0-164 C	A. Maczynski and Z. Maczynska		
EXPERIMENTAL VALUES:			
t/ ⁰ C g(1)/100g sln	x ₁ (compiler)		
	0.01006 0.6147		
10 4.57 89.47	0.00853 0.6041		
	0.00744 0.5909		
	0.00667 0.5754 0.00616 0.5634		
	0.00580 0.5486		
54 3.1 -	0.00572 -		
60 - 86.42 62 3.1 -	- 0.5336		
02 511	0.00572 – 0.00589 0.5175		
	0.00631 0.5014		
90 3.65 83.93	0.00677 0.4843		
	0.00730 0.4668		
	0.00796 0.449 0.00879 0.429		
	0.00879 0.429 0.00996 0.408		
	0.0115 0.368		
150 7.2 74.7	0.0137 0.347		
	0.0171 0.301		
	0.0228 0.241 0.0375 0.165		
1	0.0844 0.0844		
UCST is 184 ⁰ C at 33.9 wt % of cyclohexanol			
ocsi is 164 c at 55.7 wt % of cyclonexanor			
	INFORMATION		
ME THOD / AP PARATUS / PROCEDURE :	SOURCE AND PURITY OF MATERIALS:		
Alekseev's synthetic method (ref 1) was used.			
The procedure involved heating and cooling	twice distilled; m.p. 24.95°C,		
weighed amounts of (1) and (2) in a sealed	d_{4}^{25} 0.9437, n_{T}^{25} 1.4669;		
tube, 10 mm across and 80 mm long, kept in			
an oil bath. Turbidity disappearance and	0.02% of phenol impurity.		
reappearance temperatures were recorded, and the mean was adopted as the solubility	(2) not specified.		
temperature.			
	ESTIMATED ERROR:		
	Temperature: $> 100^{\circ}C \pm 0.5^{\circ}C$		
	$< 100^{\circ}C \pm 1^{\circ}C$		
	< 100 C ± 1 C		
	REFERENCES :		
	1. Anosov, V. Ya.; Pogodin, S.A.		
	Osnovyne nachala fizykokhimicheskogo		
	analiza, Izd. AN.SSSR, ML. <u>1947</u> , 122.		

COMPONENTS -	
COMPONENTS :	ORIGINAL MEASUREMENTS:
(1) Cyclohexanol; C ₆ H ₁₂ O; [108-93-0]	Skrzec, A.E.; Murphy, N.F.
	Ind. Eng. Chem. <u>1954</u> , 46, 2245-7.
(2) Water; H ₂ 0; [7732-18-5]	
VARIABLES:	PREPARED BY:
One temperature: 27 [°] C	A. Maczynski
one temperature. 27 C	A. Haczynski
EXPERIMENTAL VALUES:	
	6.7° C was reported to be 3.60 g (1)/100g sln.
The corresponding mole fraction $x_1^{}$, calculat	ed by the compiler is 6.67×10^{-3} .
The solubility of water in cyclohexanol at 2	6.7° C was reported to be 14.00 g(2)/100g sln.
The corresponding mole fraction, x_2 , calcula	ted by the compiler is 0.4752.
	INFORMATION
METHOD / APPARATUS / PROCEDURE :	SOURCE AND PURITY OF MATERIALS:
Probably the titration method was used. This method was described for the determin-	(1) E.I. du Pont de Nemours and Co., Inc.,;
ation of mutual solubilities in ternary	purified; 100% as alcohol.
systems but nothing is reported on the binary system determinations.	(2) not specified.
Sinary system determinations.	(2) not specified.
	ESTIMATED ERROR:
	Temperature: $\pm 0.5^{\circ}$ C
	REFERENCES:
	I

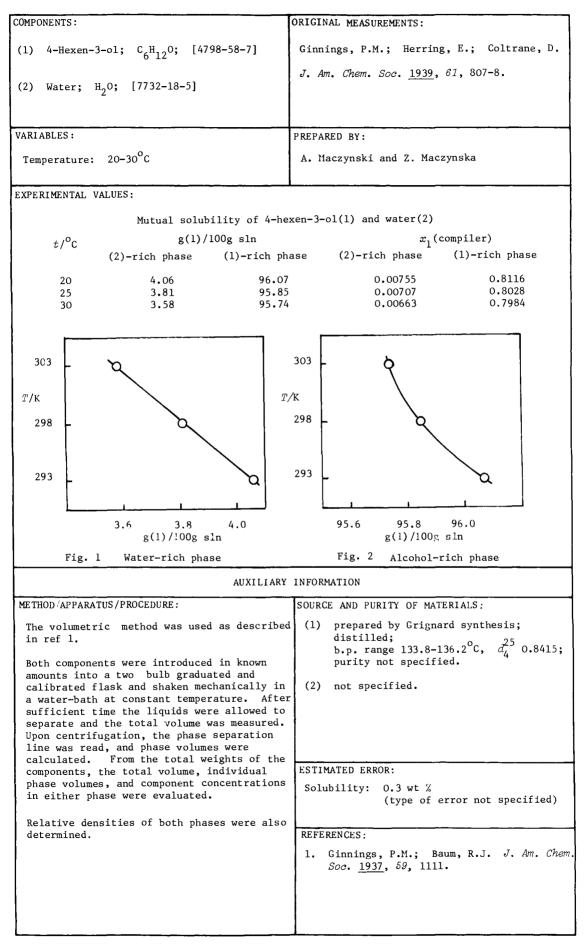
Cyclohe	exanol 2
COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Cyclohexanol; C ₆ H ₁₂ O; [108-93-0]	Tettamanti, K.; Nogradi, M; Sawinsky, J.
(2) Water; H ₂ O; [7732-18-5]	Periodica Politechnica, <u>1960</u> , 4, 201-18.
VARIABLES:	PREPARED BY:
One temperature: 20 [°] C	A. Maczynski
EXPERIMENTAL VALUES:	La manana ay amin'ny ami
The solubility of cyclohexanol in water at 2	0° C was reported to be 5.61 g(1)/100g sln.
The corresponding mole fraction x_1^{1} , calculat	ed by the compiler is 0.0106.
The solubility of water in cyclohexanol at 2	0° C was reported to be 5.3 g(2)/100g sln.
The corresponding mole fraction, $x_2^{}$, calcula	ted by the compiler is 0.24.
AUXILIARY	INFORMATION
ME THOD /APPARATUS / PROCEDURE :	SOURCE AND PURITY OF MATERIALS:
The titration method was used.	(1) not specified.
Into well-stoppered flasks one component was weighed to an accuracy of 0.01 g. Its temperature was adjusted to, and kept constant at $20.0 + 0.1^{\circ}$ C in a thermostat, then titrated with second component from a	(2) not specified.

AUXILIARY INFORMATION				
METHOD / APPARATUS / PROCEDURE :	SOURCE AND PURITY OF MATERIALS:			
The titration method was used.	(1) not specified.			
Into well-stoppered flasks one component was weighed to an accuracy of 0.01 g. Its temperature was adjusted to, and kept constant at $20.0 + 0.1^{\circ}$ C in a thermostat, then titrated with second component from a micro-buret till the appearance of turbidity.	(2) not specified.			
	ESTIMATED ERROR:			
	Not specified.			
	REFERENCES:			

COMPONENTS:	ORIGINAL MEASUREMENTS:			
(1) Cyclohexanol; C ₆ H ₁₂ 0; [108-93-0]	Lavrova, O.A.; Lesteva, T.M.			
(2) Water; H ₂ O; [7732-18-5]	Zh. Fiz. Khim., <u>1976</u> , 50, 1617; Dep. Doc. VINITI, 3813-75.			
VARIABLES:	PREPARED BY:			
Temperature: 40 and 60 ⁰ C	A. Maczynski			
EXPERIMENTAL VALUES:				
Mutual solubility of cyc	lohexanol (1) and water (2)			
$t/^{o}$ C g(1)/100g sln	x_1 (compiler)			
1	ase (2)-rich phase (1)-rich phase			
40 3.33 87.79	0.00616 0.5639			
60 3.11 86.48	0.00574 0.5349			
	INFORMATION			
METHOD/APPARATUS/PROCEDURE: The titration method was used. No details were reported in the paper.	<pre>SOURCE AND PURITY OF MATERIALS: (1) source not specified; distilled with heptane; purity 99.93 wt % with 0.07 wt % of water, b.p. 161.3°C.</pre>			
	(2) not specified.			
	ESTIMATED ERROR: Not specified.			
	REFERENCES :			

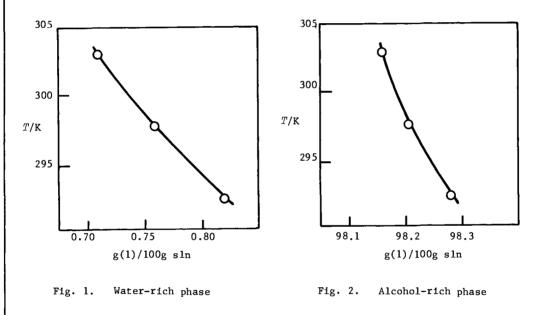


COMPONENTS: ORIGINAL MEASUREMENTS: Ginnings, P.M.; Herring, E.; Coltrane, D. (1) 1-Hexen-3-o1; $C_6H_{12}O;$ [4798-44-1] J. Am. Chem. Soc. <u>1939</u>, 61, 807-8. (2) Water; H₂O; [7732-18-5] VARIABLES: PREPARED BY: Temperature: 20-30°C A. Maczynski and Z. Maczynska EXPERIMENTAL VALUES: Mutual solubility of 1-hexen-3-ol(1) and water(2) x_1 (compiler) $t/^{\circ}C$ g(1)/100g sln (1)-rich phase (2)-rich phase (1)-rich phase (2)-rich phase 94.12 0.00500 20 2.72 0.7383 2.52 93.92 0.00463 0.7314 25 93.90 0.00432 0.7307 30 2.36 303 303 298 298 T/KT/K293 293 2.3 2.5 2.7 g(i)/100g sln² 93.8 94.0 94.2 g(1)100g sln Fig. 2. Alcohol-rich phase Fig. 1. Water-rich phase AUXILIARY INFORMATION METHOD / APPARATUS / PROCEDURE : SOURCE AND PURITY OF MATERIALS: (1) prepared by Grignard synthesis; The volumetric method was used as described distilled; in ref 1. b.p. range 133.5-134.0°C d_{4}^{25} 0.8318; purity not specified. Both components were introduced in known amounts into a two-bulb graduated and calibrated flask and shaken mechanically in (2) not specified. a water-bath at constant temperature. After sufficient time the liquids were allowed to separate and the total volume was measured. Upon centrifugation, the phase separation line was read, and phase volumes were calcualted. From the total ESTIMATED ERROR: weights of the components, the total volume, individual phase volumes, and component Solubility: 0.3 wt % concentrations in either phase were (type of error not specified) evaluated. Relative densities of both phases were also **REFERENCES**: determined. 1. Ginnings, P.M.; Baum, R.J. J. Am. Chem. Soc. 1937, 59, 1111.



COMPONENTS:	EVALUATOR:
(1) 2,2-Dimethyl-l-butanol	Z. Maczynska, Institute of Physical
(tert-pentylcarbinol); C ₆ H ₁₄ 0;	Chemistry of the Polish Academy of Sciences,
[1185-33-7]	Warsaw, Poland; and A.F.M. Harton, Murdoch
	University, Perth, Western Australia.
(2) Water; H ₂ 0; [7732-18-5]	November 1982

Solubilities in the system comprising 2,2-dimethyl-1-butanol (1) and water (2) have been reported in only two publications. Ginnings and Webb (ref 1) carried out measurements of the mutual solubilities of the two components at 293, 298 and 303 K by the volumetric method (Figures 1 and 2). Ratouis and Dode (ref 2) determined the solubility of (1) in the water-rich phase at 298 and 303 K by an analytical method, obtaining values 50% higher than ref 1. The values below, based on ref 1, are therefore tentative.



Tentative values for the mutual solubilities of 2,2-dimethyl-1-butanol (1) and water (2).

T/K	Water-rich p	Alcohol-rich	phase	
	g(1)/100g sln	$10^{3}x_{1}$	g(2)/100g sln	<i>x</i> 2
293	0.8	1.5	1.7	0.190
298	0.8	1.4	1.8	0.194
303	0.7	1.3	1.8	0.196

References

1. Ginnings, P.M.; Webb, R. J. Am. Chem. Soc. 1938, 60, 1388.

2. Ratouis, M.; Dode, M. Bull. Soc. Chim. Fr. 1965, 3318.

COMPONENTS:			ORIGINAL MEASUREMENTS:		
(1) 2,2-Dimethyl-1-butanol (tert-			Ginnings, P.M.; Webb,	R.	
pentylcarbinol); C ₆ H ₁₄ 0; [1185-33-7]			J. Am. Chem. Soc. <u>1938</u> , 60, 1388–9.		
(2) Water; H	H ₂ 0; [7732-18-5]				
VARIABLES:					
Temperature:	10. 20 ⁰ C		PREPARED BY: A. Maczynski and Z. Ma	czynska	
Temperature:	20-30 C		K. Maczyliski and 2. Ha		
EXPERIMENTAL V	ALUES:				
	Mutual solubility	of 2,2-dimeth	yl-l-butanol(l) and wat	er(2)	
t/°c	g(1)/100)g sln	$x_1(com$	piler)	
., .	-		se (2)-rich phase	(1)-rich phase	
20	0.82	98.28	0.00146	0.9097	
25	0.76	98.21	0.00135	0.9063	
30	0.71	98.16	0.00126	0.9039	
		Relative	density d_{μ}		
		heidelive	4		
	t/ ^o c W	ater-rich pha	se Alcohol-rich phas	e	
	20	0.9971	0.8598		
	25	0 .99 63	0.8551		
	30	0 .99 51	0.8511		
	<u> </u>	AUXILIARY	INFORMATION		
METHOD/APPARAT	TUS / PROCEDURE :		SOURCE AND PURITY OF M	ATERIALS:	
in ref 1.	ic method was used		(1) prepared by Grign distilled from ca b.p. range 136.9-	alcium_oxide;	
Both componer amounts into	nts were introduced a two-bulb graduat	in known ed and	$d_4^{25} \text{ 0.8498;}$ purity not specified	fied	
calibrated fl	lask and shaken mec at constant temper	hanically in		1160.	
After suffici	ient time the liqui	ds were	(2) not specified.		
was measured.	Upon centrifuga	tion, the			
phase separation line was read, and phase volumes were calculated. From the total weights of the components, the total volume, individual phase volumes, and component concentrations in either phase were evaluated.		ESTIMATED ERROR:			
		Temperature: ± 0.1°C Solubility: better	than 0.1 wt % f error not specified)		
			REFERENCES :		
			1. Ginnings, P.M.; Soc. <u>1937</u> , 59, 11	Baum, R.J. <i>J. Am. Cher</i> 11.	

COMPONENTS:	ORIG	NAL MEASUREMENTS:
 (1) 2,2-Dimethy1-l-butanol; 		uis, M.; Dode, M.;
(tert-pentylcarbinol); C ₆ H ₁₄ 0;		, Soc. Chim. Fr. 1965, 3318-22.
[1185-33-7]	2	·
(2) Water, Ψ (), [7722, 19, 5]		
(2) Water; H ₂ 0; [7732-18-5]		
VARIABLES:	PREP	ARED BY:
Temperature: 25-30 [°] C	S.C.	Valvani; S.H. Yalkowsky; A.F.M. Barton
Ringer solution also studied		
EXPERIMENTAL VALUES:		
Propo	rtion of 2,2-dim	ethyl-l-butanol (l) in water-rich phase
t/ [°] C	g(1)/100g sln	x_1 (compilers)
25	1.235	0.00220
30	1.17	0.00208
		0.00200
	AUXILIARY INFO	RMATION
METHOD ['] APPARATUS / PROCEDURE :		RMATION CE AND PURITY OF MATERIALS:
METHOD APPARATUS/PROCEDURE: In a round bottomed flask, 50 mL and a sufficient quantity of alcoh introduced until two separate laye	of water (1) ol were	CE AND PURITY OF MATERIALS: laboratory preparation; redistilled with 10:1 reflux ratio;
In a round bottomed flask, 50 mL and a sufficient quantity of alcoh introduced until two separate laye formed. The flask assembly was e	of water (1) ol were rs were quilibrated	CE AND PURITY OF MATERIALS: laboratory preparation; redistilled with 10:1 reflux ratio; b.p. 136.5-136.7 ⁰ C/770 mm Hg
In a round bottomed flask, 50 mL and a sufficient quantity of alcoh introduced until two separate laye formed. The flask assembly was e by agitation for at least 3 h in a temperature bath. Equilibrium so	of water (1) ol were rs were quilibrated constant lubility	CE AND PURITY OF MATERIALS: laboratory preparation; redistilled with 10:1 reflux ratio;
In a round bottomed flask, 50 mL and a sufficient quantity of alcoh introduced until two separate laye formed. The flask assembly was e by agitation for at least 3 h in a temperature bath. Equilibrium so was attained by first supersaturat slightly lower temperature (solubi alcohols in water decrease with in temperature) and then equilibratin	of water (1) ol were rs were quilibrated constant lubility ing at a (2) lity of creasing g at the	CE AND PURITY OF MATERIALS: laboratory preparation; redistilled with 10:1 reflux ratio; b.p. 136.5-136.7 ⁰ C/770 mm Hg
In a round bottomed flask, 50 mL and a sufficient quantity of alcoh introduced until two separate laye formed. The flask assembly was e by agitation for at least 3 h in a temperature bath. Equilibrium so was attained by first supersaturat slightly lower temperature (solubi alcohols in water decrease with in temperature) and then equilibratin desired temperature. The aqueous separated after an overnight stora	of water (1) ol were rs were quilibrated constant lubility ing at a (2) lity of creasing g at the layer was ge in a	CE AND PURITY OF MATERIALS: laboratory preparation; redistilled with 10:1 reflux ratio; b.p. 136.5-136.7°C/770 mm Hg $n_D^{25} = 1.41894$ twice distilled from silica apparatus or ion-exchanged with Sagei A20
In a round bottomed flask, 50 mL and a sufficient quantity of alcoh introduced until two separate laye formed. The flask assembly was e by agitation for at least 3 h in a temperature bath. Equilibrium so was attained by first supersaturat slightly lower temperature (solubi alcohols in water decrease with in temperature) and then equilibratin desired temperature. The aqueous separated after an overnight stora bath. The alcohol content was de reacting the aqueous solution with	of water (1) ol were rs were quilibrated constant lubility ing at a (2) lity of creasing g at the layer was ge in a termined by potassium So	CE AND PURITY OF MATERIALS: laboratory preparation; redistilled with 10:1 reflux ratio; b.p. 136.5-136.7°C/770 mm Hg $n_{\rm D}^{25} = 1.41894$ twice distilled from silica apparatus
In a round bottomed flask, 50 mL and a sufficient quantity of alcoh introduced until two separate laye formed. The flask assembly was e by agitation for at least 3 h in a temperature bath. Equilibrium so was attained by first supersaturat slightly lower temperature (solubi alcohols in water decrease with in temperature) and then equilibratin desired temperature. The aqueous separated after an overnight stora bath. The alcohol content was de reacting the aqueous solution with dichromate and titrating the exces	of water (1) ol were rs were quilibrated constant lubility ing at a (2) lity of creasing g at the layer was ge in a termined by potassium s	CE AND PURITY OF MATERIALS: laboratory preparation; redistilled with 10:1 reflux ratio; b.p. 136.5-136.7°C/770 mm Hg $n_D^{25} = 1.41894$ twice distilled from silica apparatus or ion-exchanged with Sagei A20 MATED ERROR: hubility: relative error of 2 determina- ons less than 1%.
In a round bottomed flask, 50 mL and a sufficient quantity of alcoh introduced until two separate laye formed. The flask assembly was e by agitation for at least 3 h in a temperature bath. Equilibrium so was attained by first supersaturat slightly lower temperature (solubi alcohols in water decrease with in temperature) and then equilibratin desired temperature. The aqueous separated after an overnight stora bath. The alcohol content was de reacting the aqueous solution with dichromate and titrating the exces dichromate with ferrous sulfate so the presence of phosphoric acid an	of water (1) ol were rs were quilibrated constant lubility ing at a (2) lity of creasing g at the layer was ge in a termined by potassium s lution in d	CE AND PURITY OF MATERIALS: laboratory preparation; redistilled with 10:1 reflux ratio; b.p. 136.5-136.7°C/770 mm Hg $n_D^{25} = 1.41894$ twice distilled from silica apparatus or ion-exchanged with Sagei A20 MATED ERROR: hubility: relative error of 2 determina-
In a round bottomed flask, 50 mL and a sufficient quantity of alcoh introduced until two separate laye formed. The flask assembly was e by agitation for at least 3 h in a temperature bath. Equilibrium so was attained by first supersaturat slightly lower temperature (solubi alcohols in water decrease with in temperature) and then equilibratin desired temperature. The aqueous separated after an overnight stora bath. The alcohol content was de reacting the aqueous solution with dichromate and titrating the exces dichromate with ferrous sulfate so the presence of phosphoric acid an diphenylamine barium sulfonate as	of water (1) ol were rs were quilibrated constant lubility ing at a (2) lity of creasing g at the layer was ge in a termined by potassium s lution in d	CE AND PURITY OF MATERIALS: laboratory preparation; redistilled with 10:1 reflux ratio; b.p. 136.5-136.7°C/770 mm Hg $n_D^{25} = 1.41894$ twice distilled from silica apparatus or ion-exchanged with Sagei A20 MATED ERROR: hubility: relative error of 2 determina- ons less than 1%.
In a round bottomed flask, 50 mL and a sufficient quantity of alcoh introduced until two separate laye formed. The flask assembly was e by agitation for at least 3 h in a temperature bath. Equilibrium so was attained by first supersaturat slightly lower temperature (solubi alcohols in water decrease with in temperature) and then equilibratin desired temperature. The aqueous separated after an overnight stora bath. The alcohol content was de reacting the aqueous solution with dichromate and titrating the exces dichromate with ferrous sulfate so	of water (1) ol were rs were quilibrated constant lubility ing at a (2) lity of creasing g at the layer was ge in a termined by potassium s lution in d	CE AND PURITY OF MATERIALS: laboratory preparation; redistilled with 10:1 reflux ratio; b.p. 136.5-136.7°C/770 mm Hg $n_D^{25} = 1.41894$ twice distilled from silica apparatus or ion-exchanged with Sagei A20 MATED ERROR: lubility: relative error of 2 determina- ons less than 1%. mperature: $\pm 0.05°C$
In a round bottomed flask, 50 mL and a sufficient quantity of alcoh introduced until two separate laye formed. The flask assembly was e by agitation for at least 3 h in a temperature bath. Equilibrium so was attained by first supersaturat slightly lower temperature (solubi alcohols in water decrease with in temperature) and then equilibratin desired temperature. The aqueous separated after an overnight stora bath. The alcohol content was de reacting the aqueous solution with dichromate and titrating the exces dichromate with ferrous sulfate so the presence of phosphoric acid an diphenylamine barium sulfonate as	of water (1) ol were rs were quilibrated constant lubility ing at a (2) lity of creasing g at the layer was ge in a termined by potassium s lution in d	CE AND PURITY OF MATERIALS: laboratory preparation; redistilled with 10:1 reflux ratio; b.p. 136.5-136.7°C/770 mm Hg $n_D^{25} = 1.41894$ twice distilled from silica apparatus or ion-exchanged with Sagei A20 MATED ERROR: lubility: relative error of 2 determina- ons less than 1%. mperature: $\pm 0.05°C$
In a round bottomed flask, 50 mL and a sufficient quantity of alcoh introduced until two separate laye formed. The flask assembly was e by agitation for at least 3 h in a temperature bath. Equilibrium so was attained by first supersaturat slightly lower temperature (solubi alcohols in water decrease with in temperature) and then equilibratin desired temperature. The aqueous separated after an overnight stora bath. The alcohol content was de reacting the aqueous solution with dichromate and titrating the exces dichromate with ferrous sulfate so the presence of phosphoric acid an diphenylamine barium sulfonate as	of water (1) ol were rs were quilibrated constant lubility ing at a (2) lity of creasing g at the layer was ge in a termined by potassium s lution in d	CE AND PURITY OF MATERIALS: laboratory preparation; redistilled with 10:1 reflux ratio; b.p. 136.5-136.7°C/770 mm Hg $n_D^{25} = 1.41894$ twice distilled from silica apparatus or ion-exchanged with Sagei A20 MATED ERROR: lubility: relative error of 2 determina- ons less than 1%. mperature: $\pm 0.05°C$
In a round bottomed flask, 50 mL and a sufficient quantity of alcoh introduced until two separate laye formed. The flask assembly was e by agitation for at least 3 h in a temperature bath. Equilibrium so was attained by first supersaturat slightly lower temperature (solubi alcohols in water decrease with in temperature) and then equilibratin desired temperature. The aqueous separated after an overnight stora bath. The alcohol content was de reacting the aqueous solution with dichromate and titrating the exces dichromate with ferrous sulfate so the presence of phosphoric acid an diphenylamine barium sulfonate as	of water (1) ol were rs were quilibrated constant lubility ing at a (2) lity of creasing g at the layer was ge in a termined by potassium s lution in d	CE AND PURITY OF MATERIALS: laboratory preparation; redistilled with 10:1 reflux ratio; b.p. 136.5-136.7°C/770 mm Hg $n_D^{25} = 1.41894$ twice distilled from silica apparatus or ion-exchanged with Sagei A20 MATED ERROR: lubility: relative error of 2 determina- ons less than 1%. mperature: $\pm 0.05°C$

COMPONENTS:	EVALUATOR:
(1) 2,3-Dimethy1-2-butanol	Z. Maczynska, Institute of Physical
(dimethylisopropylcarbinol); C ₆ H ₁₄ 0;	Chemistry of the Polish Academy of Sciences,
[594-60-5]	Warsaw, Poland.
(2) Water; H ₂ 0; [7732-18-5]	November 1982

Solubilities in the system comprising 2,3-dimethyl-2-butanol (1) and water (2) have been reported in only two publications (Figures 1 and 2). Ginnings and Webb (ref 1) carried out measurements of the mutual solubilities of the two components at 293, 298 and 303 K by the volumetric method. Ratouis and Dode (ref 2) determined the solubility of (1) in the water-rich phase at one temperature (303 K) by an analytical method. Their value of 3.47 g(1)/100g sln is in reasonable agreement with the value $3.76 \pm 0.1 \text{ g(1)}/100\text{ g sln}$ at this temperature of ref 1. The data are regarded as tentative, since comparison can be made only at a single temperature and the other five points are derived from a single source.

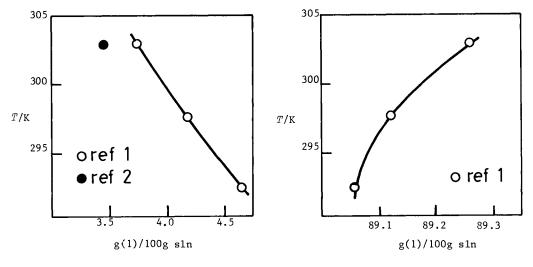


Fig. 1. Water-rich phase

Tentative values for the mutual solubilties of 2,3-dimethyl-2-butanol (1) and water (2)

Fig. 2.

Alcohol-rich phase

T/K	Water-rich phase		Alcohol-rich	phase
	g(1)/100g sln	10 ³ <i>x</i> ₁	g(2)/100g sln	<i>x</i> ₂
293	4.7	8.5	10.9	0.411
298	4.2	7.6	10.9	0.409
303	3.8	6.8	10.7	0.406

References

1. Ginnings, P.M.; Webb, R. J. Am. Chem. Soc. 1938, 60, 1388.

2. Ratouis, M.; Dode, M. Bull. Soc. Chim. Fr. 1965, 3318.

(1) 2,3-Dimethyl-2-butanol (dimethyliaspropyloarbinol); $C_{B}^{+}1_{n}$ O: (3) Water; H_{2} O: (7) O: (7) Water; H_{2} O: (7) Water;	COMPONENTS:			ORIGINAL N	EASUREMENTS:		
[594-60-5] 0.1 Min. Chem. Doi: 1200, 00, 1200 y. (2) Water; H ₂ 0; [7732-18-5] PREPARED BY: XARIABLES: A. Maczynski and Z. Maczynska EXPERIMENTAL VALUES: Mutual solubility of 2,3-dimethyl-2-butanol(1) and water(2) \$t/\$^{O}\$C g(1)/100g sln (2)-rich phase (1)-rich phase (2)-rich phase (1)-rich phase 20 4.65 20 4.65 30 3.76 30 3.76 30 3.76 89.26 0.00684 20 0.9934 Colored 0.5943 Relative density, d ₄ EXTHOMATION AUXILLARY INFORMATION MUTUAL APPROCEDURE: The volumetric method was used as described in ref 1. SOURCE AND FURITY OF MATERIALS: 10 prepared by Grigard synthesis; distilled from calcium oxide; bp. range list.0-118.0°C 22 ³⁵ 0.8118; putrity not specified. AUXILLARY INFORMATION MUXILLARY INFORMATION MUXILLARY INFORMATION MUXILIARY INFORMATION<	(1) 2,3-Dimethy1-2	-butanol		Ginnings, P.M.; Webb, R.			
VARIABLES: Temperature: $20-30^{\circ}$ C PREPARED BY: A. Maczynski and Z. Maczynska EXPERIMENTAL VALUES: Mutual solubility of 2,3-dimethyl-2-butanol(1) and water(2) $t/^{\circ}$ C g(1)/100g sin $t/^{\circ}$ C g(2)-rich phase 20 4.65 30 3.76 89.26 0.00684 20 0.9934 Relative density, d_4 $t/^{\circ}$ C Water-rich phase 20 0.9934 0.8464 25 0.9929 0.8421 30 0.9910 0.8372 METHOD/APPARATUS/PROCEDURE: The volumetric method was used as described in ref 1. Both components were introduced in known amounts into a two-bulb graduated and camporature. Solubility: Metraduated flast and shat comporature. Moded to separate and the total volumes was seesared.	0 11						
Temperature: $20-30^{\circ}$ CA. Maczynski and Z. MaczynskaEXPERIMENTAL VALUES:Hutual solubility of 2,3-dimethyl-2-butanol(1) and water(2) $t/^{\circ}$ Cg(1)/100g sln $x_1(compiler)$ (2)-rich phase(1)-rich phase(2)-rich phase(1)-rich phase204.6589.060.008520.5893254.1839.120.007630.5908303.7689.260.006840.5943Relative density, d_4 $t/^{\circ}$ CWater-rich phase200.99340.8464250.99290.8421300.99100.8372Source AND PURITY OF MATERIALS:The volumetric method was used as described in ref 1.Source AND PURITY OF MATERIALS:Source AND PURITY OF MATERIALS:The volumetric method was used as described in ref 1.Source AND PURITY OF MATERIALS:Source AND PURITY OF MATERIALS:The volumetric method was used as described in ref 1.Source AND PURITY OF MATERIALS:The volumetric method was used as described in ref 1.Source AND PURITY OF MATERIALS:The volumetric method was used as described in ref 1.Source and the total volume was measured.Source AND PURITY OF MATERIALS:The rolumetric method was used as described in ref 1.Source AND PURITY OF MATERIALS:	(2) Water; H ₂ 0;	[7732-18-5]					
EXPERIMENTAL VALUES: hutual solubility of 2,3-dimethyl-2-butanol(1) and water(2) $t/^{0}C$ g(1)/100g sln $x_{1}(compiler)$ (2)-rich phase (1)-rich phase (2)-rich phase (1)-rich phase 20 4.65 89.06 0.00852 0.5893 25 4.18 99.12 0.00763 0.5908 30 3.76 89.26 0.00684 0.5943 Relative density, d_{4} $t/^{0}C$ Water-rich phase Alcohol-rich phase 20 0.9934 0.8464 25 0.9929 0.8421 30 0.9910 0.8372 METHOD/APPARATUS/PROCEDURE: The volumetric method was used as described in ref 1. Both components were introduced in known amounts into a two-bulb graduated and calibrated flask and shaken mechanically in a water-bath at constant temperature. Alter sufficient time the liquide were allowed to separate and the total volume vas measured. Upon centifugation, the phase separation line was read, and phase volumes were calculated. From the total volume vas measured. Upon centifugation, the phase separation line was read, and phase volumes in either phase were evaluated. ESTIMATED ERROR: Temperature: $t \circ .0.1^{\circ}C$ solubility: better than 0.1 wt χ (type of error not specified) REFERENCES: 1. Ginnings, P.M.; Baum, R.J. J. Am.				PREPARED	BY:		
Mutual solubility of 2,3-dimethyl-2-butanol(1) and water(2) $t/^{0}$ Cg(1)/100g sln $x_{1}(compiler)$ (2)-rich phase(1)-rich phase(2)-rich phase204.6589.060.008520.5893254.1839.120.007630.5908303.7689.260.006840.5943Relative density, d_{4} $t/^{0}$ CWater-rich phase200.99340.8464250.99290.8421300.99100.8372AUXILIARY INFORMATIONMETHOD/APPARATUS/PROCEDURE:The volumetric method was used as described in ref 1.Both components were introduced in known amounts into a two-bub graduated and calibrated flask and shaken mechanically in a water-bat at constant temperature; and that sufficient time the liquids were allowed to separate and the total volume was measured. Upon centifugation, the phase separation line was read, and phase volumes were calculated. Prom te total weights of the component sufficient time the liquids were allowed to separate and the total volume was measured.SOURCE AND PURITY OF MATERIALS: SOURCE AND PURITY OF mage 118.0-0118.8°C d_{2}^{25} 0.8118; purity not specified.(2) not specified.(2) not specified.(2) not specified.SOURCE RENOR: Temperature: ± 0.1°C Solubility: better than 0.1 wt Z (type of error not specified)REFERENCES: 1. Ginnings, P.M.; Baum, R.J. J. Am.	Temperature: 20-30	°c		A. Maczyn	nski and Z. Ma	aczynska	
$t/^{\circ}C \qquad g(1)/100g sln \qquad x_1(compiler) \\ (2)-rich phase (1)-rich phase (2)-rich phase (1)-rich phase \\ 20 4.65 89.06 0.00852 0.5893 \\ 25 4.18 39.12 0.00763 0.5908 \\ 30 3.76 89.26 0.00684 0.5943 \\ Relative density, d_4 \\ t/^{\circ}C \qquad Water-rich phase Alcohol-rich phase \\ 20 0.9934 0.8464 \\ 25 0.9929 0.8421 \\ 30 0.9910 0.8372 \\ \hline$ METHOD/APPARATUS/PROCEDURE: The volumetric method was used as described in ref 1. \\ Both components were introduced in known amounts into a two-hulp graduated and calibrated flask and shaken mechanically in a water-bath at constant temperature. After sufficient time the Hquids were allowed to separate and the total volume was measured. Upon centrifugation, the phase separation line was tread, and phase volumes were calculated. From the total volume was measured. Upon centrifugation, the phase separation line was tread, and phase volumes were evaluated. (2) not specified. \\ ESTIMATED ERROR: Temperature: $\pm 0.1^{\circ}C$ solubility: better than 0.1 wt χ (type of error not specified) REFERENCES: 1. Ginnings, P.M.; Baum, R.J. J. Am.	EXPERIMENTAL VALUES:	·····					
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25 4.18 89.12 0.00763 0.5908 30 3.76 89.26 0.00684 0.5943 Relative density, d_4 $t/^{\circ}C$ Water-rich phase Alcohol-rich phase 20 0.9934 0.8464 25 0.9929 0.8421 30 0.9910 0.8372 METHOD/APPARATUS/PROCEDURE: The volumetric method was used as described in ref 1. Source AND PURITY OF MATERIALS: The volumetric method was used as described in ref 1. Source AND PURITY OF MATERIALS: (1) prepared by Grignard synthesis; distilled from calcium oxide; b.p. range 118.0-118.8°C d_4^{-25} 0.818; purity not specified. (2) not specified. ESTIMATED ERROR: Temperature: $\pm 0.1^{\circ}C$ Solumes, and component concentrations in either phase were evaluated. EFERENCES: 1. Ginnings, P.M.; Baum, R.J. J. Am.	(2) - r	ich phase	(1)-rich pha	ase (2)-rich phase	(1)-rich phase	
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Relative density, d_4 $t/^{\circ}C$ Water-rich phaseAlcohol-rich phase200.99340.8464250.99290.8421300.99100.8372AUXILIARY INFORMATIONMETHOD/APPARATUS/PROCEDURE:The volumetric method was used as described in ref 1.Source AND PURITY OF MATERIALS:(1) prepared by Grignard synthesis; distilled from calcium oxide; b.p. range 118.0-118.8°C d_2^{25} 0.8118; purity not specified.Source AND PURITY OF MATERIALS:(1) prepared by Grignard synthesis; distilled from calcium oxide; b.p. range 118.0-118.8°C d_2^{25} 0.8118; purity not specified.Source and the total volume was measured.Source and phase volumes were calculated. From the total weights of the components, the total volume, individual phase volumes, and component concentrations in either phase were evaluated.ESTIMATED ERROR: Temperature: $\pm 0.1^{\circ}C$ Solubility: better than 0.1 wt $\%$ (type of error not specified)REFERENCES: 1. Ginnings, P.M.; Baum, R.J. J. Am.	25	4.18	89.12		0.00763	0.5908	
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COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) 2,3-Dimethy1-2-butanol;	Ratouis, M.; Dode, M.;
(dimethylisopropylcarbinol) $C_{6}H_{14}^{1}0;$	Bull. Soc. Chim. Fr. 1965, 3318-22.
[594-60-5]	
(2) Water; H ₂ 0; [7732-18-5]	
ARIABLES:	PREPARED BY:
One temperature: 30°C	S.C. Valvani; S.H. Yalkowsky; A.F.M. Barton
Ringer solution also studied	,,
EXPERIMENTAL VALUES:	J
The proportion of 2,3-dimethyl-2-butanol (1) at 30 ⁰ C was reported to be 3.47 g(1)/100g s1	
The corresponding mole fraction solubility, $x_1 = 0.00630$.	calculated by the compiler, is
The proportion of (1) in the water-rich phas at equilibrium at 30° C was reported to be 3.	
AUXILIAR	Y INFORMATION
	Y INFORMATION SOURCE AND PURITY OF MATERIALS:
METHOD / APPARATUS / PROCEDURE :	SOURCE AND PURITY OF MATERIALS:
METHOD/APPARATUS/PROCEDURE: In a round bottomed flask, 50 mL of water and a sufficient quantity of alcohol were	
METHOD/APPARATUS/PROCEDURE: In a round bottomed flask, 50 mL of water and a sufficient quantity of alcohol were introduced until two separate layers were	SOURCE AND PURITY OF MATERIALS: (1) laboratory preparation; redistilled with 10:1 reflux ratio; b.p. 120.6°C/758.2 mm Hg
METHOD/APPARATUS/PROCEDURE: In a round bottomed flask, 50 mL of water and a sufficient quantity of alcohol were introduced until two separate layers were formed. The flask assembly was equilibrat by agitation for at least 3 h in a constant	SOURCE AND PURITY OF MATERIALS: (1) laboratory preparation; redistilled with 10:1 reflux ratio; b.p. 120.6 ^o C/758.2 mm Hg
METHOD/APPARATUS/PROCEDURE: In a round bottomed flask, 50 mL of water and a sufficient quantity of alcohol were introduced until two separate layers were formed. The flask assembly was equilibrat	SOURCE AND PURITY OF MATERIALS: (1) laboratory preparation; redistilled with 10:1 reflux ratio; b.p. 120.6°C/758.2 mm Hg $n_{\rm D}^{25} = 1.40926$
METHOD/APPARATUS/PROCEDURE: In a round bottomed flask, 50 mL of water and a sufficient quantity of alcohol were introduced until two separate layers were formed. The flask assembly was equilibrat by agitation for at least 3 h in a constant temperature bath. Equilibrium solubility was attained by first supersaturating at a slightly lower temperature (solubility of	SOURCE AND PURITY OF MATERIALS: (1) laboratory preparation; redistilled with 10:1 reflux ratio; b.p. $120.6^{\circ}C/758.2 \text{ mm Hg}$ $n_D^{25} = 1.40926$ (2) twice distilled from silica apparatus or ion-exchanged with Sagei A20
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METHOD/APPARATUS/PROCEDURE: In a round bottomed flask, 50 mL of water and a sufficient quantity of alcohol were introduced until two separate layers were formed. The flask assembly was equilibrat by agitation for at least 3 h in a constant temperature bath. Equilibrium solubility was attained by first supersaturating at a slightly lower temperature (solubility of alcohols in water decreases with increasing temperature) and then equilibrating at the desired temperature. The aqueous layer	SOURCE AND PURITY OF MATERIALS: (1) laboratory preparation; redistilled with 10:1 reflux ratio; b.p. $120.6^{\circ}C/758.2 \text{ mm Hg}$ $n_D^{25} = 1.40926$ (2) twice distilled from silica apparatus or ion-exchanged with Sagei A20
METHOD/APPARATUS/PROCEDURE: In a round bottomed flask, 50 mL of water and a sufficient quantity of alcohol were introduced until two separate layers were formed. The flask assembly was equilibrat by agitation for at least 3 h in a constant temperature bath. Equilibrium solubility was attained by first supersaturating at a slightly lower temperature (solubility of alcohols in water decreases with increasing temperature) and then equilibrating at the desired temperature. The aqueous layer was separated after an overnight storage in bath. The alcohol content was determined	SOURCE AND PURITY OF MATERIALS: (1) laboratory preparation; redistilled with 10:1 reflux ratio; b.p. 120.6°C/758.2 mm Hg $n_D^{25} = 1.40926$ (2) twice distilled from silica apparatus or ion-exchanged with Sagei A20 a ESTIMATED ERROR:
METHOD/APPARATUS/PROCEDURE: In a round bottomed flask, 50 mL of water and a sufficient quantity of alcohol were introduced until two separate layers were formed. The flask assembly was equilibrat by agitation for at least 3 h in a constant temperature bath. Equilibrium solubility was attained by first supersaturating at a slightly lower temperature (solubility of alcohols in water decreases with increasing temperature) and then equilibrating at the desired temperature. The aqueous layer was separated after an overnight storage in bath. The alcohol content was determined by reacting the aqueous solution with	SOURCE AND PURITY OF MATERIALS: (1) laboratory preparation; redistilled with 10:1 reflux ratio; b.p. 120.6°C/758.2 mm Hg $n_D^{25} = 1.40926$ (2) twice distilled from silica apparatus or ion-exchanged with Sagei A20 a ESTIMATED ERROR: Solubility: relative error of 2 determina-
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METHOD/APPARATUS/PROCEDURE: In a round bottomed flask, 50 mL of water and a sufficient quantity of alcohol were introduced until two separate layers were formed. The flask assembly was equilibrat by agitation for at least 3 h in a constant temperature bath. Equilibrium solubility was attained by first supersaturating at a slightly lower temperature (solubility of alcohols in water decreases with increasing temperature) and then equilibrating at the desired temperature. The aqueous layer was separated after an overnight storage in bath. The alcohol content was determined by reacting the aqueous solution with potassium dichromate and titrating the excess dichromate with ferrous sulfate solution in the presence of phosphoric acid	SOURCE AND PURITY OF MATERIALS: (1) laboratory preparation; redistilled with 10:1 reflux ratio; b.p. 120.6°C/758.2 mm Hg $n_D^{25} = 1.40926$ (2) twice distilled from silica apparatus or ion-exchanged with Sagei A20 (2) twice ERROR: Solubility: relative error of 2 determina- tions less than 1%. Temperature: ± 0.05°C
METHOD/APPARATUS/PROCEDURE: In a round bottomed flask, 50 mL of water and a sufficient quantity of alcohol were introduced until two separate layers were formed. The flask assembly was equilibrat by agitation for at least 3 h in a constant temperature bath. Equilibrium solubility was attained by first supersaturating at a slightly lower temperature (solubility of alcohols in water decreases with increasing temperature) and then equilibrating at the desired temperature. The aqueous layer was separated after an overnight storage in bath. The alcohol content was determined by reacting the aqueous solution with potassium dichromate and titrating the excess dichromate with ferrous sulfate	SOURCE AND PURITY OF MATERIALS: (1) laboratory preparation; redistilled with 10:1 reflux ratio; b.p. $120.6^{\circ}C/758.2$ mm Hg $n_{D}^{25} = 1.40926$ (2) twice distilled from silica apparatus or ion-exchanged with Sagei A20 (2) two error of 2 determina- tions less than 1%. Temperature: $\pm 0.05^{\circ}C$
METHOD/APPARATUS/PROCEDURE: In a round bottomed flask, 50 mL of water and a sufficient quantity of alcohol were introduced until two separate layers were formed. The flask assembly was equilibrat by agitation for at least 3 h in a constant temperature bath. Equilibrium solubility was attained by first supersaturating at a slightly lower temperature (solubility of alcohols in water decreases with increasing temperature) and then equilibrating at the desired temperature. The aqueous layer was separated after an overnight storage in bath. The alcohol content was determined by reacting the aqueous solution with potassium dichromate and titrating the excess dichromate with ferrous sulfate solution in the presence of phosphoric acid and diphenylamine barium sulfonate as an	SOURCE AND PURITY OF MATERIALS: (1) laboratory preparation; redistilled with 10:1 reflux ratio; b.p. 120.6°C/758.2 mm Hg $n_D^{25} = 1.40926$ (2) twice distilled from silica apparatus or ion-exchanged with Sagei A20 (2) twice ERROR: Solubility: relative error of 2 determina- tions less than 1%. Temperature: ± 0.05°C
METHOD/APPARATUS/PROCEDURE: In a round bottomed flask, 50 mL of water and a sufficient quantity of alcohol were introduced until two separate layers were formed. The flask assembly was equilibrat by agitation for at least 3 h in a constant temperature bath. Equilibrium solubility was attained by first supersaturating at a slightly lower temperature (solubility of alcohols in water decreases with increasing temperature) and then equilibrating at the desired temperature. The aqueous layer was separated after an overnight storage in bath. The alcohol content was determined by reacting the aqueous solution with potassium dichromate and titrating the excess dichromate with ferrous sulfate solution in the presence of phosphoric acid and diphenylamine barium sulfonate as an	SOURCE AND PURITY OF MATERIALS: (1) laboratory preparation; redistilled with 10:1 reflux ratio; b.p. 120.6°C/758.2 mm Hg $n_D^{25} = 1.40926$ (2) twice distilled from silica apparatus or ion-exchanged with Sagei A20 (2) twice ERROR: Solubility: relative error of 2 determina- tions less than 1%. Temperature: ± 0.05°C
METHOD/APPARATUS/PROCEDURE: In a round bottomed flask, 50 mL of water and a sufficient quantity of alcohol were introduced until two separate layers were formed. The flask assembly was equilibrat by agitation for at least 3 h in a constant temperature bath. Equilibrium solubility was attained by first supersaturating at a slightly lower temperature (solubility of alcohols in water decreases with increasing temperature) and then equilibrating at the desired temperature. The aqueous layer was separated after an overnight storage in bath. The alcohol content was determined by reacting the aqueous solution with potassium dichromate and titrating the excess dichromate with ferrous sulfate solution in the presence of phosphoric acid and diphenylamine barium sulfonate as an	SOURCE AND PURITY OF MATERIALS: (1) laboratory preparation; redistilled with 10:1 reflux ratio; b.p. 120.6°C/758.2 mm Hg $n_D^{25} = 1.40926$ (2) twice distilled from silica apparatus or ion-exchanged with Sagei A20 (2) twice ERROR: Solubility: relative error of 2 determina- tions less than 1%. Temperature: ± 0.05°C
METHOD/APPARATUS/PROCEDURE: In a round bottomed flask, 50 mL of water and a sufficient quantity of alcohol were introduced until two separate layers were formed. The flask assembly was equilibrat by agitation for at least 3 h in a constant temperature bath. Equilibrium solubility was attained by first supersaturating at a slightly lower temperature (solubility of alcohols in water decreases with increasing temperature) and then equilibrating at the desired temperature. The aqueous layer was separated after an overnight storage in bath. The alcohol content was determined by reacting the aqueous solution with potassium dichromate and titrating the excess dichromate with ferrous sulfate solution in the presence of phosphoric acid and diphenylamine barium sulfonate as an	SOURCE AND PURITY OF MATERIALS: (1) laboratory preparation; redistilled with 10:1 reflux ratio; b.p. 120.6°C/758.2 mm Hg $n_D^{25} = 1.40926$ (2) twice distilled from silica apparatus or ion-exchanged with Sagei A20 (2) twice ERROR: Solubility: relative error of 2 determina- tions less than 1%. Temperature: ± 0.05°C

COMPONENTS:	EVALUATOR:
(1) 3,3-Dimethy1-2-butano1	Z. Maczynska, Institute of Physical
(tert-butylmethylcarbinol); C ₆ H ₁₄ 0; [464-07-3]	Chemistry of the Polish Academy of Sciences, Warsaw, Poland.
(2) Water; H ₂ 0; [7732-18-5]	November 1982

Solubilities in the system comprising 3,3-dimethyl-2-butanol (1) and water (2) have been reported in only two publications. Ginnings and Webb (ref 1) determined the mutual solubilities of the two components at 293, 298 and 303 K by the volumetric method. Ratouis and Dode (ref 2) measured the solubility of (1) in the water-rich phase at one temperature (303 K) by an analytical method. Their value of 1.94 g(1)/100g sln is in reasonable agreement with the value $2.26 \pm 0.1 \text{ g(1)}/100\text{ g sln}$ at this temperature of ref 1. The data are regarded as tentative, since comparison can be made only at a single temperature and the other five points are derived from a single source.

	Tentative values of 3,3-dimethy1-2					
<i>Т</i> /К	T/K Water-rich phase Alcohol-rich phase					
	g(1)/100g sln	10 ³ <i>x</i> ₁	g(2)/100g sln	<i>x</i> 2		
293	2.6	4.8	7.3	0.307		
298	2.4	4.4	7.3	0.308		
303	2.3	4.1	7.3	0.310		

References

- 1. Ginnings, P.M.; Webb, R. J. Am. Chem. Soc. 1938, 60, 1388.
- 2. Ratouis, M.; Dode, M. Bull. Soc. Chim. Fr. 1965, 3318.

COMPONENTS:				ORIGINAL MEASUREMENTS:			
(1) 3,3-Dimethyl-2-butanol (<i>tert</i> -			Ginnings, P.M.; Webb, R.				
methylcarbinol); C ₆ H ₁₄ 0: [464-07-3]			J. Am. Chem. Soc. <u>1938</u> , 60, 1388-9.				
(2) Water; H ₂ 0; [7732-18-5]					-		
_							
VARIABLES: Temperature: 20-30 ⁰ C			PREPARED BY: A. Maczynski and Z. Maczynska				
EXPERIMENTAL VAL	UES:						
М	utual solubility	of 3,3-dimeth	iy1-2-	outanol(l) and wate	er(2)		
$t/^{0}$ C g(1)/100g sln			x_1 (compiler)				
			se (2)-rich phase (1)-rich phase				
20	2.64	92.74		0.00476	0.6925		
25	2.43	92.71		0.00437	0.6915		
30	2.26	92.67		0.00406	0.6902		
50	2020	,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,			0.0702		
	、 、	Relative	densi	zy, d ₄			
$t/^{\circ}$ C Water-rich phase Alcohol-rich phase							
	20	0.9955		0.8356			
	25	0.9946		0.8313			
	30	0.9936		0.8272			
	· · · · · · · · · · · · · · · · · · ·	AUXILIARY	INFOR	MATION	· · · · · · · · · · · · · · · · · · ·		
METHOD/APPARATUS					SOURCE AND PURITY OF MATERIALS:		
	The volumetric method was used as described			(1) prepared by Grignard synthesis;			
in ref 1.				distilled from cal b.p. range 119.9-2	lcium_oxide;		
Both components were introduced in known				d_{1}^{25} 0.8157;			
amounts into a two-bulb graduated and calibrated flask and shaken mechanically in a water-bath at constant tmperature. After sufficient time the liquids were allowed to separate and the total volume was measured. Upon centrifugation, the phase separation line was read, and phase volumes were calculated. From the total weights of the components, the total volume, individual phase volumes, and component concentrations in either phase were evaluated.				purity not specif:	ied.		
			(2)	not specified.			
				ATED ERROR:			
			Temperature: ± 0.1°C Solubility: better than 0.1 wt % (type of error not specified)				
			REFERENCES:				
			 Ginnings, P.M.; Baum, R.J. J. Am. Chem. Soc. <u>1937</u>, 59, 1111. 				
L			1		······································		

COMPONENTS:	ORIGINAL MEASUREMENTS:					
(1) 3,3-Dimethy1-2-butano1	Ratouis, M.; Dode, M.;					
(tert-butylmethylcarbinol); C ₆ H ₁₄ 0;	Bull. Soc. Chim. Fr. 1965, 3318-22.					
[464-07-3]						
(2) Notors II 0: [7722 18 5]						
(2) Water; H ₂ 0; [7732-18-5]						
VARIABLES:	PREPARED BY:					
One temperature: 30°C						
	S.C. Valvani; S.H. Yalkowsky; A.F.M. Barton					
Ringer solution also studied						
EXPERIMENTAL VALUES:						
The proportion of 3,3-dimethyl~2-butanol (1) in the water-rich phase at equilibrium at 30 ⁰ C was reported to be 1.94 g(1)/100g sln. The corresponding mole fraction solubility, calculated by the compilers, is						
$x_1 = 0.00348.$						
The proportion of (1) in the water-rich phase of a mixture with Ringer solution at						
equilibrium at 30° C was reported to be 1.85 g(1)/100g sln.						
AUXILIARY	INFORMATION					
METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:					
In a round bottomed flask, 50 mL of water	(1) Fluka A.G. Buchs S.G.					
and a sufficient quantity of alcohol were	redistilled with 10:1 reflux ratio;					
introduced until two separate layers were formed. The flask assembly was equilibrated	b.p. 121.2°C.					
by agitation for at least 3 h in a constant	$n_{\rm D}^{25} = 1.41330$					
temperature bath. Equilibrium solubility was attained by first supersaturating at a	(2) twice distilled from silica apparatus					
slightly lower temperature (solubility of	or ion-exchanged with Sagei A20.					
alcohols in water decreases with increasing temperature) and then equilibrating at the						
desired temperature. The aqueous layer was						
separated after an overnight storage in a bath. The alcohol content was determined	ESTIMATED ERROR:					
by reacting the aqueous solution with	Solubility: relative error of 2 determina-					
potassium dichromate and titrating the excess dichromate with ferrous sulfate solution in	Solubility: relative error of 2 determina- tions less than 1%.					
the presence of phosphoric acid and	Temperature: ± 0.05 [°] C					
diphenylamine barium sulfonate as an indicator.	REFERENCES:					

COMPONENTS:	EVALUATOR:
(1) 2-Ethy1-1-butanol; C ₆ H ₁₄ 0; [97-95-0]	A. Maczynski, Institute of Physical
(2) Water; H ₂ 0; [7732-18-5]	Chemistry of the Polish Academy of Sciences,
	Poland.
	November 1982

Solubilities in the system comprising 2-ethyl-1-butanol (1) and water (2) have been reported in only two publications. Crittenden and Hixon (ref 1) determined the mutual solubilities of the two components at one temperature (298 K), presumably by the titration method. Ratouis and Dode (ref 2) measured the solubility of (1) in the water-rich phase at 298 and 303 K by an analytical method.

The values for the solubility of (1) in (2) at 298 K are in disagreement (0.4 and 1.0 $g(1)/100g \ sln$, respectively, in ref 1 and 2). As the results in ref 2 refer to two temperatures, and are accompanied by an error estimate, these form the basis of the tentative data below.

Tentative values			
of 2-ethy1-1-but	anol (1)	and wate	r (2).

<i>Т</i> /К	T/K Water-rich phase		Alcohol-rich	phase
	g(1)/100g sln	10 ³ x ₁	g(2)/100g sln	<i>x</i> 2
298	1.0	1.8	5.6	0.25
303	0.9	1.6		

References

- 1. Crittenden, E.D., Jr.; Hixon, A.N. Ind. Eng. Chem. 1954, 46, 265.
- 2. Ratouis, M.; Dode, M. Bull. Soc. Chim. Fr. 1965, 3318.

COMPONENTS :	ORIGINAL MEASUREMENTS:
(1) 2-Ethyl-1-butanol; C ₆ H ₁₄ 0; [97-95-0]	Crittenden, E.D, Jr.; Hixon, A.N.; Ind. Eng. Chem. <u>1954</u> , 46, 265-8.
(2) Water; H ₂ 0; [7732-18-5]	
VARIABLES:	PREPARED BY:
One temperature: 25 ⁰ C	A. Maczynski
EXPERIMENTAL VALUES:	
	at 25° C was reported to be 0.4 g(1)/100 sln.
The corresponding mole fraction, x_1 , calcula	ted by the compiler is 0.0007.
The solubility of water in 2-ethyl-l-butanol	at 25° C was reported to be 5.6 g(2)/100g sln.
The corresponding mole fraction, x_2 , calcula	ted by the compiler is 0.25.
	1 1 1
AUXILIARY	INFORMATION
METHOD / AP PARATUS / PROCEDURE :	SOURCE AND PURITY OF MATERIALS:
Presumably the titration method described for ternary systems containing HCl was used.	<pre>(1) source not specified; purified;</pre>
In this method the solubility was determin-	purity not specified.
ed by bringing 100 mL samples of (1) or (2) to a temperature $25.0 \pm 0.1^{\circ}C$ and the	(2) not specified.
second component was then added from a calibrated buret, with vigorous stirring,	
until the solution became permanently cloudy.	
	ESTIMATED ERROR:
	Solubility: 2% (alcohol-rich) - 10% (water- rich).
	Temperature: ± 0.10°C
	REFERENCES ;

COMPONENTS :	ORIGINAL MEASUREMENTS:
(1) 2-Ethyl-1-butanol; C ₆ H ₁₄ 0; [97-95-0]	Ratouis, M.; Dode, M.;
	Bull. Soc. Chim. Fr. <u>1965</u> , 3318-22.
(2) Water; H ₂ 0; [7732-18-5]	
VARIABLES:	PREPARED BY:
Temperature: 25° C and 30° C	S.C. Valvani; S.H. Yalkowsky; A.F.M. Barton
Ringer solution also studied	5.6. Valvalli, 5.1. laikuwsky, A.F.M. Barton
EXPERIMENTAL VALUES:	
Proportion of 2-et	hy1-l-butanol (l) in water-rich phase
t/ ^o c g(1)/100g s1	n $10^3 x_1$ (compilers)
25 1.00	1.78
30 0.92	1.63
The proportion of (1) in the water-rich phase	
equilibrium at 30 ⁰ C was reported to be 0.90 g	(1)/100g sln.
AUXILIARY	INFORMATION
METHOD / APPARATUS / PROCEDURE :	SOURCE AND PURITY OF MATERIALS:
In a round bottomed flask, 50 mL of water	(1) Fluka A.G., Buchs S.G.
and a sufficient quantity of alcohol were introduced until two separate layers were	redistilled with 10:1 reflux ratio
formed. The flask assembly was equilibrated	b.p. 147 [°] C/763.5 mm Hg
by agitation for at least 3 h in a constant temperature bath. Equilibrium solubility	$n_{\rm D}^{25} = 1.42055$
was attained by first supersaturating at a slightly lower temperature (solubility of	(2) twice distilled from silica apparatus
alcohols in water decreases with increasing	or ion-exchanged with Sagei A20.
temperature) and then equilibrating at the desired temperature. The aqueous layer was	
separated after an overnight storage in a	
bath. The alcohol content was determined by reacting the aqueous solution with	ESTIMATED ERROR:
potassium dichromate and titrating the excess	Solubility: relative error of 2 determina- tions less than 1%.
dichromate with ferrous sulfate solution in the presence of phosphoric acid and	Temperature: $\pm 0.05^{\circ}C$
diphenylamine barium sulfonate as an	*REFERENCES :
indicator.	

COMPONENTS:	EVALUATOR:
(1) 2-Methyl-1-pentanol; C ₆ H ₁₄ 0; [105-30-6]	A. Maczynski, Institute of Physical
(2) Water; H ₂ 0; [7732-18-5]	Chemistry of the Polish Academy of Sciences,
(2) """", "2", """"""""""""""""""""""""""	Warsaw, Poland; and A.F.M. Barton, Murdoch
	University, Perth, Western Australia.
	November 1982

Solubilities in the system comprising 2-methyl-1-pentanol (1) and water (2) have been reported in only two publications. Crittenden and Hixon (ref 1) determined the mutual solubility of the two components at 298 K, presumably by the titration method. Ratouis and Dode (ref 2) used an anlytical method for the solubility of (1) in the water-rich phase at 298 and 303 K. Their value of 0.81 g(1)/100g sln at 298 K is not in agreement with the value of 0.6 g(1)/100g sln reported in ref 1, so it is possible to report only tentative values.

			utual solubilities and water (2)	
Т/К	Water-rich	phase	Alcohol-rich	phase
	g(1)/100g sln	$10^{3}x_{1}$	g(2)/100g sln	<i>x</i> ₂
298	0.81	1.4	5.4	0.24
303	0.76	1.4		

References

1. Crittenden, E.D., Jr.; Hixon, A.N. Ind. Eng. Chem. 1954, 46, 265.

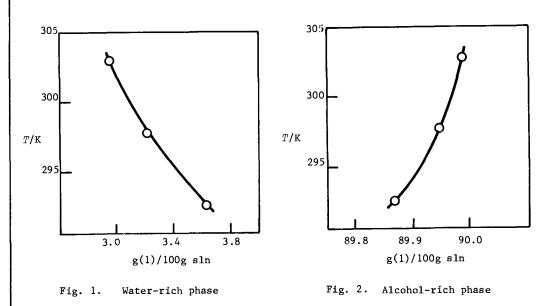
2. Ratouis, M.; Dode, M. Bull. Soc. Chim. Fr. 1965, 3318.

rittenden, E.D., Jr., Hixon, A.N. nd. Eng. Chem. <u>1954</u> , 46, 265-8. REPARED BY: . Maczynski
REPARED BY:
. Maczynski
at 25° C was reported to be 0.6 g(1)/100g
d by the compiler is 0.0011.
at 25 ⁰ C was reported to be 5.4 g(2)/100g
d by the compiler is 0.24.
IFORMATION
OURCE AND PURITY OF MATERIALS:
 source not specified; purified; purity not specified. not specified.
STIMATED ERROR: Solubility: 2% (alcohol-rich) - 10% (water-
1

COMPONENTS:	ORIGINAL MEASUREMENTS:
 2-Methyl-1-pentanol; C₆H₁₄0; 	Ratouis, M.; Dode, M.;
[105-30-6]	Bull. Soc. Chim. Fr. <u>1965</u> , 3318-22.
(2) Water; H ₂ 0; [7732-18-5]	
Δ Δ	
VARIABLES:	PREPARED BY:
Temperature: 25-30°C	S.C. Valvani; S.H. Yalkowsky; A.F.M. Barton
Ringer solution also studied	
EXPERIMENTAL VALUES:	
Proportion of 2	-methyl-l-pentanol (l) in water-rich phase
t/ ^o C g(1)/100g	x_1 (compilers)
25 0.81	0.00144
30 0.76	0.00135
AUXILIAF	Y INFORMATION
METHOD /APPARATUS / PROCEDURE :	SOURCE AND PURITY OF MATERIALS:
In a round bottomed flask, 50 mL of water and a sufficient quantity of alcohol were introduced until two separate layers were formed. The flask assembly was equilibra- ed by agitation for at least 3 h in a con- stant temperature bath. Equilibrium solubility was attained by first supersat- urating at a slightly lower temperature (solubility of alcohols in water decreases with increasing temperature) and then equilibrating at the desired temperature. The aqueous layer was separated after an overnight storage in a bath. The alcohol content was determined by reacting the aqueous solution with potassium dichromate and titrating the excess dichromate with ferrous sulfate solution in the presence of phosphoric acid and diphenylamine barium sulfonate as an indicator.	 (1) Fluka A.G. Buchs S.G. redistilled with 10:1 reflux b.p. 148-148.1°C/760 mm Hg n²⁵_D = 1.41631 (2) twice distilled from silica apparatus or ion-exchanged with Sagei A20 ESTIMATED ERROR: Solubility: relative error of 2 determina- tions less than 1%. Temperature: ± 0.05°C
L	

COMPONENTS:	EVALUATOR:
(1) 2-Methyl-2-pentanol	Z. Maczynska, Institute of Physical
(dimethyl-n-propylcarbinol, tert-hexyl	Chemistry of the Polish Academy of Sciences,
alcohol); C ₆ H ₁₄ 0; [590-36-3]	Warsaw, Poland; and A.F.M. Barton, Murdoch
(2) Water; H ₂ 0; [7732-18-5]	University, Perth, Western Australia.
	November 1982

Solubilities in the system comprising 2-methyl-2-pentanol (1) and water (2) have been reported in three publications. Ginnings and Webb (ref 1) carried out measurements of the mutual solubilities of the two components at 293, 298 and 303 K by the volumetric method (Figures 1 and 2). Addison (ref 2) determined the solubility of (1) in the water-rich phase at one temperature (293 K) by a surface tension method. Ratouis and Dode (ref 3) used an analytical method for (1) in (2), also at one temperature (303 K). The last two reported values are 10% lower than those of ref 1 for the water-rich phase, so the following figures, based on ref 1, must be regarded as tentative only.



Tentative values for the mutual solubilities of 1-methyl-2-pentanol (1) and water (2)

T/K	Water-rich	Jater-rich phase		Alcohol-rich phase	
	g(1)/100g sln	$10^{3}x_{1}$	g(2)/100g sln	<i>x</i> 2	
293	3.6	6.6	10.1	0.390	
298	3.2	5.9	10.0	0.388	
303	2.9	5.3	10.0	0.386	

References

1. Ginnings, P.M.; Webb, R. J. Am. Chem. Soc. 1938, 60, 1388.

2. Addison, C.C. J. Chem. Soc. 1945, 98.

3. Ratouis, M.; Dode, M. Bull. Soc. Chim. Fr. 1965, 3318.

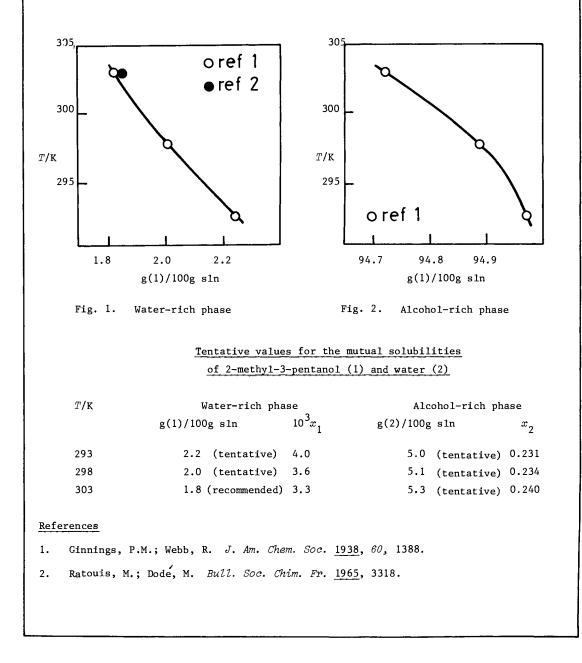
COMPONENTS:			ORIGINA	L MEASUREMENTS:	
(1) 2-Methyl-2-pentanol		Ginning	s, P.M.; Webb, R.		
(dimethyl-n-propylcarbinol, tert-hexyl		J. Am.	Chem. Soc. <u>1938</u> , 60,	1388-9.	
alcohol),	^C 6 ^H 14 ^O ; [590-36-3]				
(2) Water; H ₂ 0	; [7732-18-5]				
VARIABLES:	·····		PREPARE	D BY:	
Temperature:	20–30 [°] C		A. Macz	ynski and Z. Maczynsk	a
EXPERIMENTAL VA	LUES:				<u></u>
Mut	tual solubility of 2-m	ethy1-2-p	entanol	(1) and water (2)	
t∕°c	g(1)/100g	sln		$x_1^{}$ (comp	iler)
	(2)-rich phase	(1)-rich	phase	(2)-rich phase	(1)-rich phase
20	3.63	89.8	7	0.00660	0.6099
25	3.24	89.9		0.00586	0.6120
30	2.96	89.9	9	0.00534	0.6131
	0	elative de		-	
	$t/^{o}$ C Water	-rich pha	se Alc	ohol-rich phase	
	20	0.9935		0.8321	
	25	0.9929		0.8280	
	30	0 .99 21		0.8237	
		AUXILIARY	INFORMA	 FION	
METHOD / APPARATU	JS / PROCEDURE :		SOURCE	AND PURITY OF MATERIA	LS:
	c method was used as d	escribed	(1) E	astman best grade;	
in ref 1.				istilled, and redist alcium oxide	illed from
	ts were introduced in		Ъ	.p. range 122.4-122.6	°c
	a two-bulb graduated a ask and shaken mechani		d	²⁵ 4 0.8053	
	at constant temperatur ent time the liquids w		(2) n	ot specified	
allowed to sep	parate and the total v	olume	(or specifica	
was measured. phase separati	Upon centrifucation lon line was read, and				
volumes were o		total	L		
individual pha	ase volumes, and compo	nent		TED ERROR: ature: ± 0.1 [°] C	
concentrations evaluated.	s in either phase were		Solubi	lity: better than 0.	l wt % (type of
				not specified)	<u> </u>
			REFERE	-	-
				nnings, P.M.; Baum, R	
			J.	Am. Chem. Soc. <u>1937</u> ,	əy, 1111.

COMPONENTS:	ORIGINAL MEASUREMENTS:
<pre>(1) 2-Methyl-2-pentanol, (dimethyl-n- propylcarbinol, tert-hexyl alcohol); C₆H₁₄0; [590-36-3]</pre>	Addison, C.C. J. Chem. Soc. <u>1945</u> , 98-106.
(2) Water; H ₂ 0; [7732-18-5]	
VARIABLES:	PREPARED BY:
One tempertature: 20 [°] C	S.H. Yalkowsky; S.C. Valvani; A.F.M. Barton
EXPERIMENTAL VALUES:	
The proportion of 2-methyl-2-pentanol (1) in at 20 ⁰ C was reported to be 3.23 g(1)/100g sln The corresponding mole fraction solubility ca	
AUXILIARY	INFORMATION
METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
A surface tension method was used. Sufficient excess of (1) was added to 100mL of (2) in a stoppered flask to form a separate lens on the surface. The mixture was swirled gently, too vigorous an agita- tion giving a semi-permanent emulsion and incorrect readings. After settling, a small sample of the clear aqueous solution was withdrawn into a drop weight pipet and the surface tension determined. The swirling was continued until a constant value was obtained. The surface tension-concentra- tion curve was known, and only a slight extrapolation (logarithmic scale) was necessary to find the concentration corresponding to the equilibrium value.	(1) impure alcohols were purified by fractional distillation, the middle fraction from a distillation being redistilled; b.p. 122.0°C d_4^{20} 0.8048

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) 2-Methyl-2-pentanol	Ratouis, M.; Dode, M.;
(dimethyl-n-propylcarbinol, tert-hexyl	Bull. Soc. Chim. Fr. 1965, 3318-22.
alcohol); C ₆ H ₁₄ 0; [590-36-3].	
(2) Water, H_0 [7732-18-5].	
VARIABLES:	PREPARED BY:
One temperature: 30°C	S.C. Valvani; S.H. Yalkowsky; A.F.M. Barton
Ringer solution also studied	
EXPERIMENTAL VALUES:	
The proportion of 2-methyl-2-pentanol (1) in	the water-rich phase at equilibrium
at 30° C was reported to be 2.82 g(1)/100g slr	
	al-vlated by the compilers
The corresponding mole fraction solubility, c	acculated by the compilers,
is $x_1 = 0.00509$.	
The proportion of (1) in the water-rich phase	of a mixture with Ringer solution
at 30° C was reported to be 2.51 g(1)/100g slr	
AUXILIARY	INFORMATION
METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
In a round bottomed flask, 50 mL of water and a sufficient quantity of alochol were	 laboratory preparation; redistilled with 10:1 reflux ratio;
introduced until two separate layers were formed. The flask assembly was equilibrat-	b.p. 121.6-121.8°C/757.8 mm Hg
ed by agitation for at least 3 h in a	$n_{\rm D}^{25} = 1.40888$
constant temperature bath. Equilibrium solubility was attained by first supersat-	(2) twice distilled from silica apparatus
uration at a slightly lower temperature	or ion-exchanged with Sagei A20.
(solubility of alcohols in water decreases with increasing temperature) and then	
equilibrating at the desired temperature.	
Aqueous layer was separated after an over- night storage in a bath. The alcohol	ESTIMATED ERROR:
content was determined by reacting the aqueous solution with potassium dichromate	Solubility: relative error of 2 determina-
and titrating the excess dichromate with	tions less than 1%.
ferrous sulfate solution in the presence of phosphoric acid and diphenylamine	Temperature: ± 0.05°C
barium sulfonate as an indicator.	REFERENCES:
	1

COMPONENTS:	EVALUATOR:
(1) 2-Methyl-3-pentanol	Z. Maczynska, Institute of Physical
(isopropylethylcarbinol); C ₆ H ₁₄ 0;	Chemistry of the Polish Academy of Sciences,
[565-67-3]	Warsaw, Poland; and A.F.M. Barton, Murdoch
(2) Water; H ₂ 0; [7732-18-5]	University, Perth, Western Australia.
(2) water, ² 2°, ² 1752 10 51	November 1982.

Solubilities in the system comprising 2-methyl-3-pentanol (1) and water (2) have been reported in two publications (Figure 1 and 2). Ginnings and Webb (ref 1) carried out measurements of the mutual solubilities of the two components at 293, 298 and 303 K by the volumetric method. Ratouis and Dodé (ref 2) determined the solubility of (1) in the water-rich phase at one temperature (303 K) by an analytical method. Their value of 1.85 g(1)/100g solp at this temperature is in excellent agreement with the value 1.82 ± 0.1 g(1)/100g sln of ref 1. The 303 K value is recommended, but the other five points are derived from a single source and are regarded as tentative.



COMPONENTS	:		ORIGINAL MEA	ASUREMENTS:	
(1) 2-M	(1) 2-Methy1-3-pentano1		Ginnings. P	.M.: Wehh	. R.
(isopropylethylcarbinol); C ₆ H ₁₄ 0; [565-67-3]		Ginnings, P.M.; Webb, R. J. Am. Chem. Soc. <u>1938</u> , 60, 1388-9.			
(2) Wat	er; H ₂ 0; [7732-18-5]				
VARIABLES	:		PREPARED BY	:	
Temperat	cure: 20-30 [°] C		A. Maczynsk	i and Z. Ma	aczynska
EXPERIMENT	TAL VALUES:				
	Mutual solubili	ity of 2-methy1	-3-pentanol((1) and wate	er(2)
t/ ^o c	c g(1)/10	OOg sln		$x_1(\text{compile})$	er)
	(2)-rich phase	(1)-rich phas	e (2)-ric	h phase	(1)-rich phase
20	2.24	94.97	C	.00402	0.7689
25	2.01	94.89	C	.00360	0.7660
30	1.82	94.72	C	.00326	0.7597
		Relative de	nsity d		
		Relative de	¹¹³¹¹ , ¹¹ 4		
	t/ ^o c	Water-rich ph	ase Alco	hol-rich ph	ase
	20	0.9950		0.8323	
	25	0.9941		0.8288	
	30	0.9940		0.8249	
		AUXILIARY	INFORMATION		
ME THOD / AP	PARATUS/PROCEDURE:		SOURCE AND	PURITY OF M	MATERIALS:
The volu in ref 1	umetric method was used 1.	d as described	disti b.p.	11ed from range 126.	gnard synthesis; calcium oxide; 3-127.3°C,
	nponents were introduce into a two-bulb gradua		d_4^{25}	D.8186;	
calibrat	ted flask and shaken me	echanically in	purit	y not spec	ified.
a water-bath at constant temperature. After sufficient time the liquids were allowed to separate and the total volume was measured. Upon centrifugation, the phase separation line was read, and phase volumes were calculated. From the total weights of the components, the total volume, individual phase volumes, and component concentrations in either phase were evaluated.		(2) not s	specified.		
		ESTIMATED F	RROR:	······································	
		Temperatur Solubility	: better	C than 0.1 wt % of error not specified)	
		REFERENCES :		<u> </u>	
			ngs, P.M.; 1937, <i>59</i> , 11	Baum, R.J. J. Am. Chem. 111.	
L		······	1	<u> </u>	· · · · ·

2-Methyl-3-pentanol			
COMPONENTS: ORIGINAL MEASUREMENTS:			
 2-Methyl-3-pentanol <i>(isopropylethylearbinol);</i> C₆H₁₄0; [565-67-3] Water; H₂0; [7732-18-5] 	Ratouis, M.; Dodé, M.; Bull. Soc. Chim. Fr. <u>1965</u> , 3318-22.		
VARIABLES:	PREPARED BY:		
One temperature: 30 ⁰ C Ringer solution also studied	S.C. Valvani; S.H. Yalkowsky; A.F.M. Barton		
EXPERIMENTAL VALUES:	······································		
The proportion of 2-methyl-3-pentanol (1) in was reported to be $1.85 \text{ g}(1)/100 \text{g sln}$.	n the water-rich phase at equilibrium at 30 ⁰ C		
The corresponding mole fraction solubility,	calculated by the compilers, is $x_1 = 0.00331$.		
The proportion of (1) in the water-rich phas was reported to be 1.77 g(1)/100g s1n.	e of a mixture with Ringer solution at 30 ⁰ C		
AUXILIARY	(INFORMATION		
METHOD /APPARATUS / PROCEDURE :	SOURCE AND PURITY OF MATERIALS:		
In a round bottomed flask, 50 mL of water ar a sufficient quantity of alcohol were intro- duced until two separate layers were formed. The flask assembly was equilibrated by agitation for at least 3 h in a constant temperature bath. Equilibrium solubility	redistilled with 10:1 reflux ratio,		

(2) twice distilled from silica apparatus or ion-exchanged with Sagei A20.

bath. The alcohol content was determined by ESTIMATED ERROR: Solubility: relative error of 2 determinapotassium dichromate and titrating the excess tions less than 1%. Temperature: ±0.05°C

REFERENCES:

was attained by first supersaturation at a

slightly lower temperature (solubility of

reacting the aqueous solution with

the presence of phosphoric acid and diphenylamine barium sulfonate as an

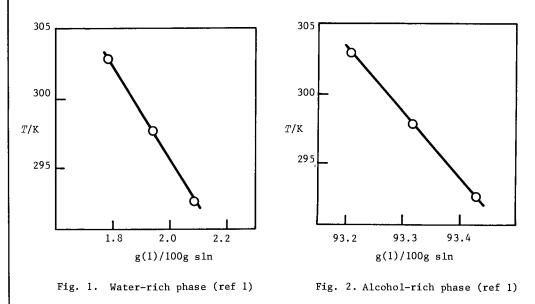
indicator.

alcohols in water decreases with increasing temperature) and then equilibrating at the desired temperature. The aqueous layer was separated after an overnight storage in a

dichromate with ferrous sulfate solution in

COMPONENTS:	EVALUATOR:		
(1) 3-Methyl-2-pentanol	Z. Maczynska, Institute of Physical		
(sec-butylmethylcarbinol); C ₆ H ₁₄ 0;	Chemistry of the Polish Academy of Sciences,		
[565-60-6]	Warsaw, Poland.		
(2) Water; H ₂ 0; [7732-18-5]	November 1982		

Solubilities in the system comprising 3-methyl-2-pentanol (1) and water (2) have been reported in two publications. Ginnings and Webb (ref 1) carried out measurements of the mutual solubilities of the two components at 293, 298 and 303 K by the volumetric method (Figure 1). Ratouis and Dode (ref 2) determined the solubility of (1) in the water-rich phase at one temperature (303 K) by an analytical method. Their value of 1.65 g(1)/100g sln at this temperature is in reasonable agreement with the value $1.79 \pm 0.1 \text{ g(1)}/100g \text{ sln of ref 1}$. The data are regarded as tentative, since comparison can be made only at a single temperature and the other five points are derived from one source.



Tentative values for the mutual solubilities of 3-methyl-2-pentanol (1) and water (2)

<i>T</i> /K	Water-rich	Water-rich phase		phase
	g(1)/100g sln	$10^{3}x_{1}$	g(2)/100g sln	<i>x</i> 2
293	2.1	3.8	6.6	0.285
298	1.9	3.5	6.7	0.289
303	1.8	3.2	6.8	0.292

References

1. Ginnings, P.M.; Webb, R. J. Am. Chem. Soc. 1938, 60, 1388.

2. Ratouis, M.; Dode, M. Bull. Soc. Chim. Fr. 1965, 3318.

COMPONENTS:		ORIGIN	AL MEASUREMENTS:	
(1) 3-Methyl-2-pentanol	(1) 3-Methyl-2-pentanol		ngs, P.M.; Webb, I	R.
(sec-butylmethylcarbinol); C	^H 14 ⁰ ;	J. Am.	Chem. Soc. <u>1938</u> ,	60, 1388-9.
[565-60-6]				
(2) Water; H ₂ 0; [7732-18-5]				
VARIABLES:		PREPAR	ED BY:	
Temperature: 20-30 [°] C		A. Mac	czynski and Z. Mac	zynska
EXPERIMENTAL VALUES:				
Mutual solubility of	of 3-methyl	-2-proj	panol(l) and water	(2)
$t/^{\circ}C$ g(1)/100g si	ln		x_1 (comp	iler)
(2)-rich phase	(1)-rich ph	ase	(2)-rich phase	(1)-rich phase
20 2.09	93.43	3	0.00375	0.7148
25 1.94	93.32	2	0.00347	0.7112
30 1.79	93.21		0.00320	0.7076
	Relative	densi	ty, <i>d</i> ₄	
t/ ^o c t	Vater-rich	phase	Alcohol-rich ph	ase
20	0.9960		0.8390	
25	0.9950		0.8356	
30	0.9939		0.8316	
	<u> </u>			
	AUXILIARY	INFORM	ATION	
METHOD/APPARATUS/PROCEDURE:			E AND PURITY OF MAT	
The volumetric method was used as in ref 1.	described		prepared by Grigna distilled from cal	cium oxide;
Both components were introduced i	n known		b.p. range 133.5-1 .25	
amounts into a two-bulb graduated	and	4	d_4^{25} 0.8231; purity	unspecified
calibrated flask and shaken mecha a water-bath at constant temperat	ure.	(2)	not specified.	
After sufficient time the liquids allowed to separate and the total				
was measured. Upon centrifugati phase separation line was read, a	•			
volumes were calculated. From t	he total	FOTIM	ATED EDDOD.	
weights of the components, the total volume, individual phase volumes, and component concentrations in either phase were evaluated.		1	erature: $\pm 0.1^{\circ}C$	
		-	bility: better t	han 0.1 wt % error not specified)
		REFER	ENCES ;	
			Ginnings, P.M.; E Soc. <u>1937</u> , 59, 111	aum, R.J. <i>J. Am. Chen</i> 1.

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) 3-Methyl-2-pentanol,	Ratouis, M.; Dode, M.;
(sec-butylmethylcarbinol); C ₆ H ₁₄ 0;	Bull. Soc. Chim. Fr. 1965, 3318-22.
[565-60-6]	2000, 500, 600, 111, <u>2000</u> , 5510 121
(2) Water; H ₂ 0; [7732-18-5]	
_	
VARIABLES:	PREPARED BY:
One temperature: 30 ⁰ C	S.C. Valvani; S.H. Yalkowsky; A.F.M. Barton.
Ringer solution also studied	
EXPERIMENTAL VALUES:	
The proportion of 3-methyl-2-pentanol (1) in	the veter-rich phase at equilibrium at
30° C was reported to be 1.65 g(1)/100g sln.	the water-fich phase at equilibrium at
The corresponding mole fraction solubility, c	alculated by the compilers is $r = 0.00295$
, , , , , , , , , , , , , , , , , , , ,	$\frac{1}{1} = \frac{1}{1}$
The proportion of (1) in the water-rich phase	of a mixture with Ringer solution at 30 ⁰ C
was reported to be $1.52 g(1)/100g sln$.	
	······································
AUXILIARY	INFORMATION
METHOD / APPARATUS / PROCEDURE :	SOURCE AND PURITY OF MATERIALS:
In a round bottomed flask, 50 mL of water	(1) Laboratory preparation;
and a sufficient quantity of alcohol were introduced until two separate layers were	redistilled with 10:1 reflux ratio;
formed. The flask assembly was equilibrate	b.p. 132.4-132.5 ⁰ C/750 mm Hg
by agitation for at least 3 h in a constant temperature bath. Equilibrium solubility	$n_{\rm D}^{25} = 1.41827$
was attained by first supersaturation at a	ע
slightly lower temperature (solubility of alcohols in water decrease with increasing	(2) twice distilled from silica apparatus
temperature) and then equilibrating at the	or ion-exchanged with Sagei A20.
desired temperature. The aqueous layer was separated after an overnight storage in a	
bath. The alcohol content was determined	ESTIMATED ERROR:
by reacting the aqueous solution with potassium dichromate and titrating the excess	Solubility: relative error of 2 determina-
dichromate with ferrous sulfate solution in	tions less than 1%.
the presence of phosphoric acid and diphenylamine barium sulfonate as an	Temperature: ±0.05 [°] C.
indicator.	REFERENCES:

COMPONENTS:	EVALUATOR:
(1) 3-Methy1-3-pentanol	Z. Maczynska, Institute of Physical
(diethylmethylcarbinol); C ₆ H ₁₄ 0;	Chemistry of the Polish Academy of Sciences,
[77-74-7]	Warsaw, Poland.
(2) Water; H ₂ 0; [7732-18-5]	November 1982

Solubilities in the system comprising 3-methyl-3-pentanol (1) and water (2) have been reported in two publications (Figures 1 and 2). Ginnings and Webb (ref 1) carried out measurements of the mutual solubilities of the two components at 293, 298 and 303 K by the volumetric method. Ratouis and Dode' (ref 2) determined the solubility of (1) in the water-rich phase at one temperature (303 K) by an analytical method. Their value of 3.57 g(1)/100 g sln at this temperature is in reasonable agreement with the value $3.81 \pm 0.1 \text{ g(1)}/100\text{ g sln}$ of ref 1. The data are regarded as tentative, since comparison can be made only at a single temperature and the other five points are derived from one source.

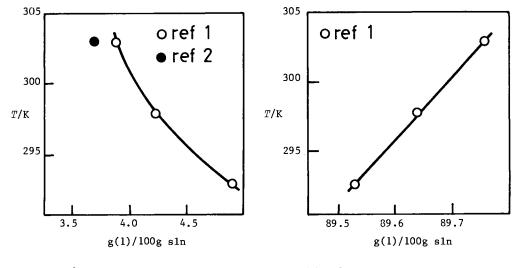


Fig. 1. Water-rich phase

Fig. 2. Alcohol-rich phase

Tentative values for the mutual solubilities of 3-methyl-3-pentanol (1) and water (2)

T/K	Water-rich p	Water-rich phase		Alcohol-rich phase	
	g(1)/100g s1n	$10^{3}x_{1}$	g(2)/100g sln	<i>x</i> ₂	
293	4.8	8.9	10.5	0.399	
298	4.3	7.8	10.4	0.396	
303	3.8	6.9	10.2	0.393	

References

1. Ginnings, P.M.; Webb, R. J. Am. Chem. Soc. 1938, 60, 1388.

2. Ratouis, M.; Dode, M. Bull. Soc. Chim. Fr. <u>1965</u>, 3318.

COMPONENTS:		ORIGINAL MEASUREMENTS:		
(1) 3-Methyl-3-pentanol		Ginnings, P.M.; Webb, R.		
(diethylmethylcarbinol); C ₆ H ₁₄ 0;		J. Am. Chem. Soc. 1938, 60, 1388-9.		
[77-7	[77-74-7]			
(2) Water	; H ₂ 0; [7731-18-5]			
VARIABLES:			PREPARED BY:	
Temperatur	e: 20-30 [°] C		A. Maczynski and Z. Ma	aczynska
EXPERIMENTAL	L VALUES:		<u> </u>	
	Mutual solubil	ity of 3-methy	1-3-pentanol(1) and wat	ter(2)
t∕°c	g(1)/100	a sln	x_1 (comp	iler)
<i>27</i> C		(1)-rich phas	-	(1)-rich phase
20	4.82	89.53	0.00885	0.6011
25	4.26	89.64	0.00778	0.6040
30	3.81	89.76	0.00693	0.6071
		Relative	e density, d_4	
	t/ ^o c	Water-rich p	ohase Alcohol-rich	phase
	20	0.9933	0.8498	
	25	0.9926	0.8454	
	30 0.9919		0.8410	
		AUXILIARY	INFORMATION	
METHOD /APPA	RATUS / PROCEDURE :		SOURCE AND PURITY OF M	1ATERIALS ;
The volum	etric method was used	l as described	(1) prepared by Gri	gnard synthesis;
in ref 1.			distilled from	calcium oxide; 6-122.8 ^o C/760 mm Hg
	onents were introduce		d_{1}^{25} 0.8242;	
	nto a two-bulb gradua d flask and shaken me		purity not spec	ified.
	r-bath at constant te ficient time the liqu	•	(2) not specified.	
allowed t	o separate and the to	otal volume		
	red. Upon centrifuga aration line was read			
	ere calculated. Fro f the components, the	om the total total volume	ESTIMATED ERROR:	
individua	1 phase volumes, and	component	Temperature: ± 0.1 ^o C	
evaluated	tions in either phase •	e were		than 0.1 wt % f error not specified)
			REFERENCES :	
			1. Ginnings, P.M.; Soc. <u>1937</u> , 59, 1	Baum, R.J. J. Am. Chem 111.

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) 3-Methyl-3-pentanol	Ratouis, M.; Dode, M.;
(diethylmethylcarbinol); C ₆ H ₁₄ 0;	Bull. Soc. Chim. Fr. 1965, 3318-22
[77-74-7]	
(2) Water; H ₂ 0; [7732-18-5]	
VARIABLES:	PREPARED BY:
One temperature: 30°C	S.C. Valvani; S.H Yalkowsky; A.F.M. Barton
Ringer solution also studied	
EXPERIMENTAL VALUES:	
The proportion of 3-methyl-3-pentanol (1) in was reported to be 3.57 g(1)/100g sln.	the water-rich phase at equilibrium at 30 ⁰ C
The corresponding mole fraction solubility,	calculated by the compilers, is $x_1 = 0.00649$
The proportion of (1) in the water-rich phas was reported to be $3.35 \text{ g}(1)/100 \text{ g sln}$.	e of a mixture with Ringer solution at 30 ⁰ C

METHOD APPARATUS/PROCEDURE: In a round bottomed flask, 50 mL of water and a sufficient quantity of alcohol were introduced until two separate layers were formed. The flask assembly was equilibrated by agitation for at least 3 h in a constant temperature bath. Equilibrium solubility	INFORMATION SOURCE AND PURITY OF MATERIALS: (1) laboratory preparation; redistilled with 10:1 reflux ratio b.p. 123-123.1°C/770.4 mm Hg n_D^{25} = 1.41665
was attained by first supersaturation at a slightly lower temperature (solubility of alcohols in water decreases with increasing temperature) and then equilibrating at the desired temperature. The aqueous layer was separated after an overnight storage in a bath. The alcohol content was determined by reacting the aqueous solution with potassium dichromate and titrating the excess dichromate with ferrous sulfate solution in the presence of phosphoric acid and diphenylamine barium sulfonate as an indicator.	 (2) twice distilled from silica apparatus or ion-exchanged with Sagei A20. ESTIMATED ERROR: Solubility: relative error of 2 determina- tions less than 1%. Temperature: ±0.05°C REFERENCES:

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) 4-Methyl-1-pentanol; C ₆ H ₁₄ 0; [626-89-1]	Ratouis, M.; Dode, M.;
	Bull. Soc. Chim. Fr. 1965, 3318-22.
(2) Water; H ₂ 0; [7732-18-5]	
VARIABLES:	PREPARED BY:
Temperature: 25° C and 30° C	S.C. Valvani; S.H. Yalkowsky; A.F.M. Barton
Ringer solution also studied	
EXPERIMENTAL VALUES:	
Proportion of 4-methyl-1-pent	anol (1) in water-rich phase
t/ ^o c g(1)/100g s1r	x_1 (compilers)
25 0.7(0.00125
25 0.76 30 0.715	0.00135 0.00127
The proportion of (1) in the water-rich phase 20°	
equilibrium at 30 [°] C was reported to be 0.70 g	(1)/100g sin.
AUXILIARY	INFORMATION
METHOD / APPARATUS / PROCEDURE :	SOURCE AND PURITY OF MATERIALS:
In a round bottomed flask, 50 mL of water and	
a sufficient quantity of alcohol were intro- duced until two separate layers were formed.	redistilled with 10:1 reflux ratio
The flask assembly was equilibrated by	b.p. 151.6-152 [°] C/760.2 mm Hg
agitation for at least 3 h in a constant temperature bath. Equilibrium solubility	$n_{\rm D}^{25} = 1.41392$
was attained by first supersaturation at a slightly lower temperature (solubility of	(2) twice distilled from silica apparatus
alcohols in water decreases with increasing temperature) and then equilibrating at the	or ion-exchanged with Sagei A20.
desired temperature. The aqueous layer was	
separated after an overnight storage in a bath. The alcohol content was determined	ESTIMATED ERROR:
by reacting the aqueous solution with potassium dichromate and titrating the excess	Solubility: relative error of 2 determina-
dichromate with ferrous sulfate solution in	tions less than 1%.
the presence of phosphoric acid and diphenylamine barium sulfonate as an	Temperature: ±0.05°C REFERENCES:
indicator.	

COMPONENTS:	EVALUATOR:
(1) 4-Methyl-2-pentanol	A. Maczynski, Institute of Physical
(isobutylmethylcarbinol); C6H140;	Chemistry of the Polish Academy of Sciences,
[108-11-2]	Warsaw, Poland; and A.F.M. Barton, Murdoch
(2) Water; H ₂ 0; [7732-18-5]	University, Perth, Western Australia.
(2) mater, 20, 20, 20, 31	November 1982

T/K

Solubilities in the system comprising 4-methyl-2-pentanol (1) and water (2) have been reported in four publications. Ginnings and Webb (ref 1) carried out measurements of the mutual solubilities of the two components at 293, 298 and 303 K by the volumetric method. Crittenden and Hixon (ref 2) used (presumably) the titration method at one temperature (298 K) for both phases and Ratouis and Dode^{\prime} (ref 3) also determined only one temperature point (303 K) of the solubility in the water-rich phase by an analytical method. Dakshinamurty *et al.* (ref 4) carried out determination of the mutual solubility of (1) and (2) at 283, 301, and 323 K by the synthetic method.

The data on the water-rich phase are collected in Figure 1. The results of ref 1, 2, 3, and of ref 4 at 301 K are in reasonable agreement. The value at 300 K is recommended, with tentative values being proposed at 280 and 320 K.

Results on the alcohol-rich phase are in poor agreement, and the proposed value at 300 K is tentative only.

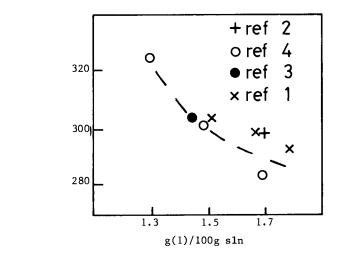


Fig. 1. Solubility of (1) in (2)

Recommended and tentative values for the mutual solubilities of 4-methyl-2-pentanol (1) and water (2)

T/KWater-rich phase Alcohol-rich phase $10^{3}x_{1}$ g(1)/100g sln g(2)/100g sln x_2 280 2 (tentative) 4 1.5 (recommended) 2.7 6 (tentative) 0.7 300 320 1 (tentative) 2

(continued next page)

COMPONENTS:	EVALUATOR:
(1) 4-Methy1-2-pentano1	A. Maczynski, Institute of Physical
(isobutylmethylcarbinol); C ₆ H ₁₄ 0;	Chemistry of the Polish Academy of Sciences,
[108-11-2]	Warsaw, Poland; and A.F.M. Barton, Murdoch
(2) Water; H ₂ 0; [7732-18-5]	University, Perth, Western Australia.
(2) water, n_2^{0} , $(7752-10-5)$	November 1982

CRITICAL EVALUATION: (continued)

References

- 1. Ginnings, P.M.; Webb, R. J. Am. Chem. Soc. 1938, 60, 1388.
- 2. Grittenden, E.D., Jr.; Hixon, A.N. Ind. Eng. Chem. 1954, 46, 265.
- 3. Ratouis, M.; Dode, M. Bull. Soc. Chim. Fr, 1965, 3318.
- Dakshinamurty, P.; Chiranjivi, C.; Rao, P.V.; Subrahmanyam, V. J. Chem. Eng. Data <u>1972</u>, 17, 379.

			ORIGI	NAL MEASUREMENTS:	
<pre>(1) 4-Methyl-2-pentanol (isobutylmethylcarbinol); C₆H₁₄0;</pre>		Ginnings, P.M.; Webb, R.			
		J. An	n. Chem. Soc. <u>1938</u> ,	60, 1388-9.	
[108-11-2];					-
(2) Water; H ₂ 0;	[7732-18-5]				
ARIABLES:	<u>_</u>		PREPA	RED BY:	
Temperature: 20	0−30 [°] C		A. Maczynski and Z. Maczynska		
EXPERIMENTAL VALUE	ES :				
	Mutual so	olubility of 4	-methy	1-2-pentanol(1) an	d water(2)
t/ ^o c	g(1)/100)g sln		x_1 (comp	iler)
(2			ase	(2)-rich phase	
20	1.79	93.79		0.00320	0.7269
25	1.64	93.65		0.00293	0.7222
30	1.52	93.45		0.00271	0.7155
		Relati	ve den	sity, d_4	
	t/ ^o c	Water-rich ph	ase	Alcohol-rich pha	se
	20	0.9956		0.8186	
	25	0.9948		0.8149	
	30	0 .99 39		0.8114	
		AUXILIARY	INFOR	MATION	
METHOD / APPARATUS /	PROCEDURE :	AUXILIARY		MATION SE AND PURITY OF MA	TERIALS :
METHOD/APPARATUS/ The volumetric m				CE AND PURITY OF MA	
			SOUR	E AND PURITY OF MA Eastman practical fractionally dist	grade; illed, and
The volumetric m in ref 1. Both components	were introduced	as described in known	SOUR	E AND PURITY OF MA Eastman practical fractionally dist redistilled from b.p. range 131.6-	grade; illed, and calcium oxide;
The volumetric m in ref l. Both components amounts into a t calibrated flask	ethod was used were introduced wo-bulb graduat and shaken med	as described in known ed and chanically in	SOUR((1)	E AND PURITY OF MA Eastman practical fractionally dist redistilled from	grade; illed, and calcium oxide;
The volumetric m in ref l. Both components amounts into a t calibrated flask a water-bath at	were introduced wo-bulb graduat and shaken med constant temper	as described in known ed and chanically in rature. After	SOUR((1)	E AND PURITY OF MA Eastman practical fractionally dist redistilled from b.p. range 131.6- d_4^{25} 0.8034.	grade; illed, and calcium oxide;
The volumetric m in ref l. Both components amounts into a t calibrated flask a water-bath at sufficient time separate and the	were introduced wo-bulb graduat and shaken med constant temper the liquids were total volume w	as described in known ed and chanically in rature. After re allowed to vas measured.	SOUR((1)	E AND PURITY OF MA Eastman practical fractionally dist redistilled from b.p. range 131.6- d_4^{25} 0.8034.	grade; illed, and calcium oxide;
The volumetric m in ref l. Both components amounts into a t calibrated flask a water-bath at sufficient time separate and the Upon centrifugat line was read, a	were introduced wo-bulb graduat and shaken med constant temper the liquids wer total volume v ion, the phase and phase volume	as described in known ed and chanically in ature. After re allowed to vas measured. separation s were	SOUR((1)	E AND PURITY OF MA Eastman practical fractionally dist redistilled from b.p. range 131.6- d_4^{25} 0.8034.	grade; illed, and calcium oxide;
The volumetric m in ref l. Both components amounts into a t calibrated flask a water-bath at sufficient time separate and the Upon centrifugat line was read, a calculated. Fr	were introduced wo-bulb graduat and shaken med constant temper the liquids wer total volume v ion, the phase and phase volume total volume, f	as described in known ed and chanically in ature. After a measured separation is were ights of the ndividual	SOUR((1) (2)	E AND PURITY OF MA Eastman practical fractionally dist redistilled from b.p. range 131.6- d_4^{25} 0.8034.	grade; illed, and calcium oxide;
The volumetric m in ref l. Both components amounts into a t calibrated flask a water-bath at sufficient time separate and the Upon centrifugat line was read, a calculated. Fr	were introduced wo-bulb graduat and shaken med constant temper the liquids were total volume w ion, the phase of the total we total volume, j ind component co	as described in known ded and chanically in cature. After re allowed to vas measured. separation es were dights of the ndividual ncentrations	(1) (2) ESTII	The AND PURITY OF MAR Eastman practical fractionally dist redistilled from b.p. range 131.6- d_4^{25} 0.8034. not specified. MATED ERROR: perature: ± 0.1 ^O C ubility: better	grade; illed, and calcium oxide; 131.8 ^o C/760 mm Hg
The volumetric m in ref 1. Both components amounts into a t calibrated flask a water-bath at sufficient time separate and the Upon centrifugat line was read, a calculated. Fr components, the phase volumes, a	were introduced wo-bulb graduat and shaken med constant temper the liquids were total volume w ion, the phase of the total we total volume, j ind component co	as described in known ded and chanically in cature. After re allowed to vas measured. separation es were dights of the ndividual ncentrations	SOURC (1) (2) ESTII Tem Sol	The AND PURITY OF MAR Eastman practical fractionally dist redistilled from b.p. range 131.6- d_4^{25} 0.8034. not specified. MATED ERROR: perature: ± 0.1 ^O C ubility: better	grade; illed, and calcium oxide; 131.8 ^o C/760 mm Hg
The volumetric m in ref 1. Both components amounts into a t calibrated flask a water-bath at sufficient time separate and the Upon centrifugat line was read, a calculated. Fr components, the phase volumes, a	were introduced wo-bulb graduat and shaken med constant temper the liquids were total volume w ion, the phase of the total we total volume, j ind component co	as described in known ded and chanically in cature. After re allowed to vas measured. separation es were dights of the ndividual ncentrations	SOURC (1) (2) ESTI Tem Sol	The AND PURITY OF MAR Eastman practical fractionally dist redistilled from b.p. range 131.6- d_4^{25} 0.8034. not specified. MATED ERROR: perature: $\pm 0.1^{\circ}C$ ubility: better (type o RENCES:	grade; illed, and calcium oxide; l31.8 ^o C/760 mm Hg than 0.1 wt % f error not specified Baum, R.J. J. Am. Cher
The volumetric m in ref 1. Both components amounts into a t calibrated flask a water-bath at sufficient time separate and the Upon centrifugat line was read, a calculated. Fr components, the phase volumes, a	were introduced wo-bulb graduat and shaken med constant temper the liquids were total volume w ion, the phase of the total we total volume, j ind component co	as described in known ded and chanically in cature. After re allowed to vas measured. separation es were dights of the ndividual ncentrations	SOURC (1) (2) ESTI Tem Sol	The AND PURITY OF MA Eastman practical fractionally dist redistilled from b.p. range 131.6- d_4^{25} 0.8034. not specified. MATED ERROR: perature: \pm 0.1 ^O C ubility: better (type o RENCES: Ginnings, P.M.;	grade; illed, and calcium oxide; l31.8 ^o C/760 mm Hg than 0.1 wt % f error not specified Baum, R.J. J. Am. Chen

COMPONENTS :	ORIGINAL MEASUREMENTS:
(1) 4-Methyl-2-pentanol	Crittenden, E.D., Jr.; Hixon, A.N.
(isobutylmethylcarbinol); C ₆ H ₁₄ 0; [108–11–2]	Ind. Eng. Chem. <u>1954</u> , 46, 265–8.
(2) Water; H ₂ 0; [7732-18-5]	
VARIABLES:	PREPARED BY:
One temperature: 25 [°] C	A. Maczynski
one temperature. 25 c	
EXPERIMENTAL VALUES:	· · · · · · · · · · · · · · · · · · ·
The solubility of 4-methyl-2-pentanol in wat sln.	er at 25 ⁰ C was reported to be 1.7 g(1)/100g
The corresponding mole fraction, $x_1^{}$, calcula	ted by the compiler is 0.0030.
The solubility of water in 4-methyl-2-pentan sln.	ol at 25 ⁰ C was reported to be 5.8 g(2)/100
The corresponding mole fraction, $x_2^{}$, calcula	ted by the compiler is 0.26
AUXILIARY	INFORMATION
METHOD / APPARATUS / PROCEDURE :	SOURCE AND PURITY OF MATERIALS:
Presumably the titration method described	 source not specified;
for ternary systems containing HCl was used. In this method the solubility was determined	
by bringing 100-mL samples of (1) or (2) to a temperature $25.0 \pm 0.1^{\circ}C$ and the second	(2) not specified.
component was then added from a calibrated	(-)
buret, with vigorous stirring, until the solution became permanently cloudy.	
	ESTIMATED ERROR: Solubility: 2% (alcohol-rich) - 10% (Water-
	rich)
	Temperature: ± 0.10°C
	REFERENCES:

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) 4-Methyl-2-pentanol	Ratouis, M.; Dode, M.;
(isobutylmethylcarbinol); C ₆ H ₁₄ 0;	Bull. Soc. Chim. Fr. <u>1965</u> , 3318-22.
[108-11-2]	
(2) Water; H ₂ 0; [7732-18-5]	
VARIABLES:	PREPARED BY:
One temperature: 30°C	S.C. Valvani; S.H. Yalkowsky; A.F.M. Barton
Ringer solution also studied	
EXPERIMENTAL VALUES:	
The proportion of 4-methyl-2-pentanol (1) in was reported to be 1.43 g(1)/100g sln.	the water-rich phase at equilibrium at 30 ⁰ C
The corresponding mole fraction solubility,	calculated by the compilers, is $x_1 = 0.00255$.

The proportion of (1) in the water-rich phase of a mixture with Ringer solution at 30° C was reported to be 1.39 g(1)/100g sln.

AUXILIARY	INFORMATION SOURCE AND PURITY OF MATERIALS:
In a round bottomed flask, 50 mL of water and a sufficient quantity of alcohol were introduced until two separate layers were formed. The flask assembly was equilibrated by agitation for at least 3 h in a constant temperature bath. Equilibrium solubility was attained by first supersaturation at a slightly lower temperature (solubility of alcohols in water decreases with increasing temperature) and then equilibrating at the desired temperature. The aqueous layer was separated after an overnight storage in a bath. The alcohol content was determined by reacting the aqueous solution with potassium dichromate and titrating the excess dichromate with ferrous sulfate solution in the presence of phosphoric acid and diphenylamine barium sulfonate as an indicator.	 n_D⁻ = 1.40919 (2) twice distilled from silica apparatus or ion-exchanged with Sagei A20. ESTIMATED ERROR: Solubility: moleting error of 2 dependent

262		Six-carbo	n Alcohols		
COMPONENTS :			ORIGINAL MEASUF	REMENTS:	
(1) 4-Methy] [108-11-	(1) 4-Methyl-2-pentanol; C ₆ H ₁₄ O; [108-11-2]		Dakshinamurty, P.; Chiranjivi, C.; Rao, P.V.; Subrahmanyam, V.		
(2) Water;	2) Water; H ₂ 0; [7732-18-5]		J. Chem. Eng. Data, <u>1972</u> , 17, 379–83.		
VARIABLES:			PREPARED BY:		
Temperature:	Temperature: 10-50°C		A. Maczynski		
EXPERIMENTAL V	VALUES:				
	Mutual solub:	ility of 4-me	thy1-2-pentano1	and wate	r
t/ ^o c	g(1)/10	OOg sln		x_1 (comp	viler)
	(2)-rich phase	(1)-rich pha	se (2)-rich	-	(1)-rich phase
10	1.7	96.7	0.	0030	0.838
28	1.5	95.7	0.	0027	0.797
50	1.3	94.7	0.	0023	0.759
	TUS/PROCEDURE:	RUNILIARI	INFORMATION SOURCE AND PUR		
The syntheti Weighed mixt in a borosil with a groun a thermomete heated or co temperature, or disappear The end poin either on he solubilities	c method was used. ures of (1) and (2) icate glass test tub d glass joint, and f r. The test tube v boled in a water bath corresponding to th ance of turbidity wa ts were reproducible ating or cooling. at required tempera graphically.	be (20 ml) Fitted with vas slowly h and the he appearance as noted. e to $\pm 0.3^{\circ}C$ The	(1) British distille b.p. ran d^{30} 0.80 (2) not spec	Drug Hous d; ge 131.5- 003 g cm ⁻³ dified. DR: ± 0.5°C.	e; 132 [°] C, n _D ³⁰ 1.4090,

1-H	exanol
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COMPONENTS:	EVALUA	TOR:	
(1) 1-Hexanol (n-hexyl alcohol); (G.T. I	G.T. Hefter and A.F.M. Barton, Murdoch	
[111-27-3]		University, Perth, Western Australia.	
(2) Water; H ₂ 0; [7732-18-5]	June,	June, 1983	
CRITICAL EVALUATION:			
Solubilities in the 1-hexanol (1)-	-water (2) system 1	have been reported	in the following
publications.		are been reperies	
P-0-100-			
Reference	<i>Т</i> /К	Phase	Method
Fühner (ref 1)	273-378	(1) in (2)	synthetic
Butler et al. (ref 2)	298	(1) in (2)	interferometric
Addison (ref 3)	293	(1) in (2)	surface tension
Laddha and Smith (ref 4)	293	mutual	titration
Donahue (ref 5)	298	mutual	analytical
Erichsen (ref 6)	273-495	mutual	synthetic
Erichsen (ref 7)	273-323	(1) in (2)	synthetic
Crittenden and Hixon (ref 8)	298	mutual	titration
Kinoshita $et \ al.$ (ref 9)	298	(1) in (2)	surface tension
Venkataratnam and Rao (ref 10)	303	mutual	turbidimetric
Ababi and Popa (ref 11)	298	mutual	turbidimetric
Chandy and Rao (ref 12)	303	mutual	turbidimetric
Hanssens (ref 13)	298	(1) in (2)	interferometric
Ratouis and Dode (ref 14)	303	(1) in (2)	analytical
Krasnov and Gartseva (ref 15)	285-313	(2) in (1)	analytical
Vochten and Petre (ref 16)	288	(1) in (2)	surface tension
Hill and White (ref 17)	278-306	(1) in (2)	interferometric
Korenman et al. (ref 18)	298	(1) in (2)	analytical
Lavrova and Lesteva (ref 19)	313-333	mutual	titration
Filippov and Markuzin (ref 20)	294-313	(2) in (1)	1
Nishino and Nakamura (ref 21)	280-350	mutual	synthetic
Tokunaga <i>et al</i> (ref 22)	288-308	(2) in (1)	analytical

The original data are compiled in the data sheets immediately following this Critical Evaluation.

In this Critical Evaluation the data of Hanssens (ref 13), Vochten and Petre (ref 16) and Korenman *et al.* (ref 18) given in weight/volume fractions are excluded from consideration as density information was not included in the original references. The graphical data of Nishino and Nakamura (ref 21) are also excluded.

In the water-rich phase the data of Addison (ref 3), Laddha and Smith (ref 4), Donahue (ref 5), Venkataratnam and Rao (ref 10), Ababi and Popa (ref 11) and Chandy and Rao (ref 12), all at either 298 or 303 K, disagree markedly from all other studies and are rejected.

In the alcohol-rich phase the low temperature (≤ 283 K) data of Erichsen (ref 6 & 7) and Krasnov and Gartseva(ref 15) disagree markedly and both are rejected. The data of Erichsen (ref 6 & 7) between 293 and 303 K are in poor agreement with all other studies (ref 5, 8, 1, 15, 20, 22) and have also been rejected as has the data of Ababi and Popa

(continued next page)

COMPONENTS :	EVALUATOR:
 (1) Hexanol (<i>n-hexyl alcohol</i>); C₆H₁₄0; [111-27-3] (2) Water; H₂0; [7732-18-5] 	G.T. Hefter and A.F.M. Barton, Murdoch University, Perth, Western Australia. June, 1983

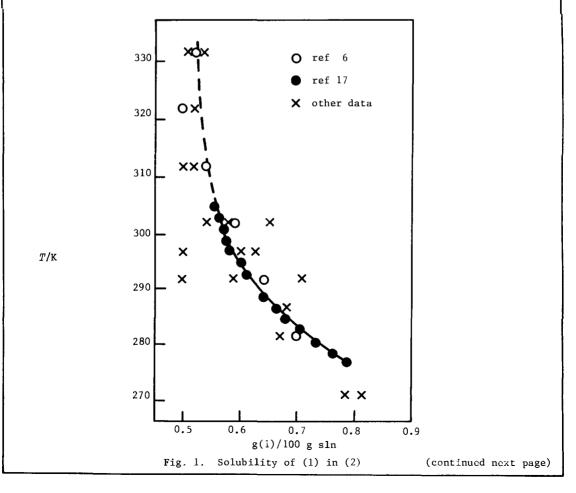
CRITICAL EVALUATION: (continued)

(ref 11). At higher temperatures Erichsen's values (ref 6 & 7) are in somewhat better agreement with other studies and have been included.

All other data are included in the Tables below. Values obtained by the Evaluators by graphical interpolation or extrapolation from the data sheets are indicated by an asterisk (*). "Best" values have been obtained by simple averaging. The uncertainty limits (σ_n) attached to the "best" values do not have statistical significance and should be regarded only as a convenient representation of the spread of reported values and not as error limits. The letter (*R*) indicates "Recommended" data. Data are "Recommended" if two or more apparently reliable studies are in reasonable agreement ($\leq \pm 5\%$ relative). For convenience the two phases will be further discussed separately.

The solubility of 1-hexanol (1) and water (2)

There is excellent agreement between the data of Fühner (ref 1) and Erichsen (ref 6 & 7) over a very wide temperature range and also with other studies (ref 17 & 19) over more limited ranges (Figure 1). This has enabled values to be recommended over an unusually wide range of temperatures (see Table below).

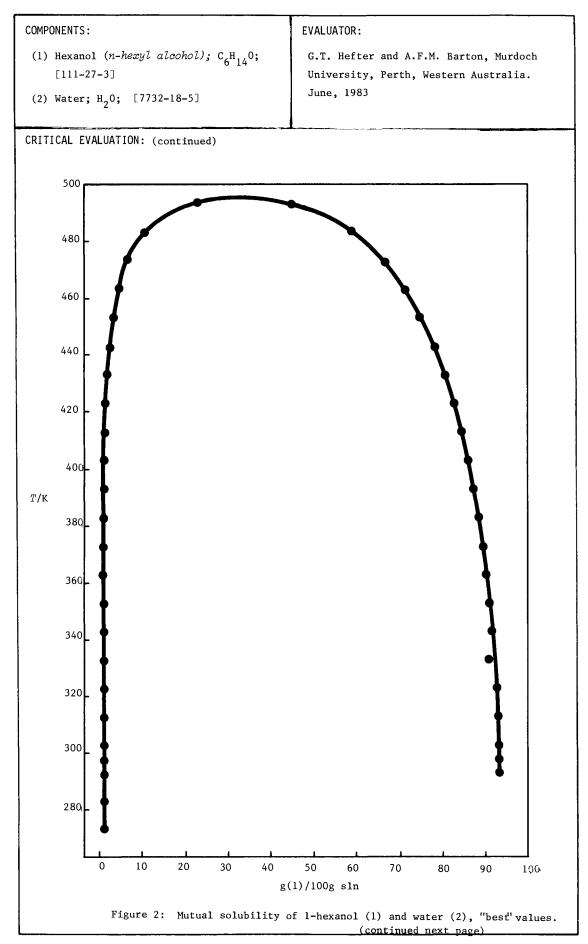


COMPONENTS	3:	EVALUATOR:	
(1) Hexar	nol (n-hexyl alcohol); C ₆ H ₁₄ 0;	G.T. Hefter and A.F.M. Barton, M	urdoch
	-27-3]	University, Perth, Western Austr	al i a
(2) Water	с; H ₂ O; [7732-18-5]	June, 1983	
	2, 2, 1, 5, 10, 5,		
CRITICAL E	EVALUATION (continued)		
	Recommended (R) and tenta	tive solubilities of	
	l-hexanol (1) in v		
	<u> </u>		
Τ/К	5	Solubility, g(1)/100g sln	
	Reported values	"Best" va	lue (±σ _n)
273	0.78 (ref 1), 0.81 (ref 6), 0.79	(ref 7) 0.79 ±	0.01 (R)
273	0.67 (ref 1), 0.70 (ref 6), 0.68		
283	0.59 (ref 1), 0.64 (ref 6), 0.62		•
293	0.57 [*] (ref 1), 0.624 (ref 2), 0.62		0102 (11)
290	0.60	(ref 9), 0.585*(ref 17) 0.60 ±	0.02 (<i>R</i>)
303	0.545 (ref 1), 0.59 (ref 6), 0.56		(-)
		$0.566 \text{ (ref 17)} 0.57 \pm $	0.02 (R)
313	0.52 (ref 1), 0.54 (ref 6), 0.56	(ref /), 0.55 (ref 1/), 0.50 (ref 19) 0.53 ±	0.02 (R)
323	0.51 (ref 1), 0.50 (ref 6), 0.51	(ref 7) 0.51 ±	0.01 (R)
333	0.53 (ref 1), 0.52 (ref 6), 0.51		0.01 (R)
343	0.565 (ref 1), 0.56 (ref 6)	0.56 ±	0.01 (R)
353	0.62 (ref 1), 0.61 (ref 6)	0.62 ±	0.01 (R)
363	0.68 (ref 1), 0.69 (ref 6)	0.69 ±	0.01 (R)
373	0.785 (ref 1), 0.80 (ref 6)	0.79 ±	0.01 (R)
383	0.89 (ref 1), 0.91 (ref 6)	0.90 ±	0.01 (R)
393	1.04 (ref 6)	1.0	
403	1.19 (ref 6)	1.2	
413	1.37 (ref 6)	1.4	
423	1.63 (ref 6)	1.6	
433	2.05 (ref 6)	2.1	
443	2.70 (ref 6)	2.7	
453	3.61 (ref 6)	3.6	
463	4.87 (ref 6)	4.9	
473	6.75 (ref 6)	6.8	
483	9.70 (ref 6)	9.7	
493	16.30 (ref 6)	16.3	

Solubility of water (2) in 1-hexanol (1)

Numerous studies (ref 5, 6, 8, 10, 12, 15, 19, 20, 22) are in good agreement over the range 298 - 313 K enabling values to be recommended. Agreement at all other temperatures is only fair and values are considered tentative only. In particular above 343 K only Erichsen's data (ref 6) are available and for reasons noted above they cannot be considered reliable without confirmatory studies.

COMPONENTS:	EVALUATOR:
 (1) Hexanol (<i>n-hexyl alcohol</i>); C₆H₁, [111-27-3] (2) Water; H₂0; [7732-18-5] 	4 ⁰ ; G.T. Hefter and A.F.M. Barton, Murdoch University, Perth, Western Australia June, 1983
-	
CRITICAL EVALUATION: (continued)	······································
Recommended (p	q) and tentative values of the solubility
of wa	ater (2) in 1-hexanol (1)
T/K	Solubility, g(2)/100g sln
Reported v	values "Best" values $(\pm \sigma_n)$
293 7.1 [*] (ref 15),6.2 [*] (ref 20)	п
	7.16 (ref 15), 6.7 [*] (ref 20)
	$7.38 (ref 22) 7.0 \pm 0.3 (R)$
303 6.8 (ref 10), 7.0 (ref 12)), 7.2 [*] (ref 15), 6.9 [*] (ref 20), 7.43 (ref 22) 7.1 ± 0.2 (R)
313 6.70 (ref 6), 7.3 (ref 15)), 7.0 (ref 19), 7.2 (ref 20) 7.1 ± 0.2 (R)
323 7.35 (ref 6)	7.4
333 8.05 (ref 6, 9.1 (ref 19)	8.6 ± 0.5
343 8.80 (ref 6)	8.8
353 9.65 (ref 6)	9.7
363 10.45 (ref 6)	10.5
373 11.30 (ref 6)	11.3
383 12.25 (ref 6)	12.3
393 13.30 (ref 6)	13.3
403 14.50 (ref 6)	14.5
413 15.85 (ref 6)	15.9
423 17.50 (ref 6)	17.5
433 19.35 (ref 6)	21.5
443 21.50 (ref 6)	24.4
453 24.40 (ref 6) 463 28.20 (ref 6)	28.2
473 33.40 (ref 6)	33.4
483 41.25 (ref 6)	41.3
493 55.35 (ref 6)	55.4
The upper critical solution temperat	ure
The UCST has been reported as 495.4	
-	
	ubility of 1-hexanol and water, taken from the
Tables above, are plotted in Figure	۷.
	(continued next page)



СОМРО	NENTS:	EVALUATOR:	
	Hexanol (<i>n-hexyl alcohol)</i> ; C ₆ H ₁₄ 0; [111-27-3] Water; H ₂ 0; [7732-18-5]	G.T. Hefter and A.F.M. Barton, Murdoch University, Perth, Western Australia. June, 1983	
CRITI	CRITICAL EVALUATION (continued)		
Pofe	Y 00 000		
1.	rences Fühner, H. Ber. Dtsch. Chem. Ges. 19	24 57 510	
2.	Butler, J.A.V.; Thomson, D.W.; Maclen		
 Addison, C.C. J. Chem. Soc. <u>1945</u>, 98. Laddha, G.S.; Smith, J.M. Ind. Eng. Chem. 1948, 40, 494. 			
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13.			
14.			
15.			
16.	Vochten, R.; Petre, G. J. Colloid In	terface Sci. <u>1973</u> , 42, 320.	
17.	Hill, D.J.T.; White, L.R. Aust. J. Chem. <u>1974</u> , 27, 1905.		
18.	Korenman, I.M.; Gorokhov, A.A.; Polozenko, G.N. Zh. Fiz. Khim. <u>1974</u> , 48, 1810; Russ. J. Phys. Chem. <u>1974</u> , 48, 1065.		
19.	Lavrova, O.A.; Lesteva, T.M. Zh. Fiz. Khim. <u>1976</u> , 50, 1617; Dep. Doc. VINITI 3813-75.		
20.	Filippov, V.V.; Markuzin, N.P.; Sazonov, V.P. Zh. Prikl. Khim. 1977, 6, 1321.		
21.	Nishino, N.; Nakamura, M. Bull. Chem	. Soc. Jpn. <u>1978</u> , 51, 1617; 54, 545.	
22.	Tokunaga, S.; Manabe, M.; Koda, M. N Hen (Memoirs Niihama Technical Colleg	iihama Kogyo Koto Semmon Gakko Kiyo, Rikogaku e, Sci. and Eng.) <u>1980</u> , 16, 96.	

1-Hexanol

1-16/	kanol 26
COMPONENTS:	ORIGINAL MEASUREMENTS:
	Fühner, H.
(1) 1-Hexanol; C ₆ H ₁₄ 0; [111-27-3]	
	Ber. Dtsch. Chem. Ges. <u>1924</u> , 57, 510-5.
(2) Water; H ₂ 0; [7732-18-5]	
VARIABLES: Temperature: 0-110 [°] C	PREPARED BY: A. Maczynski; Z. Maczynska; A. Szafranski.
	······································
EXPERIMENTAL VALUES:	······
	nexanol(1) in water (2)
$t/^{0}C$ g(1)/100g s	$\sin x_1(\text{compiler})$
0 0.78	0.00138
10 0.67	0.00119
20 0.59	0.00105
30 0.545	0.00096
40 0.52	0.00092
50 0.515	
60 0.53	0.00094
70 0.565	0.00100
80 0.62	0.00110
90 0.68	0.00121
100 0.785	0.00139
110 0.89	0.00158
AUXILIARY	INFORMATION
METHOD / APPARATUS / PROCEDURE :	SOURCE AND PURITY OF MATERIALS:
Rothmund's synthetic method (ref 1) was used.	(1) source not specified; specially purified, but no details provided.
Small amounts of (1) and (2) were sealed in a glass tube and heated with shaking in an	(2) not specified.
oil bath to complete dissolution. The	(2) not specified.
solution was cooled until a milky turbidity appeared and this temperature was adopted	
as the equilibrium temperature.	
	ESTIMATED ERROR:
	Not specified.
	REFERENCES :
	1. Rothmund, V. Z. Physik. Chem. <u>1898</u> , 20 433.

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) 1-Hexanol; C ₆ H ₁₄ 0; [111-27-3] (2) Water; H ₂ 0; [7732-18-5]	Butler, J.A.V.; Thomson, D.W.; Maclennan, W.H. <i>J. Chem. Soc.</i> <u>1933</u> , 674-86.
VARIABLES:	PREPARED BY:
One temperature: 25 ⁰ C	S.H. Yalkowsky; S.C. Valvani; A.F.M. Barton

EXPERIMENTAL VALUES:

The proportion of 1-hexanol (1) in the water-rich phase at equilibrium at 25° C was reported to be 0.624 g(1)/100g sln, the mean of seven determinations (0.637, 0.625, 0.622, 0.615, 0.611, 0.627, 0.634 g(1)/100g sln).

The corresponding mole fraction solubility was reported as $x_1 = 0.00111$.

AUXILIARY INFORMATION		
METHOD/APPARATUS/PROCEDURE: An analytical method was used, with a U-tube apparatus having two internal stoppers. Suitable quantities of (1) and (2) were placed in one of the connected vessels and shaken in a thermostat for some hours. The liquid was allowed to separate into two layers, the heavier aqueous layer being separated by raising the stoppers and allowing part of the liquid to run into the connected vessel. A weighed portion of the separated sln was diluted with about an equal quantity of (2) and the resulting sln compared with calibration slns in an interferometer. To avoid the possibility of reading the position of the wrong fringe, 2 cells (1 cm and 5 cm) were used. The method was unsuitable for analysis of alcohol -rich slns, as no stoppered interferometer	ESTIMATED ERROR: Solubility: the result is the mean of seven determinations agreeing within 0.013 g(1)/ 100g sln.	
cell was available.	REFERENCES :	

COMPONENTS :	ORIGINAL MEASUREMENTS:
(1) 1-Hexanol; C ₆ H ₁₄ 0; [111-27-3]	Addison, C.C.
(2) Water; H ₂ O; [7732-18-5]	J. Chem. Soc. <u>1945</u> , 98-106.
VARIABLES:	PREPARED BY:
One temperature: 20 ⁰ C	S.H. Yalkowsky; S.C. Valvani; A.F.M. Barton
EXPERIMENTAL VALUES:	1

The proportion of 1-hexanol (1) in the water-rich phase at equilibrium at 20° C was reported to be 0.706 g(1)/100g sln.

The corresponding mole fraction solubility, calculated by the compilers, is $x_1 = 0.00125$.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

A surface tension method was used. Sufficient excess of (1) was added to 100 mL of (2) in a stoppered flask to form a separate lens on the surface. The mixture was swirled gently, too vigorous an agitation being avoided as this gave a semipermanent emulsion and incorrect readings. After settling, a small sample of the clear aqueous solution was withdrawn into a drop weight pipet and the surface tension determined. The swirling was continued until a constant value was obtained. The surface tension - concentration curve was known, and only a slight extrapolation (logarithmic scale) was necessary to find the concentration corresponding to the equilibrium value.

SOURCE AND PURITY OF MATERIALS:

(1) impure alcohols were purified by fractional distillation, the middle fraction from a distillation being redistilled;
 b.p. 157.5°C d₄²⁰ 0.8194

 $n_{\rm D}^{20}$ 1.4182

(2) not stated

ESTIMATED ERROR:

Solubility: ± 0.5%

REFERENCES:

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) 1-Hexanol; C ₆ H ₁₄ 0; [111-27-3]	Laddha, G.S.; Smith, J.M.
(1) 1 minuter, 56-14-, [2) 51	Ind. Eng. Chem. <u>1948</u> , 40, 494-6.
(2) Water; H ₂ O; [7732-18-5]	1100 Dirigi Orizini. <u>1910</u> , 10, 1910.
VARIABLES:	PREPARED BY:
One temperature: 20 ⁰ C	A. Maczynski
EXPERIMENTAL VALUES:	
The solubility of 1-hexanol in water at 20° C	was reported to be $0.5 g(1)/100g sln$.
The corresponding mole fraction, x_1 , calculat	<i>.</i>
The corresponding more traction, w ₁ , careara	
The solubility of water in 1-hexanol at 20 ⁰ C	was reported to be 5.7 $g(2)/100 \text{sln}$.
The corresponding mole fraction, x_{γ} calculat	
The corresponding more fraction, we carculat	cu by the compiler is 0.20.
	INFORMATION
METHOD /APPARATUS / PROCEDURE :	SOURCE AND PURITY OF MATERIALS: (1) Carbide and Carbon Chemicals Co.,
The titration method was used.	<pre>(1) Carbide and Carbon Chemicals Co., technical grade; b.p. range 156.5-157°C, d²⁰ 0.820.</pre>
One component was placed in a 20° C constant-temperature bath for 1 h . Then titration	
was carried out in several steps, in order that the mixture could be frequently returned	(2) distilled.
to the constant-temperature bath to ensure maintenance of the 20°C temperature. The	
end point was taken when turbidity appeared over the entire solution.	
	ESTIMATED ERROR:
	Not specified.
	REFERENCES:
	Į

COMPONENTS:		ORIGINAL MEASUREMENTS:
(1) 1-Hexanol; C ₆ H ₁₄ 0; [11	1-27-3]	Donahue, D.J.; Bartell, F.E.
(2) Water; H ₂ 0; [7732-18-5]	J. Phys. Chem. <u>1952</u> , 56, 480–4.
VARIABLES:		PREPARED BY:
One temperature: 25°C		A.F.M. Barton
EXPERIMENTAL VALUES:		
	Density	Mutual solubilities
	$g mL^{-1}$	x_1 g(1)/100g sln (compiler)
Alcohol-rich phase	0.8284	0.712 93.3
Water-rich phase	0.9962	0.00110 ^a 0.62
^a From ref 1.		
	AUXILIARY	INFORMATION
METHOD/APPARATUS/PROCEDURE:		SOURCE AND PURITY OF MATERIALS;
Mixtures were placed in gl		(1) "best reagent grade";
flasks and were shaken int at least 3 days in a water	ermittently for bath. The	fractional distillation
organic phase was analyzed	for water content	(2) purified
by the Karl Fischer method phase was analyzed interfe	and the aqueous rometrically. The	
solubility measurements fo	rmed part of a	
study of water-organic lique tensions.	uid interfacial	
		ESTIMATED ERROR:
		Temperature: ±0.1°C
		REFERENCES:
		(1) Butler, J.A.V.; Thomson, D.W.;
		Maclennan, W.H. J. Chem. Soc. 1933, 67
1		

COMPONENTS:			ORIGINAL MEASUREMENTS:
(1) 1-Hexanol; C (2) Water; H ₂ O;	5 ^H 14 ^O ; [111-27-3] [7732-18-5]		Erichsen, L. von Brennst. Chem. <u>1952</u> , 33, 166-72.
VARIABLES:	<u> </u>		PREPARED BY:
Temperature: 0-22	o°c		S.H. Yalkowsky and Z. Maczynska
EXPERIMENTAL VALUES	: Mutual s	olubility	y of 1-hexanol (1) and water (2)
t/ ^o C		.ch phase ^x 1	(1)-rich phase
0	0.81	0.001	14 95.55 0.7911
10	0.70	0.001	
20	0.64 0.59	0.001 0.001	
30 40	0.59	0.001	
50	0.50	0.000	
60	0.52	0.000	
70	0.56	0.001	
80	0.61	0.001	
90	0.69	0.001	
100 110	0.80 0.91	0.001	
120	1.04	0.001	
130	1.19	0.002	
140	1.37	0.002	
150	1.63	0.002	
160	2.05	0.003	
170 180	2.70 3.61	0.005	
190	4.87	0.009	
200	6.75	0.012	
210	9.70	0.018	
220	16.30	0.034	42 44.65 0.1245
The UCST is 222.	2 [°] C		
	A	UXILIARY	INFORMATION
METHOD / APPARATUS / PH	ROCEDURE :		SOURCE AND PURITY OF MATERIALS:
The synthetic met	hod was used.		 Merck, or Ciba, or industrial product; distilled and chemically free from
glass ampules.	were carried out i These were placed	in an	isomers; b.p. 156.4-156.5 [°] C (751 mm Hg) ²⁰ 1.4184. n _D
windows. Cloud a thermocouple wo	quipped with two g points were measur und around the amp was repeated twic	red with pule.	(2) not specified.
			ESTIMATED ERROR:
			Not specified.
			REFERENCES :

1-Hexanol

	2-18-5]	27-3]	ORIGINAL MEASUREMENTS: Erichsen, L. von Naturwissenschaften <u>1952</u> , 39, 41-2. PREPARED BY: A. Maczynski and Z. Maczynska	
(2) Water; H ₂ O; [773 VARIABLES: Temperature: O-50 [°] C EXPERIMENTAL VALUES:	2-18-5]	27-3]	Naturwissenschaften <u>1952</u> , 39, 41-2. PREPARED BY:	
(2) Water; H ₂ O; [773 VARIABLES: Temperature: O-50 [°] C EXPERIMENTAL VALUES:	2-18-5]	- 	Naturwissenschaften <u>1952</u> , 39, 41-2. PREPARED BY:	
VARIABLES: Temperature: 0-50 [°] C EXPERIMENTAL VALUES:			PREPARED BY:	
Temperature: 0-50 ⁰ C EXPERIMENTAL VALUES:	Sol	·,		
Temperature: 0-50 ⁰ C EXPERIMENTAL VALUES:	Sol			
EXPERIMENTAL VALUES:	Sol		A. Maczynski and Z. Maczynska	
	 Sol			
	Sol		<u>1 </u>	
	Sol			
		ubility of 1-	-hexanol (1) in water (2)	
	t∕°c	x_1	g(1)/100g sln (compiler)	
	0	0.0014	0.79	
	10	0.0012	0.68	
	20	0.0011	0.62	
	30	0.0010	0.56	
	40	0.0010	0.56	
	50	0.0009	0.51	
		AUXILIAR	Y INFORMATION	-
METHOD/APPARATUS/PROCED	URE:		SOURCE AND PURITY OF MATERIALS:	
The synthetic method w	as used.		(1) not specified.	
No details were report	ed in th	e paper.	(2) not specified.	
			ESTIMATED ERROR:	
			Not specified.	
			Not specified.	
			REFERENCES :	

COMPONENTS :	ORIGINAL MEASUREMENTS:
(1) 1-Hexanol; C ₆ H ₁₄ O; [111-27-3]	Crittenden, E.D., Jr.; Hixon, A.N.;
6 14	Ind. Eng. Chem. <u>1954</u> , 46, 265-8.
(2) Water; H ₂ 0; [7732-18-5]	
VARIABLES:	PREPARED BY:
One temperature: 25 ⁰ C	A. Maczynski
EXPERIMENTAL VALUES:	
The solubility of 1-hexanol in water at 25 ⁰ C	
The corresponding mole fraction, $x_1^{}$, calcula	ted by the compiler is 0.0011.
The solubility of water in 1-hexanol at 25 ⁰ C	was reported to be 7.2 g(2)/100g sln.
The corresponding mole fraction, $x_2^{}$, calcula	ted by the compiler is 0.31.
	INFORMATION
METHOD /APPARATUS / PROCEDURE :	SOURCE AND PURITY OF MATERIALS:
Presumably the titration method described	 source not specified;
for ternary systems containing HCl was used.	purified;
In this method the solubility was determined by bringing 100-mL samples of (1) or (2) to	
a temperature $25.0 \pm 0.1^{\circ}$ C and the second component was then added from a calibrated	(2) not specified.
buret, with vigorous stirring, until the solution became permanently cloudy.	
	ESTIMATED ERROR:
	Temperature: ± 0.10 [°] C. Solubility: 2% (alcohol-rich)-10% (water-
	rich)
	REFERENCES:

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) 1-Hexanol; C ₆ H ₁₄ 0; [111-27-3] (2) Water; H ₂ 0; [7732-18-5]	Kinoshita, K.; Ishikawa, H.; Shinoda, K. Bull. Chem. Soc. Jpn. <u>1958</u> , 31, 1081-4.
VARIABLES:	PREPARED BY:
One temperature: 25°C	S.H. Yalkowsky; S.C. Valvani; A.F.M. Barton

EXPERIMENTAL VALUES:

The equilibrium concentration of 1-hexanol (1) in the water-rich phase at 25° C was reported to be 0.059 mol(1)/L sln. The mass percentage solubility was reported as 0.60 g(1)/100g sln, and the corresponding mole fraction solubility, calculated by the compilers, is $x_1 = 0.00106$.

AUXILIARY	INFORMATION
METHOD / APPARATUS / PROCEDURE :	SOURCE AND PURITY OF MATERIALS:
The surface tension in aqueous solutions of alcohols monotonously decreases up to their saturation concentration and remains constant in the heterogeneous region (ref 1-4). Surface tension was measured by the drop weight method, using a tip 6 mm in diameter, the measurements being carried out in a water thermostat. From the (surface tension) - (logarithm of concentration) curves the saturation points were determined as the intersections of the curves with the horizontal straight lines passing through	b.p. 155.7 - 156°C (2) not stated
the lowest experimental points.	ESTIMATED ERROR: Temperature: ± 0.05%
	Solubility: within 4%
	bolubility. within 4%
	 REFERENCES: (1) Motylewski, S. Z. Anorg. Chem. <u>1904</u>, 38, 410 (2) Taubamann, A. Z. physik. Chem. <u>1932</u>, A161, 141 (3) Zimmerman, H.K, Jr. Chem. Rev. <u>1952</u>, 51, 25 (4) Shinoda, K.; Yamanaka, T.; Kinoshita, K. J. Phys. Chem. <u>1959</u>, 63, 648

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) 1-Hexanol; C ₆ H ₁₄ 0; [111-27-3]	Venkataratnam, A.; Rao, R.I.
6 14	J. Sci. Ind. Res. <u>1958</u> , 17B, 108-10.
(2) Water; H ₂ 0; [7732-18-5]	<u> </u>
VARIABLES:	PREPARED BY:
One temperature: 30°C	A. Maczynski
EXPERIMENTAL VALUES:	
The solubility of 1-hexanol in water at 30° C	was reported to be 0.4 g(l)/100 sln.
The corresponding mole fraction, x_1 , calculat	ted by the compiler is 7×10^{-4} .
The solubility of water in 1-hexanol at 30°C	was reported to be 6.8 $g(2)/100g \ sln$.
The corresponding mole fraction, $x_2^{}$, calculated on the corresponding mole fraction, $x_2^{}$, calculated on the correspondence of the correspondenc	Led by the complifier is 0.29.
AUXILIARY	INFORMATION
ME THOD / APPARATUS / PROCEDURE :	SOURCE AND PURITY OF MATERIALS:
The method of appearance and disappearance	(1) source not specified;
of turbidity described in ref 1 was used.	distilled; b.p. 157°C, n ³⁰ 1.4188, d ³⁰ 0.8179 g/ml
No details were reported in the paper.	
	(2) distilled; free from carbon dioxide.
	ESTIMATED ERROR:
	Not enabled
	Not specified.
	REFERENCES:
	1. Othmer, D.F.; White, R.E.; Trueger, E.
	Ind. Eng. Chem. <u>1941</u> , 33, 1240.

1-Hexanol

COMPONENTS :	ORIGINAL MEASUREMENTS:
COTFORENTS.	URIGINAL MEASUREMENTS:
(1) 1-Hexanol; C ₆ H ₁₄ 0; [111-27-3]	Ababi, V.; Popa, A.
(2) Water; H ₂ 0; [7732-18-5]	An. Stiint. Univ. "Al. I. Cuza" Iasi. <u>1960</u> , 6, 929-42.
VARIABLES:	PREPARED BY:
One temperature: 25 [°] C	A. Maczynski
EXPERIMENTAL VALUES:	
The solubility of 1-hexanol in water at 25 ⁰ C	
The corresponding mole fraction, $x_1^{}$, calcula	ted by the compiler is 9 x 10^{-4} .
The solubility of water in 1-hexanol at 25 ⁰ C	was reported to be 7.9 g(2)/100g sln.
The corresponding mole fraction, $x_2^{}$, calcula	ted by the compiler is 0.33.
-	
AUXILIARY	INFORMATION
METHOD / APPARATUS / PROCEDURE :	SOURCE AND PURITY OF MATERIALS:
The turbidimetric method was used.	(1) Merck analytical reagent;
Ternary solubilities were described in the	used as received.
paper but nothing was reported on the method for binary solubilities.	(2) not specified.
	ESTIMATED ERROR:
	Not specified.
	REFERENCES:

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) 1-Hexanol; C ₆ H ₁₄ O; [111-27-3]	Chandy, C.A.; Rao, M.R.
	J. Chem. Eng. Data <u>1962</u> , 7, 473-5.
(2) Water; H ₂ O; [7732-18-5]	
VARIABLES:	PREPARED BY:
One temperature: 30 ⁰ C	A. Maczynski
EXPERIMENTAL VALUES:	
The solubility of 1-hexanol in water at 30 ⁰ C	was reported to be 0.65 $g(1)/100g \ sln$.
The corresponding mole fraction, $x_1^{}$, calcula	
_	
The solubility of water in 1-hexanol at 30 ⁰ C	was reported to be 7.0 g(2)/100g sln.
The corresponding mole fraction, $x_2^{}$, calcula	ted by the compiler is 0.30.
AUXILIARY	INFORMATION
ME THOD / APPARATUS / PROCEDURE :	SOURCE AND PURITY OF MATERIALS:
The method of appearance and disappearance	(1) Jean A. du Crocq, Jr. Ltd., (Holland);
of turbidity described in ref 1 was used.	distilled; b.p. range 156-156.5 [°] C.
No details were reported in the paper.	
	<pre>(2) distilled; free from carbon dioxide.</pre>
	ESTIMATED ERROR:
	Not specified.
	REFERENCES :
	1. Othmer, D.F.; White, R.E.; Trueger, E.
	Ind. Eng. Chem. <u>1941</u> , 33, 1240.

1-He>	anol 281
COMPONENTS: (1) 1-hexanol; C ₆ H ₁₄ 0; [111-27-3] (2) Water; H ₂ 0; [7732-18-5]	ORIGINAL MEASUREMENTS: * Hanssens, I. Associatie van normal alcoholen en hun affiniteit voor water en organische solventen Doctoraatsproefschrift, Leuven, <u>1969</u> . Huyskens, P.; Mullens, J.; Gomez, A.; Tack, J.
VARIABLES: One temperature; 298 K	Bull. Soc. Chim. Belg. <u>1975</u> , 84, 253-62. PREPARED BY: M.C. Haulait-Pirson; A.F.M. Barton
EXPERIMENTAL VALUES: The concentration of 1-hexanol (1) in the wat 0.0581 mol(1)/L sln, (0.0585 in the 1975 pub water (2) in the alcohol-rich phase was repor The corresponding solubilities on a mass/volu are 5.9 g(1)/L sln, and 135.0 g(2)/L sln, res (The temperature was unspecified in the Thesi published paper).	lished paper), and the concentration of ted as 7.493 mol(2)/L sln. me basis, calculated by the compilers, pectively.
AUXILIARY	INFORMATION
METHOD/APPARATUS/PROCEDURE: (1) and (2) were equilibrated using a cell described in ref 1. The Rayleigh M75 interference refractometer with the cell M160 for liquids was used for the determina- tion of the concentrations. Cell thick- nesses were 1, 3 and 10 cm depending on the concentration range. Standard solutions covering the whole range of concentrations investigated were used for the calibration.	SOURCE AND PURITY OF MATERIALS: (1) Merck p.a. (2) distilled
	ESTIMATED ERROR: Solubility: ± 0.00036 - 0.05 mol(1)/L sln, depending on the concentration REFERENCES: 1. Meeussen, E.; Huyskens, P.

J. Chim. Phys. 1966, 63, 845.

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COMPONENTS: (1) 1-Hexanol; C ₆ H ₁₄ 0; [111-27-3] (2) Water; H ₂ 0; [7732-18-5]	ORIGINAL MEASUREMENTS: Ratouis, M.; Dode, M.; Bull. Soc. Chim. Fr. <u>1965</u> , 3318-22.
VARIABLES: One temperature: 30 ⁰ C Ringer solution also studied	PREPARED BY: S.C. Valvani; S.H. Yalkowsky; A.F.M. Barton
reported to be 0.58 g(1)/100g sln. The corresponding mole fraction solub	he water-rich phase at equilibrium at 30° C was ility, calculated by the compilers, is $x_1 = 0.00103$. ch phase of a mixture with Ringer solution at 30° C

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE: In a round bottomed flask, 50 mL of water and a sufficient quantity of alcohol were introduced until two separate layers were The flask assembly was equilibrated formed. by agitation for at least 3 h in a constant temperature bath. Equilibrium solubility was attained by first supersaturation at a slightly lower temperature (solubility of alcohols in water decreases with increasing temperature) and then equilibrating at the desired temperature. The aqueous layer was separated after an overnight storage in The alcohol content was determined a bath. by reacting the aqueous solution with potassium dichromate and titrating the excess dichromate with ferrous sulfate solution in the presence of phosphoric acid and diphenylamine barium sulfonate as an indicator.

SOURCE AND PURITY OF MATERIALS:

- (1) Fluka A.G. Buchs S.G.; redistilled with 10:1 reflux ratio; b.p. 157^oC/760 mm Hg
 - $n_{\rm D}^{25} = 1.41607$
- (2) twice distilled from silica apparatus or ion-exchanged with Sagei A20.

ESTIMATED ERROR:

Solubility: relative error of 2 determinations less than 1%.

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Temperature: ±0.05<sup>o</sup>C.
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REFERENCES:

	ORIGINAL MEASUREMENTS:
(1) 1-Hexanol; C ₆ H ₁₄ 0; [111-27-3]	Krasnov, K.S., Gartseva, L.A.
(2) Water; H ₂ 0; [7732-18-5]	Izv. Vysshykh Uchebn. Zavedenii, Khim. Khim. Tekhnol. <u>1970</u> , 13, 9 52–6.
VARIABLES:	PREPARED BY:
Temperature: 12-40 [°] C	A. Maczynski and Z. Maczynska
EXPERIMENTAL VALUES:	<u> </u>
Solubility of wat	ter (2) in 1-hexanol (1)
t/ ^o C g(2)/100	Og sln x_2 (compiler)
12 7.	12 0.303
25 7.	16 0.304
40 7.	31 0.309
I	
AUXILIARY	INFORMATION
AUXILIARY METHOD / APPARATUS / PROCEDURE :	INFORMATION SOURCE AND PURITY OF MATERIALS;
	_

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) 1-Hexanol; C ₆ H ₁₄ O; [111-27-3] (2) Water; H ₂ O; [7732-18-5]	Vochten, R.; Petre, G. J. Colloid Interface Sci. <u>1973</u> , 42, 320-7.
VARIABLES: One temperature: 15 [°] C EXPERIMENTAL VALUES:	PREPARED BY: S.H. Yalkowsky; S.C. Valvani; A.F.M. Barton

The equilibrium concentration of 1-hexanol (1) in the water-rich phase at 15° C was reported to be 0.066 mol(1)/L sln.

The corresponding mass/volume solubility, calculated by the compilers, is 6.75 g(1)/L sln.

AUXILIARY	INFORMATION

METHOD / APPARATUS / PROCEDURE : SOURCE AND PURITY OF MATERIALS: (1) purified by distillation and The solubility was obtained from the surface tension of saturated solutions, preparative gas chromatography; measured by the static method of Wilhelmy b.p. 157.0°C/760 mm Hg (platinum plate). The apparatus consisted of an electrobalance (R.G. Cahn) connected (2) triply distilled from permanganate with a high impedance null detector (Fluke solution type 845 AR). An all-Pyrex vessel was used. ESTIMATED ERROR: Temperature: $\pm 0.1^{\circ}C$ Solubility: (probably standard deviation) ± 0.001 mo1(1)/L s1n. REFERENCES:

1-Hexanol

COMPONENTS :		1	ORIGINAL MEACHDEMENTE.		
			ORIGINAL MEASUREMENTS:		
(1) 1-Hexanol; C ₆ H ₁₄ O; [111-27-3]		27-3]	Hill, D.J.T.; White, L.R.		
(2) Water; H ₂ 0; [7732-18-5]			Aust. J. Chem., <u>1974</u> , 27, 1905–16.		
VARIABLES:			PREPARED BY:		
Temperature: 279-306	К		A. Maczynski		
EXPERIMENTAL VALUES:	Solu	ubility of 1-1	hexanol (1) in water (2)		
	<i>т</i> /к	x_1	g(1)/100g sln (compiler)		
	278.66	0.001398	0.7879		
	280.00	0.001358	0.7655		
	281.83	0.001308	0.7375		
	284.15	0.001252	0.7061		
	286.09	0.001209	0.6820		
	287.83	0.001179	0.6651		
	290.19	0.001139	0.6427		
	293.86	0.001085	0.6124		
296.14 0.001060			0.5984		
		0.001034	0,5838		
	300.14	0.001021	0.5764		
	302.09	0.001010	0.5702		
	304.07	0.0009986	0.5639		
	306.24	0.0009846	0.5560		
		AUXILIARY	INFORMATION		
METHOD / APPARATUS / PROCE	DURE:		SOURCE AND PURITY OF MATERIALS:		
The interferometric	method was	used.	(1) Fluka puriss grade;		
The interferometric method was used. The saturated solutions of (1) were prepar- ed in an equilibrium flask and solution concentrations were determined from their refractive index using a Zeiss interfero- meter and appropriate calibration curves. Duplicate determinations were always within the error limits calculated from the curve fit to the calibration measurements (0.5% at the 95% confidence level).		solution from their interfero- ion curves. always within om the curve	b.p. 335.7 K (20 mm Hg), n ²⁵ 1.4150, 99.5% purity.		
Numerous technical details were reported		e reported	ESTIMATED ERROR:		
in the paper.			Temperature: ± 0.02 [°] C Solubility: < 0.5% (accuracy at 95% confidence level)		
			REFERENCES :		

COMPONENTS:	ORIGINAL MEASUREMENTS:		
(1) 1-Hexanol; C ₆ H ₁₄ 0; [111-27-3]	Korenman, I.M.; Gorokhov, A.A.; Polozenko,		
(2) Water; H ₂ 0; [7732-18-5]	G.N. Zhur. Fiz. Khim. <u>1974</u> , 48, 1810–2; *Russ. J. Phys. Chem. <u>1974</u> , 48, 1065–7 _.		
VARIABLES:	PREPARED BY:		
One temperature: 25 [°] C	A.F.M. Barton		
was reported to be 0.058 mol(1)/L sln ar alcohol-rich phase was reported to be 3.59	9 mol(2)/L sln. volume basis, calculated by the compiler,		

AUXILIARY	INFORMATION
METHOD APPARATUS/PROCEDURE: The two liquids were shaken in a closed vessel at 25.0±0.1°C until equilibrium was established. The soly of the alcohol in the aqueous phase was determined on a Tsvet-1 chromatograph with a flame-ionisation de- tector. The sorbent was a polyethylene glycol adipate deposited on Polychrom-1 (10% of the mass of the carrier). The 1 m column had an internal diameter 4 um, its temp 140°C, and the flow of the carrier gas (nit- rogen) 50 mL min ⁻¹ . The soly of water in the alcohol was determined on a UKh ⁻¹ uni- versal chromatograph under isothermal con- ditions (150°C) with a heat-conductivity detector. The 1 m by 6 mm column was filled with Polysorb. The carrier gas was helium (50 mL min ⁻¹). The study formed part of an investigation of salting-out by alkali halides of higher alcohol-water systems.	ESTIMATED ERROR:

COMPONENTS:			ORIGI	NAL MEASUREMENTS:	
(1) 1-Hexanol; C ₆ H ₁₄ 0; [111-27-3]		Lavrova, O.A.; Lesteva, T.M.			
0 14		Zh. F	iz. Khim., 1976, 5	0, 1617. Dep. Doc.	
(2) Water; H	1 ₂ 0; [7732-18-5]	ľ		<i>I</i> , 3813–75	5
VARIABLES:			PREPA	RED BY:	
Temperature:	40 and 60°C		A. Ma	czynski	
EXPERIMENTAL	ALUES:		L <u></u>	· • · · · · · · · · · · · · · · · · · ·	
	Mutual s	solubility of	1-hexa	nol(1) and water	(2)
t/°c	g(1)/100g	g sln		x_1 (compi	ler)
			se	(2)-rich phase	
40	0.50	93.0		0.0008	0.701
60	0.51	90.9		0.00090	0.638
		AUXILIARY	INFOR		
METHOD APPARA	TUS / DDOCEDUDE .				TEDIALC
METHOD/APPARA	TUS/PROCEDURE:			E AND PURITY OF MA	
The titrati	on method was used.	,	(1)	source not specif	
No details	were reported in th	ne paper.		distilled with he purity 99.95 wt %	with 0.05 wt % water,
	·	r - r			$157.0^{\circ}C, d_4^{20}$ 0.8186
					197.0.0, a ₄ 0.0100
			(2)	not specified.	
			ESTI	MATED ERROR:	
				Not specified.	
			DEPE	DENCLO	
			REFE	RENCES :	
			1		

COMPONENTS:		ORIGINAL MEASUREMENTS:
	1	Filippov, V.V.; Markuzin, N.P.;
(1) 1-Hexanol; C ₆ H ₁₄ 0; [111-27-3]		Sazonov, V.P.
(2) Water; H ₂ 0; [7732-18-5]		Zh. Prikl. Khim. <u>1977</u> , 6, 1321-4.
_		
VARIABLES:		PREPARED BY:
Temperature: 21-40 ⁰ C		A. Maczynski and Z. Maczynska
EXPERIMENTAL VALUES:		
Solubili	ity of war	ter in l-hexanol
t/ ^o c	<i>x</i> ₂	g(2)/100g sln
21.0	0.276	6.30
23.0	0.283	6.50
40.0	0.305	7.18
	AUXILIARY	INFORMATION
METHOD/APPARATUS/PROCEDURE:		SOURCE AND PURITY OF MATERIALS:
Not specified		(1) pure grade reagent;
		purified; purity not specified.
		(2) twice distilled
		ESTIMATED ERROR:
		Not specified.
		REFERENCES:

COMPONENTS:	ORIGINAL MEASUREMENTS:		
(1) 1-Hexanol; C ₆ H ₁₄ 0; [111-27-3] (2) Water; H ₂ 0; [7732-18-5]	Nishino, N.; Nakamura, M. Bull. Chem. Soc. Jpn. <u>1978</u> , 51, 1617-20; <u>1981</u> , 54, 545-8.		
VARIABLES:	PREPARED BY:		
Temperature: 275-360 K	G.T. Hefter		

EXPERIMENTAL VALUES:

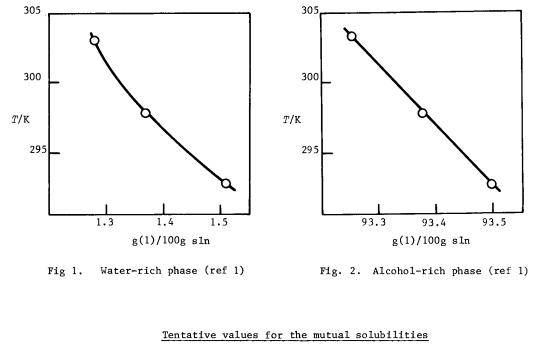
The mutual solubility of (1) and (2) in mole fractions are reported over the temperature range in graphical form. Graphical data are also presented for the heat of evaporation of (1).

AUXILIARY	INFORMATION
METHOD/APPARATUS/PROCEDURE: The turbidimetric method was used. Twenty to thirty glass ampoules containing aqueous solutions of ca . 5 cm ³ of various concentra- tions near the solubility at room tempera- ture were immersed in a water thermostat. The distinction between clear and turbid ampoules was made after equilibrium was established (ca . 2h). The smooth curve drawn to separate the clear and turbid regions was regarded as the solubility	 SOURCE AND PURITY OF MATERIALS: (1) G.R. grade (various commercial sources given); dried over calcium oxide; kept in ampoules over magnesium powder. (2) Deionized, refluxed for 15h with potassium permanganate then distilled.
curve.	ESTIMATED ERROR: Not stated
	REFERENCES :

COMPONENTS:		ORIGINAL MEASUREM	ENTS:	
(1) 1-Hexanol; C ₆ H ₁₄ 0; [111-27-3]		Tokunaga, S.; Manabe, M.; Koda, M.		
(2) Water; H ₂ 0; [7732-18	-5]		to Semmon Gakko Kiyo,	
(2) water, 120, 17752 10		-	moirs Niihama Technical	
		college, sci. an	d Eng.) <u>1980</u> , 16, 96-101.	
ARIABLES:		PREPARED BY:	<u> </u>	
Temperature: 15-35 ⁰ C		A.F.M. Barton		
EXPERIMENTAL VALUES:				
S	olubility of water (in the alcohol 	-rich phase	
t/ ^o c	g(2)/100g sln	<i>x</i> ₂	mol(1)/mol(2)	
15	7.13	0.303	2.29	
20	7.30	0.309	2.25	
25	7.38	0.311	2.22	
30	7.43	0.313	2.19	
35	7.57	0.317	2.16	
	AUXILIARY	INFORMATION	5	
METHOD / APPARATUS / PROCEDURI	3:	SOURCE AND PURIT	Y OF MATERIALS:	
The mixtures of 1-hexano		(1) distilled;	l e stalla la sas	
(-10mL) were stirred magn stoppered vessel and allo		chromatogra	es detectable by gas phy	
10-12h in a water thermos rich phase was analyzed :		(2) deionized;		
Fischer titration.		distilled p	rior to use	
		ESTIMATED ERROR:		
		Temperature: ±	0.1 [°] C	
			ch result is the mean of ree determinations.	
		REFERENCES ;		
		KEFEKENCES:		
		REFERENCES :		
		KEFLKENCES :		
		REFERENCES :		
		REFERENCES :		

COMPONENTS:	EVALUATOR:
(1) 2-Hexanol (n-butylmethylcarbinol);	Z. Maczynska, Institute of Physical
с ₆ н ₁₄ 0; [626-93-7]	Chemistry of the Polish Academy of Sciences,
(2) Water; H ₂ 0; [7732-18-5]	Warsaw, Poland; and A.F.M. Barton, Murdoch
(2) "	University, Perth, Western Australia.
	November 1982.
	1

Solubilities in the system comprising 2-hexanol (1) and water (2) have been reported in four publications. Ginnings and Webb (ref 1) carried out measurements of the mutual solubilities in the two phases at 293, 298 and 303 K by the volumetric method (Figures 1 and 2). Ratouis and Dode (ref 2) determined the solubility of (1) in the water-rich phase at one temperature (303 K) by an analytical method. Their value of 1.19 g(1)/100 g sln is in good agreement with the value $1.28 \pm 0.1 \text{ g(1)}/100 \text{ g sln}$ of ref 1. Nishino and Nakamura provided graphical information only of the solubility of (1) in (2) (ref 3) and (2) in (1) (ref 4). Since direct comparison is possible for only a single data point, the data of ref 1 are regarded as tentative.



of 2-hexanol (1) and water (2)

<i>Т</i> /к	Water-rich	Water-rich phase		Alcohol-rich phase	
	g(1)/100g sln	$10^{3}x_{1}$	g(2)/100g sln	^x 2	
293	1.5	2.7	6.5	0.283	
298	1.4	2.4	6.6	0.287	
303	1.3	2.3	6.7	0.292	
References					
1. Ginnings,	P.M.; Webb, R. J. Am.	Chem. Soc. <u>19</u>	<u>38</u> , <i>60</i> , 1388.		
2. Ratouis,	M.; Dode, M. Bull. Soc.	Chim. Fr. <u>19</u>	65, 3318.		
3. Nishino,	N.; Nakamura, M. Bull. C	them. Soc. Jp	n. <u>1978</u> , 51, 1617.		

4. Nishino, N.; Nakamura, M. Bull. Chem. Soc. Jpn. <u>1981</u>, 54, 545.

COMPONENTS:			ORIGINAL MEASU	REMENTS:	
(1) 2-Hexanol (n-butylmethylcarbinol);		Ginnings, P.M.; Webb, R.			
с ₆ н ₁₄ 0 [623-93-7]		J. Am. Chem. S	50c. 1938,	<i>60</i> , 1388-9.	
(2) Water;	(2) Water; H ₂ 0; [7732-18-5]				-
VARIABLES:			PREPARED BY:		
Temperature:	20–30 [°] C		A. Maczynski and Z. Maczynska		
EXPERIMENTAL	VALUES:				
	Mutual sc	olubility of 2-	hexanol(1) and	water(2)	
t/°c	g(1)/100)o eln		<i>r</i> (c	compiler)
07 0	(2)-rich phase		e (2)-rich	T	
20	1.51	93.50	0.0	0270	0.7171
25	1.37	93.38	0.0	0244	0.7132
30	1.28	93.25	0.0	0228	0.7089
		Relativ	ve density, d_{4}		
			4		
	t/ ^o C	Water-rich ph	nase Alcoho	l-rich pha	ise
	20	0 .99 65	0	.8264	
	25	0.9954		.8231	
	30	0.9942	0	.8194	
		··· ··· ······························			i
		AUXILIARY	INFORMATION		
	ATUS/PROCEDURE:		SOURCE AND PUR		
The volumet in ref l.	ric method was used	l as described		best grad ed, and re	le; edistilled from calcium
	nents were introduce		b.p. rat	nge 139.0-	-140.0°C, d_4^{25} 0.8108,
calibrated	to a two-bulb gradua flask and shaken me	chanically	(2) not spe	cified.	
	-bath at constant te Lcient time the liqu				
allowed to was measure	separate and the to ed. Upon centrifug				
phase separ	ation line was read	l, and phase			
weights of	volumes were calculated. From the total weights of the components, the total volume,		ESTIMATED ERR	OR:	
individual phase volumes, and component concentrations in either phase were evaluated.		Temperature:	± 0.1°C		
		Solubility:		than 0.1 wt % f error not specified)	
		REFERENCES:			
			, P.M.; E <u>7</u> , <i>59</i> , 111	Baum, R.J. J. Am. Chem. Ll.	
L					

exanol 293
ORIGINAL MEASUREMENTS: Ratouis, M.; Dode, M.; Bull. Soc. Chim. Fr. <u>1965</u> , 3318-22.
PREPARED BY: S.C. Valvani; S.H. Yalkowsky; A.F.M. Barton
r-rich phase at equilibrium at 30° C calculated by the compilers is $x_1 = 0.00212$. se of a mixture with Ringer solution at 30° C
Y INFORMATION
SOURCE AND PURITY OF MATERIALS: (1) Fluka A.G. Buchs S.G. redistilled with 10:1 reflux ratio b.p. 138.6-138.8°C/770 mm Hg $n_D^{25} = 1.41269$

294 Six-carbo	n Alcohols
COMPONENTS: (1) 2-Hexanol (<i>n-buty lmethy learbinol</i>) C ₆ H ₁₄ 0; [626-93-7] (2) Water; H ₂ 0; [7732-18-5]	ORIGINAL MEASUREMENTS: Nishino, N.; Nakamura, M. Bull. Chem. Soc. Jpn. <u>1978</u> , 51, 1617-20; <u>1981</u> , 54, 545-8.
VARIABLES: Temperature: 275 - 360 K	PREPARED BY: G.T. Hefter
EXPERIMENTAL VALUES:	
The mutual solubility of (1) and (2) in mole temperature range in graphical form. Graphi heat of evaporation of (1)	
	INFORMATION
METHOD /APPARATUS / PROCEDURE :	SOURCE AND PURITY OF MATERIALS:
The turbidimetric method was used. Twenty to thirty glass ampoules containing aqueous solutions of σa . 5 cm of various concentra- tions near the solubility at room temperature were immersed in a water thermostat. The distinction between clear and turbid ampoules was made after equilibrium was established (σa . 2h). The smooth curve drawn to separate the clear and turbid regions was regarded as the solubility curve.	 (1) G.R. grade (various commercial sources given); dried over calcium oxide; kept in ampoules over magnesium powder. (2) Deionized, refluxed for 15h with
	ESTIMATED ERROR: Not stated REFERENCES:

COMPONENTS:	EVALUATOR:
(1) 3-Hexanol (n-propylethylcarbinol)	Z. Maczynska, Institute of Physical
C ₆ H ₁₄ 0; [623-37-0]	Chemistry of the Polish Academy of Sciences,
(2) Water; H ₂ 0; [7732-18-5]	Warsaw, Poland; and A.F.M. Barton, Murdoch
	University, Perth, Western Australia.
	November 1982

Solubilities in the system comprising 3-hexanol (1) and water (2) have been reported in four publications. Ginnings and Webb (ref 1) carried out measurements of the mutual solubilities in the two phases at 293, 298 and 303 K by the volumetric method (Figures 1 and 2). Ratouis and Dodé (ref 2) determined the solubility of (1) in the water-rich phase at one temperature (303 K) by an analytical method. Their value of 1.36 g(1)/100g sln is in good agreement with the value 1.49 ± 0.1 g(1)/100g sln of ref 1. Nishino and Nakamura provided graphical information only of the solubility of (1) in (2) (ref 3) and of (2) in (1) (ref 4). Since direct comparison is possible for only a single data point, the data of ref 1 are regarded as tentative.

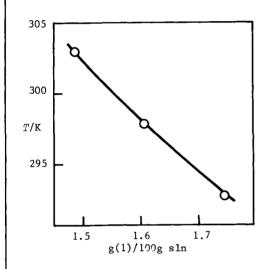


Fig. 1. Water-rich phase (ref 1)

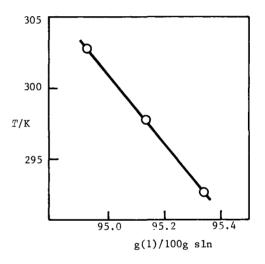


Fig. 2. Alcohol-rich phase (ref 2)

Tentative values for the mutual solubilities of 3-hexanol (1) and water (2)

<i>Т</i> /К	Water-rich	phase	Alcohol-rich	phase
	g(1)/100g sln	$10^{3}x_{1}$	g(2)/100g sln	<i>x</i> 2
293	1.8	3.1	4.7	0.217
298	1.6	2.9	4.9	0.225
303	1.5	2.7	5.1	0.232
References				
l. Ginnings, P.	M.; Webb, R. J. Am. C	Them. Soc. <u>1938</u> ,	60, 1388.	
2. Ratouis, M.;	Dode, M. Bull. Soc.	Chim. Fr. 1965,	3318.	
3. Nishino, N.;	Nakamura, M. Bull. C	Them. Soc. Jpn.	<u>1978</u> , <i>51</i> , 1617.	
4. Nishino, N.;	Nakamura, M. Bull. C	Them. Soc. Jpn.	<u>1981, 54, 545.</u>	

COMPONENTS:	ORIC	GINAL MEASUREMENTS:		
<pre>(1) 3-Hexanol (n-propylethylcarbinol); C₆H₁₄0; [623-37-0] (2) Water; H₂0; [7732-18-5]</pre>		Ginnings, P.M.; Webb, R. J. Am. Chem. Soc. <u>1938</u> , 60, 1388-9.		
VARIABLES: Temperature: 20-30 ⁰ C	1	PREPARED BY: A. Maczynski and Z. Maczynska		
-				
EXPERIMENTAL VALUES: Mutual solub	oility of 3-hexa	anol(1) and water(2)		
t/ ^o C g(1)/100g	sln	x_1 (comp	iler)	
		(2)-rich phase		
20 1.75	95.34	0.00313	0.7829	
25 1.61	95.14	0.00286	0.7753	
30 1.49	94.93	0.00266	0.7675	
	Relative dens	sity, d_{μ}		
t/ ⁰ C Water-rich phase Alcohol-rich phase				
20	0.9952	0.8264		
25	0.9951	0.8225		
	AUXILIARY INFO	ORMATION		
METHOD/APPARATUS/PROCEDURE: The volumetric method was used as described in ref. 1. Both components were introduced in known amounts into a two-bulb graduated and calibrated flask and shaken mechanically in a water-bath at constant temperature. After sufficient time the liquids were allowed to separate and the total volume was measured. Upon centrifugation, the phase separation line was read, and phase volumes were calculated. From the total weights of the components, the total volume, individual phase volumes, and component concentrations in either phase were evaluated.		(type o	nard synthesis; alcium oxide; -135.0°C, fied. than 0.1 wt % f error not specified) 	

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) 3-Hexanol (n-propylethylcarbinol)	Ratouis, M.; Dodé, M.;
$C_6 H_{14} 0; [623-37-0]$	Bull. Soc. Chim. Fr. <u>1965</u> , 3318-22.
÷ -,	<u> </u>
(2) Water; H ₂ 0 [7732-18-5]	
VARIABLES:	PREPARED BY:
One temperature: 30°C	S.C. Valvani; S.H. Yalkowsky; A.F.M. Barton
Ringer solution also studied	
EXPERIMENTAL VALUES:	
The proportion of 3-hexanol (1) in the water-	rich phone at equilibrium at 30 ⁰ C area
reported to be 1.36 $g(1)/100g$ sln.	fich phase at equilibrium at 50 C was
The corresponding mole fraction solubility, o	alculated by the compilers is
$x_1 = 0.00243.$	alculated by the complicity, is
The proportion of (1) in the water-rich phase	of a mixture with Ringer solution at 30° C
was reported to be $1.25 \text{ g}(1)/100\text{g sln}$.	
	······································
	INFORMATION
METHOD/APPARATUS/PROCEDURE:	INFORMATION SOURCE AND PURITY OF MATERIALS:
In a round bottomed flask, 50 mL of water	SOURCE AND PURITY OF MATERIALS: (1) Fluka A.G., Buchs S.G.
In a round bottomed flask, 50 mL of water and a sufficient quantity of alcohol were	SOURCE AND PURITY OF MATERIALS: (1) Fluka A.G., Buchs S.G. redistilled with 10:1 reflux ratio
In a round bottomed flask, 50 mL of water and a sufficient quantity of alcohol were introduced until two separate layers were formed. The flask assembly was equilibrate	SOURCE AND PURITY OF MATERIALS: (1) Fluka A.G., Buchs S.G. redistilled with 10:1 reflux ratio b.p. 136.1-136.2°C
In a round bottomed flask, 50 mL of water and a sufficient quantity of alcohol were introduced until two separate layers were formed. The flask assembly was equilibrate by agitation for at least 3 h in a constant	<pre>SOURCE AND PURITY OF MATERIALS: (1) Fluka A.G., Buchs S.G. redistilled with 10:1 reflux ratio</pre>
In a round bottomed flask, 50 mL of water and a sufficient quantity of alcohol were introduced until two separate layers were formed. The flask assembly was equilibrate by agitation for at least 3 h in a constant temperature bath. Equilibrium solubility was attained by first supersaturation at a	SOURCE AND PURITY OF MATERIALS: (1) Fluka A.G., Buchs S.G. redistilled with 10:1 reflux ratio b.p. 136.1-136.2°C $n_{\rm D}^{25}$ = 1.41392
In a round bottomed flask, 50 mL of water and a sufficient quantity of alcohol were introduced until two separate layers were formed. The flask assembly was equilibrate by agitation for at least 3 h in a constant temperature bath. Equilibrium solubility was attained by first supersaturation at a slightly lower temperature (solubility of	SOURCE AND PURITY OF MATERIALS: (1) Fluka A.G., Buchs S.G. redistilled with 10:1 reflux ratio b.p. 136.1-136.2°C
In a round bottomed flask, 50 mL of water and a sufficient quantity of alcohol were introduced until two separate layers were formed. The flask assembly was equilibrate by agitation for at least 3 h in a constant temperature bath. Equilibrium solubility was attained by first supersaturation at a slightly lower temperature (solubility of alcohols in water decreases with increasing temperature) and then equilibrating at the	SOURCE AND PURITY OF MATERIALS: (1) Fluka A.G., Buchs S.G. redistilled with 10:1 reflux ratio b.p. 136.1-136.2°C $n_{\rm D}^{25}$ = 1.41392 (2) twice distilled from silica apparatus
In a round bottomed flask, 50 mL of water and a sufficient quantity of alcohol were introduced until two separate layers were formed. The flask assembly was equilibrate by agitation for at least 3 h in a constant temperature bath. Equilibrium solubility was attained by first supersaturation at a slightly lower temperature (solubility of alcohols in water decreases with increasing	SOURCE AND PURITY OF MATERIALS: (1) Fluka A.G., Buchs S.G. redistilled with 10:1 reflux ratio b.p. 136.1-136.2°C $n_{\rm D}^{25}$ = 1.41392 (2) twice distilled from silica apparatus
In a round bottomed flask, 50 mL of water and a sufficient quantity of alcohol were introduced until two separate layers were formed. The flask assembly was equilibrate by agitation for at least 3 h in a constant temperature bath. Equilibrium solubility was attained by first supersaturation at a slightly lower temperature (solubility of alcohols in water decreases with increasing temperature) and then equilibrating at the desired temperature. The aqueous layer was separated after an overnight storage in a bath. The alcohol content was determined	SOURCE AND PURITY OF MATERIALS: (1) Fluka A.G., Buchs S.G. redistilled with 10:1 reflux ratio b.p. 136.1-136.2°C $n_D^{25} = 1.41392$ (2) twice distilled from silica apparatus or ion-exchanged with sagei A20.
In a round bottomed flask, 50 mL of water and a sufficient quantity of alcohol were introduced until two separate layers were formed. The flask assembly was equilibrate by agitation for at least 3 h in a constant temperature bath. Equilibrium solubility was attained by first supersaturation at a slightly lower temperature (solubility of alcohols in water decreases with increasing temperature) and then equilibrating at the desired temperature. The aqueous layer was separated after an overnight storage in	 SOURCE AND PURITY OF MATERIALS: (1) Fluka A.G., Buchs S.G. redistilled with 10:1 reflux ratio b.p. 136.1-136.2°C n²⁵_D = 1.41392 (2) twice distilled from silica apparatus or ion-exchanged with sagei A20. ESTIMATED ERROR: Solubility: relative error of 2 determina-
In a round bottomed flask, 50 mL of water and a sufficient quantity of alcohol were introduced until two separate layers were formed. The flask assembly was equilibrate by agitation for at least 3 h in a constant temperature bath. Equilibrium solubility was attained by first supersaturation at a slightly lower temperature (solubility of alcohols in water decreases with increasing temperature) and then equilibrating at the desired temperature. The aqueous layer was separated after an overnight storage in a bath. The alcohol content was determined by reacting the aqueous solution with potassium dichromate and titrating the excess dichromate with ferrous sulfate	SOURCE AND PURITY OF MATERIALS: (1) Fluka A.G., Buchs S.G. redistilled with 10:1 reflux ratio b.p. 136.1-136.2°C $n_D^{25} = 1.41392$ (2) twice distilled from silica apparatus or ion-exchanged with sagei A20. ESTIMATED ERROR: Solubility: relative error of 2 determina- tions less than 1%.
In a round bottomed flask, 50 mL of water and a sufficient quantity of alcohol were introduced until two separate layers were formed. The flask assembly was equilibrate by agitation for at least 3 h in a constant temperature bath. Equilibrium solubility was attained by first supersaturation at a slightly lower temperature (solubility of alcohols in water decreases with increasing temperature) and then equilibrating at the desired temperature. The aqueous layer was separated after an overnight storage in a bath. The alcohol content was determined by reacting the aqueous solution with potassium dichromate and titrating the excess dichromate with ferrous sulfate solution in the presence of phosphoric acid and diphenylamine barium sulfonate as an	 SOURCE AND PURITY OF MATERIALS: (1) Fluka A.G., Buchs S.G. redistilled with 10:1 reflux ratio b.p. 136.1-136.2°C n²⁵_D = 1.41392 (2) twice distilled from silica apparatus or ion-exchanged with sagei A20. ESTIMATED ERROR: Solubility: relative error of 2 determina- tions less than 1%. Temperature: ±0.05°C
In a round bottomed flask, 50 mL of water and a sufficient quantity of alcohol were introduced until two separate layers were formed. The flask assembly was equilibrate by agitation for at least 3 h in a constant temperature bath. Equilibrium solubility was attained by first supersaturation at a slightly lower temperature (solubility of alcohols in water decreases with increasing temperature) and then equilibrating at the desired temperature. The aqueous layer was separated after an overnight storage in a bath. The alcohol content was determined by reacting the aqueous solution with potassium dichromate and titrating the excess dichromate with ferrous sulfate solution in the presence of phosphoric acid	SOURCE AND PURITY OF MATERIALS: (1) Fluka A.G., Buchs S.G. redistilled with 10:1 reflux ratio b.p. 136.1-136.2°C $n_D^{25} = 1.41392$ (2) twice distilled from silica apparatus or ion-exchanged with sagei A20. ESTIMATED ERROR: Solubility: relative error of 2 determina- tions less than 1%.
In a round bottomed flask, 50 mL of water and a sufficient quantity of alcohol were introduced until two separate layers were formed. The flask assembly was equilibrate by agitation for at least 3 h in a constant temperature bath. Equilibrium solubility was attained by first supersaturation at a slightly lower temperature (solubility of alcohols in water decreases with increasing temperature) and then equilibrating at the desired temperature. The aqueous layer was separated after an overnight storage in a bath. The alcohol content was determined by reacting the aqueous solution with potassium dichromate and titrating the excess dichromate with ferrous sulfate solution in the presence of phosphoric acid and diphenylamine barium sulfonate as an	 SOURCE AND PURITY OF MATERIALS: (1) Fluka A.G., Buchs S.G. redistilled with 10:1 reflux ratio b.p. 136.1-136.2°C n²⁵_D = 1.41392 (2) twice distilled from silica apparatus or ion-exchanged with sagei A20. ESTIMATED ERROR: Solubility: relative error of 2 determina- tions less than 1%. Temperature: ±0.05°C
In a round bottomed flask, 50 mL of water and a sufficient quantity of alcohol were introduced until two separate layers were formed. The flask assembly was equilibrate by agitation for at least 3 h in a constant temperature bath. Equilibrium solubility was attained by first supersaturation at a slightly lower temperature (solubility of alcohols in water decreases with increasing temperature) and then equilibrating at the desired temperature. The aqueous layer was separated after an overnight storage in a bath. The alcohol content was determined by reacting the aqueous solution with potassium dichromate and titrating the excess dichromate with ferrous sulfate solution in the presence of phosphoric acid and diphenylamine barium sulfonate as an	 SOURCE AND PURITY OF MATERIALS: (1) Fluka A.G., Buchs S.G. redistilled with 10:1 reflux ratio b.p. 136.1-136.2°C n²⁵_D = 1.41392 (2) twice distilled from silica apparatus or ion-exchanged with sagei A20. ESTIMATED ERROR: Solubility: relative error of 2 determina- tions less than 1%. Temperature: ±0.05°C
In a round bottomed flask, 50 mL of water and a sufficient quantity of alcohol were introduced until two separate layers were formed. The flask assembly was equilibrate by agitation for at least 3 h in a constant temperature bath. Equilibrium solubility was attained by first supersaturation at a slightly lower temperature (solubility of alcohols in water decreases with increasing temperature) and then equilibrating at the desired temperature. The aqueous layer was separated after an overnight storage in a bath. The alcohol content was determined by reacting the aqueous solution with potassium dichromate and titrating the excess dichromate with ferrous sulfate solution in the presence of phosphoric acid and diphenylamine barium sulfonate as an	 SOURCE AND PURITY OF MATERIALS: (1) Fluka A.G., Buchs S.G. redistilled with 10:1 reflux ratio b.p. 136.1-136.2°C n²⁵_D = 1.41392 (2) twice distilled from silica apparatus or ion-exchanged with sagei A20. ESTIMATED ERROR: Solubility: relative error of 2 determina- tions less than 1%. Temperature: ±0.05°C

298 Six-carbor	n Alcohols
COMPONENTS: (1) 3-Hexanol (n-propylethylcarbinol) C ₆ H ₁₄ 0; [623-37-0] (2) Water; H ₂ 0; [7732-18-5]	ORIGINAL MEASUREMENTS: Nishino, N.; Nakamura, M. Bull. Chem. Soc. Jpn. <u>1978</u> , 51, 1617-20; <u>1981</u> , 54, 545-8 PREPARED BY: G.T. Hefter fractions are reported over the
AUXILIARY	INFORMATION
METHOD APPARATUS/PROCEDURE: The tubidimetric method was used. Twenty to thirty glass ampoules containing aqueous solutions of ca . 5 cm of various concentra- tions near the solubility at room tempera- ture were immersed in a water thermostat. The distinction between clear and turbid ampoules was made after equilibrium was established (ca . 2h). The smooth curve drawn to separate the clear and turbid regions was regarded as the solubility curve.	 SOURCE AND PURITY OF MATERIALS: (1) G.R. grade (various commercial sources given); dried over calcium oxide; kept in ampoules over magnesium powder. (2) Deionized, refluxed for 15h with potassium permanganate then distilled. ESTIMATED ERROR: Not stated

REFERENCES:

COMPONENTS:	ORIGINAL MEASUREMENTS:
 (1) 2,3,3-Trimethyl-2-butanol; C₇H₁₆0; [594-83-2] (2) Water; H₂0; [7732-18-5] 	Ginnings, P.M.; Hauser, M. J. Am. Chem. Soc. <u>1938</u> , 60, 2581-2.
VARIABLES: One temperature: 40° C EXPERIMENTAL VALUES: The mutual solubility of 2,3,3-trimethyl-2-bu 2.20 and 94.72 g(1)/100g sln. The corresponding mole fractions x_1 calculate and 0.7355. The relative densities of the water-rich and respectively.	d by the compilers are 3.47 x 10^{-3}
AUXILIARY METHOD/APPARATUS/PROCEDURE: The volumetric method was used as described in ref 1. Both components were introduced in known amounts into a two-bulb graduated and calibrated flask and shaken mechanically in a water-bath at constant temperature. After sufficient time the liquids were allowed to separate and the total volume was measured. Upon centrifugation, the phase separation line was read, and phase volumes were calculated. From the total weights of the components, the total volume, individual phase volumes, and component concentrations in either phase were evaluated.	<pre>INFORMATION SOURCE AND PURITY OF MATERIALS: (1) prepared by Grignard synthesis; distilled from calcium oxide; b.p. range 130.3-130.8°C, d²⁵ 0.8380; purity not specified. (2) not specified. (2) not specified. (2) not specified. ESTIMATED ERROR: Solubility: better than 0.1 wt % (type of error not specified) REFERENCES: 1. Ginnings, P.M.; Baum, R.J. J. Am. Chem. Soc. 1937, 59, 1111.</pre>

COMPONENTS :	ORIGINAL MEASUREMENTS:	
(1) 2,2-Dimethyl-1-pentanol; C ₇ H ₁₆ 0;	Ratouis, M.; Dodé, M.	
[2370-12-9]	Bull. Soc. Chim. Fr. <u>1965</u> , 3318–22	
(2) Water: H ₂ 0; [7732-18-5]		
VARIABLES: Temperature: 25 ⁰ C and 30 ⁰ C	PREPARED BY: S.C. Valvani; S.H. Yalkowsky; A.F.M. Barton	
-	S.C. Valvani; S.H. falkowsky; A.F.M. barton	
Ringer solution also studied		
EXPERIMENTAL VALUES:		
Proportion of 2,2-dimet	hyl-l-pentanol (1) in water-rich phase	
t/ ^o C g(1)/100	$\log \sin 10^4 x_1$ (compilers)	
25 0.36	5.6	
30 0.34	5.3	
The proportion of (1) in the water-rich phase	e of a mixture with Ringer solution at	
equilibrium at 30 ⁰ C was reported to be 0.30 g	g(1)/100g sln.	
-1		
AUXILIARY	INFORMATION	
AUXILIARY METHOD/APPARATUS/PROCEDURE:	INFORMATION SOURCE AND PURITY OF MATERIALS:	
		
METHOD/APPARATUS/PROCEDURE: In a round bottomed flask, 50 mL of water and a sufficient quantity of alcohol were	SOURCE AND PURITY OF MATERIALS:	
METHOD/APPARATUS/PROCEDURE: In a round bottomed flask, 50 mL of water and a sufficient quantity of alcohol were introduced until two separate layers were	SOURCE AND PURITY OF MATERIALS: (1) Fluka A.G. Buchs S.G.; redistilled with 10:1 reflux ratio	
METHOD/APPARATUS/PROCEDURE: In a round bottomed flask, 50 mL of water and a sufficient quantity of alcohol were introduced until two separate layers were formed. The flask assembly was equilibrated	SOURCE AND PURITY OF MATERIALS: (1) Fluka A.G. Buchs S.G.; redistilled with 10:1 reflux ratio b.p. 153.8-154 ⁰ C/758.4 mm Hg	
METHOD/APPARATUS/PROCEDURE: In a round bottomed flask, 50 mL of water and a sufficient quantity of alcohol were introduced until two separate layers were formed. The flask assembly was equilibrated by agitation for at least 3h in a constant temperature bath. Equilibrium solubility	SOURCE AND PURITY OF MATERIALS: (1) Fluka A.G. Buchs S.G.; redistilled with 10:1 reflux ratio	
METHOD/APPARATUS/PROCEDURE: In a round bottomed flask, 50 mL of water and a sufficient quantity of alcohol were introduced until two separate layers were formed. The flask assembly was equilibrated by agitation for at least 3h in a constant temperature bath. Equilibrium solubility was attained by first supersaturation at a	SOURCE AND PURITY OF MATERIALS: (1) Fluka A.G. Buchs S.G.; redistilled with 10:1 reflux ratio b.p. 153.8-154 ⁰ C/758.4 mm Hg	
METHOD/APPARATUS/PROCEDURE: In a round bottomed flask, 50 mL of water and a sufficient quantity of alcohol were introduced until two separate layers were formed. The flask assembly was equilibrated by agitation for at least 3h in a constant temperature bath. Equilibrium solubility	SOURCE AND PURITY OF MATERIALS: (1) Fluka A.G. Buchs S.G.; redistilled with 10:1 reflux ratio b.p. 153.8-154°C/758.4 mm Hg $n_D^{25} = 1.42556$	
METHOD/APPARATUS/PROCEDURE: In a round bottomed flask, 50 mL of water and a sufficient quantity of alcohol were introduced until two separate layers were formed. The flask assembly was equilibrated by agitation for at least 3h in a constant temperature bath. Equilibrium solubility was attained by first supersaturation at a slightly lower temperature (solubility of alcohols decreases with increasing temperature) and then equilibrating at the	SOURCE AND PURITY OF MATERIALS: (1) Fluka A.G. Buchs S.G.; redistilled with 10:1 reflux ratio b.p. 153.8-154°C/758.4 mm Hg $n_D^{25} = 1.42556$ (2) twice distilled from silica apparatus	
METHOD/APPARATUS/PROCEDURE: In a round bottomed flask, 50 mL of water and a sufficient quantity of alcohol were introduced until two separate layers were formed. The flask assembly was equilibrated by agitation for at least 3h in a constant temperature bath. Equilibrium solubility was attained by first supersaturation at a slightly lower temperature (solubility of alcohols decreases with increasing temperature) and then equilibrating at the desired temperature. The aqueous layer was	SOURCE AND PURITY OF MATERIALS: (1) Fluka A.G. Buchs S.G.; redistilled with 10:1 reflux ratio b.p. 153.8-154°C/758.4 mm Hg $n_D^{25} = 1.42556$ (2) twice distilled from silica apparatus	
METHOD/APPARATUS/PROCEDURE: In a round bottomed flask, 50 mL of water and a sufficient quantity of alcohol were introduced until two separate layers were formed. The flask assembly was equilibrated by agitation for at least 3h in a constant temperature bath. Equilibrium solubility was attained by first supersaturation at a slightly lower temperature (solubility of alcohols decreases with increasing temperature) and then equilibrating at the	 SOURCE AND PURITY OF MATERIALS: (1) Fluka A.G. Buchs S.G.; redistilled with 10:1 reflux ratio b.p. 153.8-154°C/758.4 mm Hg n²⁵ = 1.42556 (2) twice distilled from silica apparatus or ion-exchanged with Sagei A20 	
METHOD/APPARATUS/PROCEDURE: In a round bottomed flask, 50 mL of water and a sufficient quantity of alcohol were introduced until two separate layers were formed. The flask assembly was equilibrated by agitation for at least 3h in a constant temperature bath. Equilibrium solubility was attained by first supersaturation at a slightly lower temperature (solubility of alcohols decreases with increasing temperature) and then equilibrating at the desired temperature. The aqueous layer was separated after an overnight storage in a bath. The alcohol content was determined by reacting the aqueous solution with potassium	 SOURCE AND PURITY OF MATERIALS: (1) Fluka A.G. Buchs S.G.; redistilled with 10:1 reflux ratio b.p. 153.8-154°C/758.4 mm Hg n²⁵ = 1.42556 (2) twice distilled from silica apparatus or ion-exchanged with Sagei A20 ESTIMATED ERROR: 	
METHOD/APPARATUS/PROCEDURE: In a round bottomed flask, 50 mL of water and a sufficient quantity of alcohol were introduced until two separate layers were formed. The flask assembly was equilibrated by agitation for at least 3h in a constant temperature bath. Equilibrium solubility was attained by first supersaturation at a slightly lower temperature (solubility of alcohols decreases with increasing temperature) and then equilibrating at the desired temperature. The aqueous layer was separated after an overnight storage in a bath. The alcohol content was determined by reacting the aqueous solution with potassium dichromate and titrating the excess	 SOURCE AND PURITY OF MATERIALS: (1) Fluka A.G. Buchs S.G.; redistilled with 10:1 reflux ratio b.p. 153.8-154°C/758.4 mm Hg n²⁵ = 1.42556 (2) twice distilled from silica apparatus or ion-exchanged with Sagei A20 ESTIMATED ERROR: 	
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METHOD/APPARATUS/PROCEDURE: In a round bottomed flask, 50 mL of water and a sufficient quantity of alcohol were introduced until two separate layers were formed. The flask assembly was equilibrated by agitation for at least 3h in a constant temperature bath. Equilibrium solubility was attained by first supersaturation at a slightly lower temperature (solubility of alcohols decreases with increasing temperature) and then equilibrating at the desired temperature. The aqueous layer was separated after an overnight storage in a bath. The alcohol content was determined by reacting the aqueous solution with potassium dichromate and titrating the excess dichromate with ferrous sulfate solution in the presence of phosphoric acid and	 SOURCE AND PURITY OF MATERIALS: (1) Fluka A.G. Buchs S.G.; redistilled with 10:1 reflux ratio b.p. 153.8-154°C/758.4 mm Hg n²⁵ = 1.42556 (2) twice distilled from silica apparatus or ion-exchanged with Sagei A20 ESTIMATED ERROR: Solubility: relative error of 2 determinations less than 1% 	
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METHOD/APPARATUS/PROCEDURE: In a round bottomed flask, 50 mL of water and a sufficient quantity of alcohol were introduced until two separate layers were formed. The flask assembly was equilibrated by agitation for at least 3h in a constant temperature bath. Equilibrium solubility was attained by first supersaturation at a slightly lower temperature (solubility of alcohols decreases with increasing temperature) and then equilibrating at the desired temperature. The aqueous layer was separated after an overnight storage in a bath. The alcohol content was determined by reacting the aqueous solution with potassium dichromate and titrating the excess dichromate with ferrous sulfate solution in the presence of phosphoric acid and diphenylamine barium sulfonate as an	 SOURCE AND PURITY OF MATERIALS: (1) Fluka A.G. Buchs S.G.; redistilled with 10:1 reflux ratio b.p. 153.8-154°C/758.4 mm Hg n²⁵ = 1.42556 (2) twice distilled from silica apparatus or ion-exchanged with Sagei A20 ESTIMATED ERROR: Solubility: relative error of 2 determinations less than 1% Temperature: ± 0.05°C 	
METHOD/APPARATUS/PROCEDURE: In a round bottomed flask, 50 mL of water and a sufficient quantity of alcohol were introduced until two separate layers were formed. The flask assembly was equilibrated by agitation for at least 3h in a constant temperature bath. Equilibrium solubility was attained by first supersaturation at a slightly lower temperature (solubility of alcohols decreases with increasing temperature) and then equilibrating at the desired temperature. The aqueous layer was separated after an overnight storage in a bath. The alcohol content was determined by reacting the aqueous solution with potassium dichromate and titrating the excess dichromate with ferrous sulfate solution in the presence of phosphoric acid and diphenylamine barium sulfonate as an	 SOURCE AND PURITY OF MATERIALS: (1) Fluka A.G. Buchs S.G.; redistilled with 10:1 reflux ratio b.p. 153.8-154°C/758.4 mm Hg n²⁵ = 1.42556 (2) twice distilled from silica apparatus or ion-exchanged with Sagei A20 ESTIMATED ERROR: Solubility: relative error of 2 determinations less than 1% Temperature: ± 0.05°C 	
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300

COMPONENTS:	EVALUATOR:
 (1) 2, 2-Dimethyl-3-pentanol; C₇H₁₆0; [3970-62-5] (2) Water; H₂0; [7732-18-5] 	Z. Maczynska, Institute of Physical Chemistry of the Polish Academy of Sciences, Warsaw, Poland. November 1982

Solubilities in the system comprising 2,2-dimethyl-3-pentanol (1) and water (2) have been reported in two publications. Ginnings and Hauser (ref 1) carried out measurements of the mutual solubilities in the two phases at 293, 298 and 303 K by the volumetric method (Figures 1 and 2). Ratouis and Dode' (ref 2) determined the solubility of (1) in the water-rich phase at one temperature (303 K) by an analytical method. Their value of 0.72 g(1)/100g sln is in good agreement with the value 0.79 \pm 0.1 g(1)/100g sln of ref 1. However, as the comparison involves a single point and as the other five points are derived from only one source, the data are regarded as tentative.

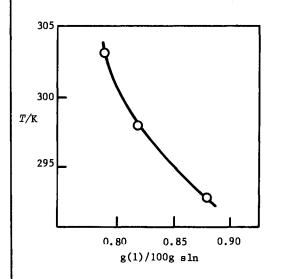


Fig. 1. Water-rich phase (ref 1)

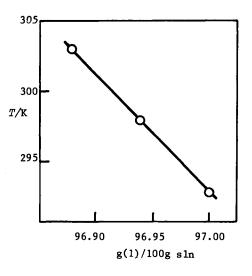


Fig. 2. Alcohol-rich phase (ref 1)

Tentative values	for the mutual	solubilities
of 2,2-dimethyl-	-3-pentanol (1)	and water (2)

I/K	Water-rich phase		Alcohol-rich phase	
	g(1)/100g sln	$10^{3}x_{1}$	g(2)/100g sln	<i>x</i> 2
293	0.88	1.4	3.0	0.166
298	0.82	1.3	3.1	0.169
303	0.79	1.2	3.1	0.172

References:

1. Ginnings, P.M.: Hauser, M. J. Am. Chem. Soc. 1938, 60, 2581.

2. Ratouis, M.; Dode, M. Bull. Soc. Chim. Fr. <u>1965</u>, 3318.

COMPONENTS :		ORIGI	NAL MEASUREMENTS:		
<pre>(1) 2,2-Dimethy1-3-pentanol; [3970-62-5]</pre>	^C 7 ^H 16 ^O ;	Ginr	ings, P.M.; Hauser,	М.	
[3970-62-5]		J. A	m. Chem. Soc. <u>1938</u> ,	60, 2581-2.	
(2) Water; H ₂ 0; [7732-18-5]					
VARIABLES:		PREPA	RED BY:		
Temperature: 20-30 ⁰ C		A. M	aczynski and Z. Macz	ynska	
EXPERIMENTAL VALUES:					
Mutual solubility	of 2,2-dimeth	ny1-3-	pentanol(1) and wate	r(2)	
t/ ^o C g(1)/10	Og sln		$x_1^{(compil}$	er)	
(2)-rich phase	(1)-rich pł	nase	(2)-rich phase	(1)-rich phase	
20 0.88	97.00)	0.00137	0.8336	
25 0.82	96.94	ŀ	0.00128	0.8308	
30 0.79	96.88	3	0.00123	0.8280	
	Relative	densi	ty, <i>d</i> ,		
t/ ^o c			Alcohol-rich phase		
20	_	130			
20	0.9971 0.9962		0.8329 0.8289		
30	0.9950		0.8253		
	AUXILIARY	INFOR	ΜΑΤΙΩΝ		
ME THOD / APPARATUS / PROCEDURE :			SOURCE AND PURITY OF MATERIALS:		
The volumetric method was used	as described	(1)	prepared by Grignar		
in ref 1.			distilled from calc b.p. range 134.7-13	ium_oxide;	
Both components were introduced amounts into a two-bulb graduat			d_{4}^{25} 0.8224;	5.1 0,	
calibrated flask and shaken me	chanically in		purity not specifie	d.	
a water-bath at constant temper sufficient time the liquids we	re allowed to	(2)	not specified.		
separate and the total volume of Upon centrifugation, the phase					
line was read, and phase volume calculated. From the total we	es were				
components, the total volume, individual phase volumes, and component concentrations			MATED ERROR:	- 0 1 1	
in either phase was evaluated.	JICENTIALIONS	501	ubility: better tha (type of e	rror not specified)	
		REFF	RENCES :		
		1.		um, R.J. J. Am. Chem.	
			<u> </u>		

2,2-Dimethyl-3-pentanol				
COMPONENTS :	ORIGINAL MEASUREMENTS:			
 2,2-Dimethyl-3-pentanol; C₇H₁₆0; 	Ratouis, M.; Dodé, M.			
[3970-62-5]	Bull. Soc. Chim. Fr. <u>1965</u> , 3318-22.			
(2) Water; H ₂ 0; [7732-18-5]				
VARIABLES:	PREPARED BY:			
One temperature: 30 ⁰ C	S.C. Valvani; S.H. Yalkowsky; A.F.M. Barton			
Ringer solution also studied				
EXPERIMENTAL VALUES:				
The proportion of 2,2-dimethy1-3-pentanol (1) at 30 ⁰ C was reported to be 0.72 g(1)/100g sln	-			
The corresponding mole fraction solubility, c	alculated by the compilers, is $x_1 = 0.00112$.			
The proportion of (1) in the water-rich phase 30°C was reported to be 0.64 g(1)/100g sln.	of a mixture with Ringer solution at			
AUXILIARY	INFORMATION			
METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:			
In a round bottomed flask, 50 mL of water and a sufficient quantity of alcohol were introduced until two separate layers were formed. The flask assembly was equilibrated by agitation for at least 3h in a constant temperature bath. Equilibrium solubility was attained by first supersaturation at a slightly lower temperature (solubility of alcohols in water decreases with increasing temperature) and then equilibrating at the desired temperature. The aqueous layer was separated after an overnight storage in a	 (1) laboratory preparation; redistilled with 10:1 reflux ratio b.p. 135.4°C/768.2 mm Hg n²⁵ = 1.42358 (2) twice distilled from silica apparatus or ion-exchanged with Sagei A20. 			
bath. The alcohol content was determined by reacting the aqueous solution with potassium dichromate and titrating the excess dichromate with ferrous sulfate solution in the presence of phosphoric acid and diphenylamine barium sulfonate as an indicator.				

COMPONENTS:	EVALUATOR:
(1) 2,3-Dimethy1-2-pentanol; C ₇ H ₁₆ 0;	Z. Maczynska, Institute of Physical
[4911-70-0]	Chemistry of the Polish Academy of Sciences,
(2) Water; H ₂ 0; [7732-18-5]	Warsaw, Poland
(2) water, "2°, [7732 10 5]	November 1982

Solubilities in the system comprising 2,3-dimethyl-2-pentanol (1) and water (2) have been reported in two publications. Ginnings and Hauser (ref 1) carried out measurements of the mutual solubilities in the two phases at 293, 298 and 303 K by the volumetric method (Figure 1). Ratouis and Dode (ref 2) determined the solubility of (1) in the water-rich phase at one temperature (303 K) by an anlytical method. Their value of 1.15 g(1)/100g sln agrees poorly with the value 1.40 \pm 0.1 g(1)/100g sln of ref 1. The results are regarded as tentative.

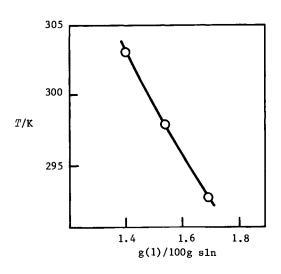


Fig. 1 Solubility of (1) in (2) (ref 1)

Tentative values for the mutual solubilities of 2,3-dimethyl-2-pentanol (1) and water (2)

<i>Т</i> /к	Water-rich phase		Alcohol-rich phase	
	g(1)/100g sln	$10^{3}x_{1}$	g(2)/100g sln	<i>x</i> 2
293	1.7	2.7	6.3	0.30
298	1.5	2.4	6.3	0.30
303	1.4	2.2	6.3	0.30

References

1. Ginnings, P.M.; Hauser, M. J. Am. Chem. Soc. 1938, 60, 2581

2. Ratouis, M.; Dode, M. Bull. Soc. Chim. Fr. <u>1965</u>, 3318

COMPONENTS:	<u></u>		ORIGINA	L MEASUREMENTS:	
(1) 2,3-Dime [4911-70-	thyl-2-pentanol; C -0]	7 ^H 16 ⁰ ;		ngs, P.M.; Hauser <i>Chem. Soc</i> . <u>1938</u> ,	
(2) Water; 1	H ₂ 0; [7732-18-5]				
VARIABLES:			PREPARE	CD BY:	
Temperature:	20–30 [°] C		A. Ma	czynski and Z. Mac	zynska
EXPERIMENTAL V	ALUES:		L. <u></u>		
	Mutual solubility	of 2,3-dimeth	y1-2-pe	ntanol(l) and wate	er(2)
t/ ^o C	g(1)/10 (2)-rich phase		ase	x _l (comp (2)-rich phase	
20	1.69	93.69		0.00265	0.6971
25	1.54	93.69		0.00242	0.6971
30	1.40	93.71		0.00219	0.6978
		Relative d	ensitv.	d.	
	t∕ ^o C Wa			cohol-rich phase	
	20	0.9964		0.8477	
	25	0.9955		0.8441	
	30	0.9943		0.8404	
		AUXILIARY	INFORM	TION	
METHOD /APPARA	TUS/PROCEDURE:		SOURCE	AND PURITY OF MAT	TERIALS:
The volumetric method was used as described in ref 1. Both components were introduced in known amounts into a two-bulb graduated and calibrated flask and shaken mechanically in a water-bath at constant temperature. After sufficient time the liquids were allowed to separate and the total volume was measured. Upon centrifugation, the phase separation line was read, and phase volumes were calculated. From the total weights of the components, the total volume, individual phase volumes, and component concentrations in either phase were evaluated.		(2) ESTIMA Solub	prepared by Grigna distilled from cal b.p. range 138.5- d ₄ ²⁵ 0.8307; purity not specif: not specified. MTED ERROR: ility: better that (type of o	Lcium oxide; L39.5°C, ied.	
				innings, P.M.; Ba oc. <u>1937</u> , 59, 111	aum, R.J. J. Am. Chem 1.

06 Seven-carbon Alcohols				
COMPONENTS: (1) 2,3-Dimethyl-2-pentanol; C ₇ H ₁₆ 0; [4911-70-0] (2) Water; H ₂ 0; [7732-18-5]	ORIGINAL MEASUREMENTS: Ratouis, M.; Dodé, M. Bull. Soc. Chim. Fr. <u>1965</u> , 3318-22.			
VARIABLES: One temperature: 30 ⁰ C Ringer solution also studied	PREPARED BY: S.C. Valvani; S.H. Yalkowsky; A.F.M. Barton			
The proportion of 2,3-dimethyl-2-pentanol (1) at 30°C was reported to be 1.15 g(1)/100g sln The corresponding mole fraction solubility, c The proportion of (1) in the water-rich phase 30°C was reported to be 1.02 g(1)/100g sln.	. alculated by the compilers, is $x_1 = 0.00180$.			
AUXILIARY	INFORMATION			
METHOD/APPARATUS/PROCEDURE: In a round bottomed flask, 50 mL of water and a sufficient quantity of alcohol were introduced until two separate layers were formed. The flask assembly was equilibrated	SOURCE AND PURITY OF MATERIALS: (1) laboratory preparation; redistilled with 10:1 reflux ratio b.p. 84.4°C/97 mm Hg			

by agitation for at least 3h in a constant temperature bath. Equilibrium solubility was attained by first supersaturation at a

slightly lower temperature (solubility of

by reacting the aqueous solution with

potassium dichromate and titrating the

excess dichromate with ferrous sulfate

indicator.

solution in the presence of phosphoric acid and diphenylamine barium sulfonate as an

alcohols in water decreases with increasing temperature) and then equilibrating at the desired temperature. The aqueous layer was separated after an overnight storage in a bath. The alcohol content was determined

- $n_{\rm D}^{25} = 1.42348$
- (2) twice distilled from silica apparatus or ion-exchanged with Sagei A20

ESTIMATED ERROR:

Solubility: relative error of 2 determinations less than 1% Temperature: ± 0.05°C

REFERENCES:

COMPONENTS:	EVALUATOR:		
(1) 2,3-Dimethy1-3-pentanol; C ₇ H ₁₆ 0;	Z. Maczynska, Institute of Physical		
[595-41-5]	Chemistry of the Polish Academy of Sciences,		
(2) Water; H ₂ 0; [7732-18-5]	Warsaw, Poland		
(-,	November 1982		

Solubilities in the system comprising 2,3-dimethyl-3-pentanol (1) and water (2) have been reported in two publications (Figure 1). Ginnings and Hauser (ref 1) carried out measurements of the mutual solubilities in the two phases at 293, 298 and 303 K by the volumetric method. Ratouis and Dode (ref 2) determined the solubility of (1) in the water-rich phase at one temperature (303K) by an analytical method. Their value of 1.41 g(1)/100g sln is in excellent agreement with the value 1.43 \pm 0.1 g(1)/100g sln of ref 1. However, the comparison involves a single point and as the remaining five points are derived from only one source, the data are regarded as tentative.

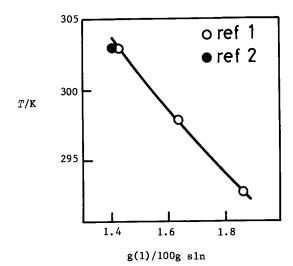


Fig. 1 Solubility of (1) in (2)

Tentative values for the mutual solubilities of 2,3-dimethy1-3-pentanol (1) and water (2)

Т/К	Water-rich phase		Alcohol-rich phase		
	g(1)/100g sln	$10^{3}x_{1}$	g(2)/100g sln	<i>*</i> 2	
293	1.9	2.9	5.9	0.29	
298	1.6	2.6	5.9	0.29	
303	1.4	1.4	5.9	0.29	

References

1. Ginnings, P.M.; Hauser, M. J. Am. Chem. Soc. 1938, 60, 2581.

2. Ratouis, M.; Dode, M. Bull. Soc. Chim. Fr. 1965, 3318.

evaluated. REFERENCES: 1. Ginnings. P.M.; Baum, R.J. J. Am. Che	COMPONENTS:	ORIGINAL MEASUREMENTS:
[535-41-5] J. Am. Chem. Soc. 1938, 80, 2581-2. (2) Water; H ₂ 0; [7732-18-5] J. Am. Chem. Soc. 1938, 80, 2581-2. (2) Water; H ₂ 0; [7732-18-5] PREPARED BY: A. Maczynski and Z. Maczynska EXPERIMENTAL VALUES: Mutual solubility of 2,3-dimethyl-3-pentanol(1) and water(2) A. Maczynski and Z. Maczynska $t/^{O_C}$ g(1)/100g sln (2)-rich phase (1)-rich phase (2)-rich phase (1)-rich phase 20 $x_1(compiler)$ (2)-rich phase (1)-rich phase 20 $x_1(compiler)$ (2)-rich phase 20 20 1.87 94.11 0.00294 0.7123 25 1.64 94.12 0.00224 0.7127 30 1.43 94.12 0.00224 0.7127 Relative density, d ₄ t/"OC AUXILLARY INFORMATION MUTLIARY INFORMATION <td>(1) 2,3-Dimethyl-3-pentanol; C₂H₁₆0;</td> <td>Ginnings, P.M.; Hauser, M.</td>	(1) 2,3-Dimethyl-3-pentanol; C ₂ H ₁₆ 0;	Ginnings, P.M.; Hauser, M.
VARIABLES: Temperature: 20-30°C EXPERIMENTAL VALUES: Mutual solubility of 2,3-dimethyl-3-pentanol(1) and water(2) t/°C g(1)/100g sln s, (compiler) (2)-rich phase (1)-rich phase (2)-rich phase (1)-rich phase 20 1.87 94.11 0.00294 0.7123 25 1.64 94.12 0.00258 0.7127 30 1.43 94.12 0.00224 0.7127 Relative density, d ₄ t/°C Water-rich phase Alcohol-rich phase 20 0.9965 0.8513 25 0.9961 0.8430 METHOD/APPARATUS/PROCEDURE: The volumetric method was used as described in ref 1. PHOD/APPARATUS/PROCEDURE: The volumetric method was used as described in ref 1. Ne THOD/APPARATUS/PROCEDURE: The volumetric method was used as described in ref 1. Not components were introduced in known mounts into a two-bulb graduated and calibrated flask and shaken mechanically in a water-bala constant temperature. After sufficient time the liquids were allowed to separate and the total volume was measured. Upon centrifygation, the phase were calculated. From the total weights in the bild phase volumes, individual phase volumes, individual phase volumes, and component evaluated. REFERENCES: 1. Ginnings. P.M.; Baum, R.J. J. Am. Che	[595-41-5] 7 10	J. Am. Chem. Soc. <u>1938</u> , 60, 2581–2.
International product of the components, were introduced in known maounts into a two-bulb graduated and calibrated flask and shaken mechanically in a water-bulb graduated and calibrated flask and shaken mechanically in a water-bulb graduated and calibrated flask and shaken mechanically in a water-bulb graduated and calibrated flask and shaken mechanically in a water-bulb graduated and calibrated flask and shaken mechanically in a water-bulb graduated and calibrated flask and shaken mechanically in a water-bulb graduated and calibrated flask and shaken mechanically in a water-bulb graduated and calibrated flask and shaken mechanically in a water-bulb graduated and calibrated flask and shaken mechanically in a water-bulb graduated and calibrated flask and shaken mechanically in a water-bulb graduated and calibrated flask and shaken mechanically in a water-bulb graduated and calibrated flask and shaken mechanically in a water-bulb graduated and calibrated flask and shaken were waluated. Source AND PURITY OF MATERIALS: (1) prepared by Grignard synchesis; distilled from calcium oxide; bp. range 139.6%; distilled from calcium oxide; br. ranger 139.6%; distilled from calcium oxide; br. range 139.6%; distill	(2) Water; H ₂ O; [7732-18-5]	
EXPERIMENTAL VALUES: Mutual solubility of 2,3-dimethyl-3-pentanol(1) and water(2) $t/^{0}C$ g(1)/100g sln x1(compiler) (2)-rich phase (1)-rich phase (2)-rich phase (1)-rich phase 20 1.87 94.11 0.00294 0.7123 25 1.64 94.12 0.00238 0.7127 30 1.43 94.12 0.00224 0.7127 Relative density, d_4 $t/^{0}C$ Water-rich phase Alcohol-rich phase 20 0.9965 0.8513 25 0.9961 0.8470 30 0.9945 0.8430 METHOD/AFPARATUS/FROCEDURE: The volumetric method was used as described in ref 1. Both components were introduced in known amounts into a two-bulb graduated and calibrated flask and shaken mechanically in a water-bath at constant temperature. After sufficient ine the liquids were allowed to separate and the total volumes separation line was read, and phase volumes were calculated. From the total veights of the components, the total volumes, and component comentrations in either phase were evaluated. REFERENCES: 1. Cinnings. P.M.; Baum, R.J. J. Am. Che	VARIABLES:	PREPARED BY:
Mutual solubility of 2,3-dimethyl-3-pentanol(1) and water(2) $t/^{O}C$ g(1)/100g sin $x_1(compiler)$ (2)-rich phase(1)-rich phase(2)-rich phase201.8794.110.00294251.6494.120.00258301.4394.120.00224301.4394.120.00224Relative density, d_4 $t/^{O}C$ Water-rich phase200.99650.8513250.99610.8470300.99450.8430AUXILIARY INFORMATIONMUXILIARY INFORMATIONMUXILIARY INFORMATIONMUXILIARY INFORMATIONAUXILIARY INFORMATIONAUXILIARY INFORMATIONMUXILIARY INFORMATIONAUXILIARY INFORMATIONAUXILIA	Temperature: 20-30 ⁰ C	A. Maczynski and Z. Maczynska
$\frac{t/^{\circ}C}{(2)-rich phase} (1)-rich phase} (2)-rich phase (1)-rich phase (1)-rich phase (2)-rich phase (1)-rich phase (1)-rich phase (2)-rich phase (1)-rich phase (2)-rich phase (1)-rich phase (2)-rich phase (2)-ri$	EXPERIMENTAL VALUES:	
(2)-rich phase (1)-rich phase (2)-rich phase (1)-rich phase (2)-rich phase (1)-rich phase (2)-rich phase (1)-rich phase (2) -rich phase (1)-rich phase (2) -rich phase (2) -r	Mutual solubility of 2,3-dimethy	1-3-pentanol(1) and water(2)
$\frac{25}{30} 1.64 \qquad 94.12 \qquad 0.00258 \qquad 0.7127$ $30 \qquad 1.43 \qquad 94.12 \qquad 0.00224 \qquad 0.7127$ Relative density, d_4 $\frac{t/^{0}C}{C} Water-rich phase \qquad Alcohol-rich phase$ $20 \qquad 0.9965 \qquad 0.8513$ $25 \qquad 0.9961 \qquad 0.8430$ $30 \qquad 0.9945 \qquad 0.8430$ $\frac{AUXILIARY INFORMATION}{30 \qquad 0.9945 \qquad 0.8430}$ $\frac{AUXILIARY INFORMATION}{10 \qquad 0.9945 \qquad 0.8430}$		x_1 (compiler) ase (2)-rich phase (1)-rich phase
30 1.43 94.12 0.00224 0.7127 Relative density, d_4 t^{j^0} C Water-rich phase Alcohol-rich phase 20 0.9965 0.8513 25 0.9961 0.8470 30 0.9945 0.8430 AUXILIARY INFORMATION METHOD/APPARATUS/PROCEDURE: Source and purity of MATERIALS: The volumetric method was used as described in ref 1. Source and purity of MATERIALS: The volumetric method was used as described in ref 1. Source and purity of MATERIALS: Source and purity of specified from calcium oxide; b-p. range 139.6-139.8°C; d_2^{15} 0.8365; purity not specified. Constant temperature. After sufficient time the liquids were allowed to separate and the total volume, super sease and phase volumes were calculated. From the total wolume, individual phase volumes, and component concentrations in either phase were evaluated. Solubility: better than 0.1 wt % (type of error not specified) REFERENCES: 1. Ginnings. P.M.; Baum, R.J. J. Am. Che	20 1.87 94.11	0.00294 0.7123
Relative density, d_4 Relative density, d_4 $t/^{\circ}C$ Water-rich phase200.99650.8513250.99610.8470300.99450.8430AUXILIARY INFORMATIONMETHOD/APPARATUS/PROCEDURE:The volumetric method was used as described in ref 1.Source AND PURITY OF MATERIALS:(1) prepared by Grignard synthesis; distilled from calcium oxide; b.p. range 139.6-139.8°C, d_2^{25} 0.8365; purity not specified.(2) not specified.(1) colspan="2">(1) colspan	25 1.64 94.12	0.00258 0.7127
$t/^{\circ}C$ Water-rich phaseAlcohol-rich phase200.99650.8513250.99610.8470300.99450.8430AUXILIARY INFORMATIONMETHOD/APPARATUS/PROCEDURE:The volumetric method was used as described in ref 1.Both components were introduced in known amounts into a two-bulb graduated and calibrated flask and shaken mechanically in a water-bath at constant temperature. After sufficient time the liquids were allowed to separate and the total volume was measured. Upon centrifugation, the phase separation line was read, and phase volumes were calculated. From the total weights of the components, the total volume, individual phase volumes, and component concentrations in either phase were evaluated.Solubility: better than 0.1 wt % (type of error not specified)REFERENCES: 1. Ginnings. P.M.; Baum, R.J. J. Am. Che	30 1.43 94.12	0.00224 0.7127
20 0.9965 0.8513 25 0.9961 0.8470 30 0.9945 0.8430 AUXILIARY INFORMATION METHOD/APPARATUS/PROCEDURE: The volumetric method was used as described in ref 1. Both components were introduced in known amounts into a two-bulb graduated and calibrated flask and shaken mechanically in a water-bath at constant temperature. After sufficient time the liquids were allowed to separate and the total volume was measured. Upon centrifugation, the phase separation line was read, and phase volumes, individual phase volumes, and component concentrations in either phase were evaluated. Solucte AND PURITY OF MATERIALS: SURCE AND PURITY OF MATERIALS: Source AND PURITY OF MATERIALS: (1) prepared by Grignard synthesis; distilled from calcium oxide; b.p. range 139.6-139.8°C, d_2 0.8365; purity not specified. (2) not specified. <	Relative	density, d_4
250.99610.8470300.99450.8430AUXILIARY INFORMATIONMETHOD/APPARATUS/PROCEDURE:The volumetric method was used as described in ref 1.The volumetric method was used as described in ref 1.Both components were introduced in known amounts into a two-bulb graduated and calibrate flask and shaken mechanically in a water-bath at constant temperature. After sufficient time the liquids were allowed to separate and the total volume was measured. Upon centrifugation, the phase separation line was read, and phase volumes were calculated.SOURCE AND PURITY OF MATERIALS: (1) prepared by Grignard synthesis; distilled from calcium oxide; b.p. range 139.6-139.8°C, d_{d_{1}}^{25} 0.8365; purity not specified.(2) not specified.(1) colspan="2">(1) cols	$t/^{o}$ C Water-rich phas	se Alcohol-rich phase
30 0.9945 0.8430 AUXILIARY INFORMATION METHOD/APPARATUS/PROCEDURE: The volumetric method was used as described in ref 1. Both components were introduced in known amounts into a two-bulb graduated and calibrated flask and shaken mechanically in a water-bath at constant temperature. After sufficient time the liquids were allowed to separate and the total volume was measured. Upon centrifugation, the phase separation line was read, and phase volumess were calculated. From the total weights of the components, the total volume, individual phase volumes, and component concentrations in either phase were evaluated. REFERENCES: 1. Ginnings. P.M.; Baum, R.J. J. Am. Che	20 0.9965	
AUXILIARY INFORMATIONMETHOD/APPARATUS/PROCEDURE:SOURCE AND PURITY OF MATERIALS:The volumetric method was used as described in ref 1.SOURCE AND PURITY OF MATERIALS:Both components were introduced in known amounts into a two-bulb graduated and calibrated flask and shaken mechanically in a water-bath at constant temperature. After sufficient time the liquids were allowed to separate and the total volume was measured. Upon centrifugation, the phase separation line was read, and phase volumes were calculated. From the total weights of the components, the total volume, individual phase volumes, and component concentrations in either phase were evaluated.SOURCE AND PURITY OF MATERIALS: (1) prepared by Grignard synthesis; distilled from calcium oxide; b.p. range 139.6-139.8°C, d_{Δ}^{2} 0.8365; purity not specified.(2) not specified.(2) not specified.(2) not specified.ESTIMATED ERROR: Solubility: better than 0.1 wt % (type of error not specified)REFERENCES: 1. Ginnings. P.M.; Baum, R.J. J. Am. Che	25 0.9961	0.8470
METHOD/APPARATUS/PROCEDURE:SOURCE AND PURITY OF MATERIALS:The volumetric method was used as described in ref 1.SOURCE AND PURITY OF MATERIALS:Both components were introduced in known amounts into a two-bulb graduated and calibrated flask and shaken mechanically in a water-bath at constant temperature. After sufficient time the liquids were allowed to separate and the total volume was measured. Upon centrifugation, the phase separation line was read, and phase volumes were calculated. From the total weights of the components, the total volume, individual phase volumes, and component concentrations in either phase were evaluated.SOURCE AND PURITY OF MATERIALS:(1) prepared by Grignard synthesis; distilled from calcium oxide; b.p. range 139.6-139.8°C, d_4^{25} 0.8365; purity not specified.(2) not specified.(2) not specified.(2) not specified.ESTIMATED ERROR: Solubility: better than 0.1 wt % (type of error not specified)REFERENCES: 1. Ginnings. P.M.; Baum, R.J. J. Am. Che	30 0.9945	0.8430
METHOD/APPARATUS/PROCEDURE:SOURCE AND PURITY OF MATERIALS:The volumetric method was used as described in ref 1.SOURCE AND PURITY OF MATERIALS:Both components were introduced in known amounts into a two-bulb graduated and calibrated flask and shaken mechanically in a water-bath at constant temperature. After sufficient time the liquids were allowed to separate and the total volume was measured. Upon centrifugation, the phase separation line was read, and phase volumes were calculated. From the total weights of the components, the total volume, individual phase volumes, and component concentrations in either phase were evaluated.SOURCE AND PURITY OF MATERIALS:(1) prepared by Grignard synthesis; distilled from calcium oxide; b.p. range 139.6-139.8°C, d_4^{25} 0.8365; purity not specified.(2) not specified.(2) not specified.(2) not specified.ESTIMATED ERROR: Solubility: better than 0.1 wt % (type of error not specified)REFERENCES: 1. Ginnings. P.M.; Baum, R.J. J. Am. Che		
 The volumetric method was used as described in ref 1. Both components were introduced in known amounts into a two-bulb graduated and calibrated flask and shaken mechanically in a water-bath at constant temperature. After sufficient time the liquids were allowed to separate and the total volume was measured. Upon centrifugation, the phase separation line was read, and phase volumes were calculated. From the total weights of the components, the total volume, individual phase volumes, and component concentrations in either phase were evaluated. (1) prepared by Grignard synthesis; distilled from calcium oxide; b.p. range 139.6-139.8°C, 2²⁵ d.4 0.8365; purity not specified. (2) not specified. (3) ESTIMATED ERROR: (4) Solubility: better than 0.1 wt % (type of error not specified) (4) REFERENCES: (4) Ginnings. P.M.; Baum, R.J. J. Am. Chemer (the specified) 		
50e. <u>1937</u> , 59, 1111.	The volumetric method was used as described in ref 1. Both components were introduced in known amounts into a two-bulb graduated and calibrated flask and shaken mechanically in a water-bath at constant temperature. After sufficient time the liquids were allowed to separate and the total volume was measured. Upon centrifugation, the phase separation line was read, and phase volumes were calculated. From the total weights of the components, the total volume, individual phase volumes, and component concentrations in either phase were	 prepared by Grignard synthesis; distilled from calcium oxide; b.p. range 139.6-139.8°C, d²⁵₄ 0.8365; purity not specified. not specified. not specified. ESTIMATED ERROR: Solubility: better than 0.1 wt % (type of error not specified)

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) 2,3-Dimethy1-3-pentanol; C ₇ H ₁₆ 0;	Ratouis, M.; Dodé, M.
[595-41-5]	Bull. Soc. Chim. Fr. 1965, 3318-22.
(2) Water; H ₂ 0; [7732-18-5]	
VARIABLES:	PREPARED BY:
One temperature: 30°C	S.C. Valvani; S.H. Yalkowsky; A.F.M. Barton
Ringer solution also studied	

EXPERIMENTAL VALUES:

The proportion of 2,3-dimethyl-3-pentanol (1) in the water-rich phase at equilibrium at 30° C was reported to be 1.41 g(1)/100g sln.

The corresponding mole fraction solubility, calculated by the compilers, is $x_1 = 0.00221$.

The proportion of (1) in the water-rich phase of a mixture with Ringer solution at 30° C was reported to be 1.31 g(1)/100g sln.

INFORMATION
INFORMATION SOURCE AND PURITY OF MATERIALS: (1) laboratory preparation; redistilled with 10:1 reflux ratio b.p. 60.2-60.3°C/40 mm Hg $n_D^{25} = 1.42671$ (2) twice distilled from silica apparatus or ion-exchanged with Sagei A20 ESTIMATED ERROR: Solubility: relative error of 2 determinations less than 1% Temperature: ± 0.05°C REFERENCES;

COMPONENTS:	ORIGINAL MEASUREMENTS	:	
 2,4-Dimethy1-1-pentanol; C₇H₁₆0; 	Ratouis, M.; Dodé, M.		
[6305-71-1]	Bull. Soc. Chim. Fr. 1965, 3318-22.		
(2) Water; H ₂ 0; [7732-18-5]			
VARIABLES:	PREPARED BY:		
Temperature: 25°C and 30°C		-lloughest A. T. M. Doubou	
Ringer solution also studied	S.C. Valvani; S.H. Y	alkowsky; A.F.M. Barton	
EXPERIMENTAL VALUES:	····		
Proportion of 2,4-dimethyl	-l-pentanol (l) in wat	ter-rich phase	
$t/^{o}$ c g(1) (100- 1	104	
25	1)/100g s1n	$10^4 x_1$ (compilers)	
30	0.30 0.285	4.7 4.42	
00	0.205	4.42	
The proportion of (1) in the water-rich phase		nger solution at	
equilibrium at 30 ⁰ C was reported to be 0.265	g(1)/100g sln.		
AUXILIARY	INFORMATION		
METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF	MATERIALS:	
In a round bottomed flask, 50 mL of water and a sufficient quantity of alcohol were	(1) Fluka A.G. Buchs		
introduced until two separate layers were	b.p. 158.2-159°C	10:1 reflux ratio	
formed. The flask assembly was equilibrated by agitation for at least 3h in a constant	$n_{\rm p}^{25} = 1.42009$	6//53.6 mm Hg	
temperature bath. Equilibrium solubility	$n_{\rm D} = 1.42009$		
was attained by first supersaturation at a slightly lower temperature (solubility of		from silica apparatus	
alcohols in water decreases with increasing	or ion-exchanged	with Sagei A20	
temperature) and then equilibrating at the desired temperature. The aqueous layer			
was separated after an overnight storage in a bath. The alcohol content was determined	ESTIMATED ERROR:		
by reacting the aqueous solution with	Colubellet and and add	o orror of ?	
potassium dichromate and titrating the excess dichromate with ferrous sulfate solution in	-	nations less than 1%	
the presence of phosphoric acid and	Temperature: ± 0.05	°c	
diphenylamine barium sulfonate as an indicator.	REFERENCES :		
	1		

COMPONENTS :	EVALUATOR:
 (1) 2,4-Dimethyl-2-pentanol; C₇H₁₆0; [625-06-9] (2) Water; H₂0; [7732-18-5] 	Z. Maczynska, Institute of Physical Chemistry of the Polish Academy of Sciences, Warsaw, Poland November 1982

Solubilities in the system comprising 2,4-dimethyl-2-pentanol (1) and water (2) have been reported in two publications. Ginnings and Hauser (ref 1) carried out measurements of the mutual solubilities at 293, 298 and 303 K by the volumetric method (Figure 1). Ratouis and Dode['] (ref 2) determined the solubility of (1) in the water-rich phase at one temperature (303 K) by an analytical method. Their value of 0.98 g(1)/100g sln is in reasonable agreement with the value 1.22 ± 0.1 g(1)/100g sln of ref 1. The data are regarded as tentative, since comparison can be made only at a single temperature and the other five points are derived from one reference.

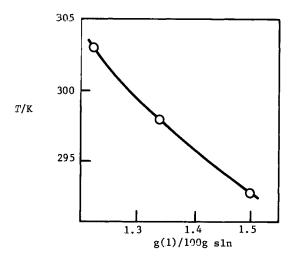


Fig. 1 Solubility of (1) in (2) (ref 1)

Tentative	values	for	the	mutual	<u>l solubili</u>	ties
of 2.4-dir	nethvl-	2-per	itano	51 (1)	and water	(2)

Т/К	Water-rich p	hase	Alcohol-rich	phase
	g(1)/100g sln	10 ³ <i>x</i> ₁	g(2)/100g sln	<i>x</i> 2
293	1.5	2.4	6.5	0.31
298	1.3	2.1	6.5	0.31
303	1.2	1.9	6.5	0.31

References

1. Ginnings, P.M.; Hauser, M. J. Am. Chem. Soc. 1938, 60, 2581.

COMPONENTS :			ORIGI	AL MEASUREME	NTS:	
(1) 2,4-Dimethyl-2-pentanol; C ₇ H ₁₆ 0;		Ginnings, P.M.; Hauser, M.				
[625-06-9]		/ 10	J. AI	n. Chem. Soc.	<u>1938</u> , 60	2581-2.
(2) Water; H ₂ 0;	[7732-18-5]					
VARIABLES:			PREPA	RED BY:		
Temperature: 20-3	o°c		A. M	aczynski and	Z. Maczyr	iska
EXPERIMENTAL VALUES			1 0	1/1)	1	
Mutua	l solubility o	t 2,4-dimethy	71-2-p	entanol(l) an	id water(2	.)
t/ ^o c	g(1)/100g	sln		x_1	(compiler	-)
(2)-	rich phase	(1)-rich pha	ase	(2)-rich ph	ase	(1)-rich phase
20	1.50	93.4	9	0.002	35	0.6900
25	1.34	93.4	8	0.002	10	0.6897
30	1.22	93.4	9	0.001	.91	0.6900
		Relative	doneit	v d		
		Relative	uensit	y, "4		
	t∕ ^o c W	ater-rich ph	ase	Alcohol-rich	h phase	
	20	0.9962		0.8279		
	25	0.9954		0.8240		
		AUXILIARY	INFOR	1ATION		
METHOD/APPARATUS/PF	ROCEDURE:		SOURC	E AND PURITY	OF MATER	IALS:
The volumetric met	hod was used a	s described	(1)	prepared by		
in ref 1.				distilled fr b.p. range 1		
Both components we amounts into a two				d_4^{25} 0.8100;		
calibrated flask a a water-bath at co	and shaken mech	anically in		purity not a	specified	
sufficient time th	ne liquids were	allowed		not specifie	ed.	
	centrifugation,	the phase				
separation line wa were calculated.	is read, and ph From the tota		POTI	ATED ERROR:		
of the components, the total volume individual phase volumes, and component			bility: bett	tor than	0 1+ %	
concentrations in evaluated.	either phase w	ere				or not specified)
			REFE	RENCES:		
				Ginnings, P.M Soc. <u>1937</u> , 59		, R.J. J. Am. Chem.
L			1			

ORIGINAL MEASUREMENTS:				
Ratouis, M.; Dodé, M.				
Bull. Soc. Chim. Fr. <u>1965</u> , 3318-22.				
PREPARED BY:				
S.C. Valvani; S.H. Yalkowsky; A.F.M. Barton				
) in the water-rich phase at equilibrium at				
calculated by the compilers, is $x_1 = 0.00153$.				
e of a mixture with Ringer solution at 30 ⁰ C				

	INFORMATION
METHOD/APPARATUS/PROCEDURE: In a round bottomed flask, 50 mL of water and a sufficient quantity of alcohol were introduced until two separate layers were formed. The flask assembly was equilibrated by agitation for at least 3h in a constant temperature bath. Equilibrium solubility was attained by first supersaturation at a slightly lower temperature (solubility of alcohols in water decreases with increasing temperature) and then equilibrating at the desired temperature. The aqueous layer was separated after an overnight storage in a bath. The alcohol content was determined by reacting the aqueous solution with potassium dichromate and titrating the excess dichromate with ferrous sulfate solution in the presence of phosphoric acid and diphenylamine barium sulfonate as an indicator.	<pre>SOURCE AND PURITY OF MATERIALS: (1) laboratory preparation; redistilled with 10:1 reflux ratio b.p. 132.3-133.6°C/752.4 mm Hg n²⁵_D = 1.41216 (2) twice distilled from silica apparatus or ion-exchanged with Sagei A20 ESTIMATED ERROR: Solubility: relative error of 2 determinations less than 1% Temperature: ± 0.05°C REFERENCES:</pre>

COMPONENTS:	EVALUATOR:
(1) 2,4-Dimethy1-3-pentanol	Z. Maczynska, Institute of Physical
(diisopropylcarbinol); C ₇ H ₁₆ 0;	Chemistry of the Polish Academy of Sciences,
[600-36-2]	Warsaw, Poland
(2) Water; H ₂ 0; [7732-18-5]	November 1982.
-	

Solubilities in the system comprising 2,4-dimethyl-3-pentanol (1) and water (2) have been reported in two publications. Ginnings and Hauser (ref 1) carried out measurements of the mutual solubilities in the two phases at 293, 298 and 303 K by the volumetric method (Figures 1 and 2). Ratouis and Dode (ref 2) determined the solubility of (1) in the water-rich phase at one temperature (303 K) by an analytical method, their value of 0.61 g(1)/100g sln being in good agreement with the value of 0.67 \pm 0.1 g(1)/100g sln of ref 1. However, as the comparison involves a single point and as the remaining five points are derived from only one source, the data are regarded as tentative.

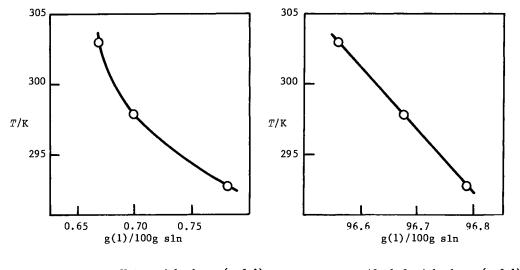


Fig. 1. Water-rich phase (ref 1)

Fig. 2. Alcohol-rich phase (ref 1)

Tentative values for the mutual solubilities of 2,4-dimethy1-3-pentanol (1) and water (2)

T/K	Water-ric	Water-rich phase		n ph ase
	g(1)/100g sln	$10^{3}x_{1}$	g(2)/100g sln	<i>x</i> 2
293	0.78	1.2	3.2	0.176
298	0.70	1.1	3.3	0.181
303	0.67	1.0	3.4	0.187

References

1. Ginnings, P.M.; Hauser, M. J. Am. Chem. Soc. 1938, 60, 2581.

COMPONENTS:			ORIGIN	AL MEASUREMENTS	:
(1) 2.4 - Dime	thy1-3-pentano1;		Ginni	ngs, P.M.; Hau	ser. M.
	popylcarbinol); C ₇ H ₁	.0 :			38, 60, 2581-2.
[600-36-	· •	6-,	U. AVI.	onem. 500. <u>1</u> 5	<u>50</u> , 00, 2501-2.
(2) Water; H	1,0; [7732-18-5]				
VARIABLES:	2 , 2 , 2 , 2 , 2 , 2 , 2 , 2 , 2 , 2 ,		PREPAR	ED BY:	
Temperature:	20–30 [°] C		A. Ma	zynski and Z.	Maczynska
EXPERIMENTAL V	ALUES:		_		
	Mutual solubility o	f 2,4-dimethy	1-3-pe	ntanol(1) and w	ater(2)
t∕°c	g(1)/100g	sln		<i>x</i> 1 (co	mpiler)
	(2)-rich phase	(1)-rich pha	se	–	(1)-rich phase
20	0.78	96.79)	0.00122	0.8237
25	0.70	96.68	5	0.00109	0.8186
30	0.67	96.56		0.00104	0.8131
30		,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,		0.00101	,
		Relative	densi	y, d ₄	
	t/ ⁰ C Wat	er-rich phase	Alo	cohol-rich phase	e
	20	0,9974		0.8351	
	25	0.9965		0.8315	
	30	0.9955		0.8271	
		AUXILIARY			
METHOD/APPARA	TUS/PROCEDURE:		SOURCI	E AND PURITY OF	MATERIALS:
in ref l. Both compone amounts into	ric method was used ents were introduced o a two-bulb graduat flask and shaken med	in known ed and	(1)	• • •	
sufficient t separate and Upon centrif	n at constant temper time the liquids wer d the total volume w fugation, the phase ad, and phase volume	e allowed to was measured. separation	(2)	not specified.	
calculated.	From the total we the total volume, i		ESTIM	ATED ERROR:	
phase volume	es, and component contained.	ncentrations	Solu		than 0.1 wt % of error not specified)
			RE F E F	ENCES:	
				Ginnings, P.M.; <i>Chem. Soc</i> . <u>1937</u>	Baum, R.J. <i>J. Am.</i> 7, 59, 1111.

316 Seven-carbo	Seven-carbon Alcohols		
COMPONENTS:	ORIGINAL MEASUREMENTS:		
 (1) 2,4-Dimethy1-3-pentanol (diisopropylearbinol); C₇H₁₆0; [600-36-2] (2) Nature H. 0: [7722, 18, 5] 	Ratouis, M.; Dodé, M. Bull. Soc. Chim. Fr. <u>1965</u> , 3318-22 _.		
(2) Water; H ₂ 0; [7732-18-5]			
VARIABLES: One temperature: 30 ⁰ C Ringer solution also studied EXPERIMENTAL VALUES:	PREPARED BY: S.C. Valvani; S.H. Yalkowsky; A.F.M. Barton		
The proportion of 2,4-dimethyl-3-pentanol (1) 30°C was reported to be 0.61 g(1)/100g sln. The corresponding mole fraction solubility, c The proportion of (1) in the water-rich phase was reported to be 0.53 g(1)/100g sln.	alculated by the compilers, is $x_1 = 0.00095$.		
METHOD/APPARATUS/PROCEDURE: In a round bottomed flask, 50 mL of water and a sufficient quantity of alcohol were introduced until two separate layers were formed. The flask assembly was equilibrated by agitation for at least 3h in a constant temperature bath. Equilibrium solubility was attained by first supersaturation at a slightly lower temperature (solubilities of alcohols in water decrease with increasing temperature) and then equilibrating at the desired temperature. The aqueous layer was separated after an overnight storage in a bath. The alcohol content was determined by	 n_D²⁵ = 1.42265 (2) twice distilled from silica apparatus or ion-exchanged with Sagei A20 		
reacting the aqueous solution with potassium dichromate and titrating the excess dichromate with ferrous sulfate solution in the presence of phosphoric acid and diphenylamine barium sulfonate as an indicator.	Solubility: relative error of 2 determinations less than 1% Temperature: ± 0.05°C REFERENCES:		

	ORIGINAL MEASUREMENTS:
(1) 4,4-Dimethyl-l-pentanol; C ₇ H ₁₆ 0;	Ratouis, M.; Dodé, M.
[3121-79-7]	Bull. Soc. Chim. Fr. 1965, 3318-22.
2) Water; H ₂ 0; [[] 7732-18-5]	~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~
2	
RIABLES:	PREPARED BY:
Cemperature: 25 ⁰ C and 30 ⁰ C	S.C. Valvani; S.H. Yalkowsky; A.F.M. Bartor
Ringer solution also studied	
XPERIMENTAL VALUES:	
Proportion of 4,4-dimethy1-1-pe	ntanol (1) in water-rich phase
t/ ^o C g(1)/100g sln	$10^4 x_1$ (compilers)
25 0.335	5.20
30 0.325	5.05
AUXILIARY	INFORMATION
	INFORMATION SOURCE AND PURITY OF MATERIALS:
AUXILIARY METHOD/APPARATUS/PROCEDURE: In a round bottomed flask, 50 mL of water and a sufficient quantity of alcohol were introduced until two separate layers were formed. The flask assembly was equilibrated by agitation for at least 3h in a constant temperature bath. Equilibrium solubility was attained by first supersaturation at a slightly lower temperature (solubilities of alcohols in water decrease with increasing temperature) and then equilibrating at the desired temperature. Aqueous layer was separated after an overnight storage in a bath. The alcohol content was determined by reacting the aqueous solution with potassium	 SOURCE AND PURITY OF MATERIALS: (1) laboratory preparation; redistilled with 10:1 reflux ratio b.p. 162.9-163.3°C/755.5 mm Hg n²⁵_D = 1.41853 (2) twice distilled from silica apparatus or ion-exchanged with Sagei A20 ESTIMATED ERROR:

COMPONENTS :	EVALUATOR:
(1) 3-Ethy1-3-pentanol; C7H ₁₆ O;	A.Maczynski, Institute of Physical
[597-49-9]	Chemistry of the Polish Academy of Sciences,
(2) Water; H ₂ 0; [7732-18-5]	Warsaw, Poland.
	November 1982

Solubilities in the system comprising 3-ethyl-3-pentanol (1) and water (2) have been reported in two publications (Figure 1). Ginnings and Hauser (ref 1) carried out measurements of the mutual solubilities in the two phases at 293, 298, 303 and 313 K by the volumetric method. The value of the solubility of water in the alcohol-rich phase at 313 K is inconsistent with those obtained at the lower temperature. Ratouis and Dode (ref 2) determined the solubility of (1) in the water-rich phase at one temperature (303 K) by an analytical method, their value of 1.45 g(1)/100g sln being in excellent agreement with that of 1.50 ± 0.1 g(1)/100g sln of ref 1. However, as the comparison involves a single point and as the remaining points are derived from only one source, the data are regarded as tentative.

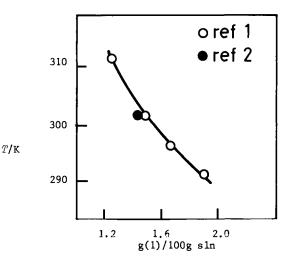


Fig. 1. Solubility of (1) in (2)

Tentative values	for the	mutual	solubilities
of 3-ethy1-3-pent	tanol (1) and wa	ater (2)

T/K	Water-rich		Alcohol-rio	ch phase
	g(1)/100g sln	$10^{3}x_{1}$	g(2)/100g sln	<i>x</i> ₂
293	1.9	3.0	5.75	0.282
298	1.7	2.6	5.76	0.283
303	1.5	2.4	5.79	0.283
313	1.3	2.0	-	-

References

1. Ginnings, P.M.; Hauser, M. J. Am. Chem. Soc. 1938, 60, 2581.

COMPONENTS:			ORIGINAL 1	MEASUREMENTS:	
(1) 3-Ethyl-3-pentanol; C ₇ H ₁₆ 0;		Ginnings, P.M.; Hauser, M.			
[597-49-9]			nem. Soc. <u>1938</u> ,		
			e. Am. Cr	<i>tem. 500.</i> <u>1750</u> ,	00, 2381-2.
(2) Water;	H ₂ 0; [7732-18-5]				r.
VARIABLES:	·		PREPARED	BY:	
Temperature:	20-40 [°] C		A. Maczyn	nski and Z. Mac	zynska
			L		
EXPERIMENTAL	VALUES:				
	Mutual solubility	of 3-ethy1-3-p	entanol(1)) and water(2)	
t∕°c	g(1)/100	g sln		$x_1^{(compi}$	ler)
	(2)-rich phase		se (2	-	(1)-rich phase
20	1.91	94.25		0.00301	0.7176
25	1.68	94.24		0.00264	0.7172
30	1.50	94.21		0.00235	0.7161
40	1.26	94.31		0.00197	0.7198
		Relative	density,	^d 4	
	$t/^{o}$ C Wat	er-rich phase	Alcoh	ol-rich phase	
	20	0.9964		0.8541	
	25	0.9957		0.8502	
30 0.9945			0.8457		
40 0.9921			0.8366		
		AUXILIARY	INFORMATI	ON	
ME THOD / APPAR	ATUS/PROCEDURE:		SOURCE AL	ND PURITY OF MA	TERIALS:
The volume in ref 1.	tric method was used	as described		epared by Grign stilled from ca	
Both compor	nents were introduce	d in known		p. range 143.1- ⁵ 0.8402;	-143.2°C,
amounts int	to a two-bulb gradua flask and shaken me	ted and	4	U.8402; rity not specif	ind
in a water-	-bath at constant te	mperature.			ieu.
	icient time the liqu separate and the to		(2) no	t specified.	
was measure	ed. Upon centrifug ration line was read				
volumes wer	re calculated. Fro	m the total	ESTIMATE	D ERROR:	
individual	the components, the phase volumes, and	component	1	ity: better th	uan 0.1 wt %
concentrations in either phase were evaluated.				error not specified)	
			REFERENC	ES;	
				nings, P.M.; E n. Soc. <u>1937</u> , 5	
			1		
			L		

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) 3-Ethy1-3-pentanol; C ₇ H ₁₆ 0; [597-49-9]	Ratouis, M.; Dodé, M.
(2) Water; H ₂ 0; [7732-18-5]	Bull. Soc. Chim. Fr. 1965, 3318-22.
VARIABLES:	PREPARED BY:
One temperature: 30°C	S.C. Valvani; S.H. Yalkowsky; A.F.M. Barton
Ringer solution also studied	
EXPERIMENTAL VALUES:	•

The proportion of 3-ethyl-3-pentanol (1) in the water-rich phase at equilibrium at 30° C was reported to be 1.45 g(1)/100g sln.

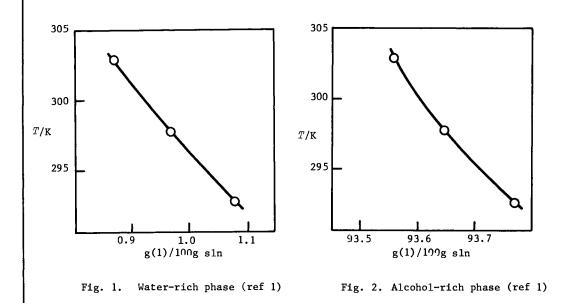
The corresponding mole fraction solubility, calculated by the compilers, is $x_1 = 0.00228$.

The proportion of (1) in the water-rich phase of a mixture with Ringer solution at 30° C was reported to be 1.32 g(1)/100g sln.

AUXILIARY INFORMATION			
In a round bottomed flask, 50 mL of water and a sufficient quantity of alcohol were introduced until two separate layers were formed. The flask assembly was equilibrated by agitation for at least 3h in a constant temperature bath. Equilibrium solubility was attained by first supersaturation at a slightly lower temperature (solubility of alcohols in water decreases with increasing temperature) and then equilibrating at the desired temperature. The aqueous layer was separated after an overnight storage in a	 SOURCE AND PURITY OF MATERIALS: (1) laboratory preparation; redistilled with 10:1 reflux ratio b.p. 140-140.2°C/761 mm Hg n²⁵_D = 1.42716 (2) twice distilled from silica apparatus or ion-exchanged with Sagei A20 		
	ESTIMATED ERROR: Solubility: relative error of 2 determinations less than 1% Temperature: ± 0.05 ^o C REFERENCES:		

COMPONENTS:	EVALUATOR:
(1) 2-Methyl-2-hexanol; C ₇ H ₁₆ 0;	Z. Maczynska, Institute of Physical
[625-23-0]	Chemistry of the Polish Academy of Sciences,
(2) Water; H ₂ O; [7732-18-5]	Warsaw, Poland.
(-,,	November 1982

Solubilities in the system comprising 2-methyl-2-hexanol (1) and water (2) have been reported in two publications. Ginnings and Hauser (ref 1) carried out measurements of the mutual solubilities in the two phases at 293, 298 and 303 K by the volumetric method (Figures 1 and 2). Ratouis and Dode (ref 2) determined the solubility of (1) in the water-rich phase at one temperature (303 K) by an analytical method, and their value of 0.82 g(1)/100g sln is in good agreement with the value 0.87 \pm 0.1 g(1)/100g sln of ref 1. However, as the comparison involves a single point and as the other five points are derived from only one source, the data are regarded as being tentative.



Tentative values for the mutual solubilities of 2-methyl-2-hexanol (1) and water (2)

T/K	Water-rich	-	Alcohol-ric	h ph as e
	g(1)/100g sln	$10^{3}x_{1}$	g(2)/100g sln	<i>x</i> 2
293	1.1	1.7	6.2	0.300
298	1.0	1.5	6.3	0.303
303	0.9	1.3	6.4	0.307

References

1. Ginnings, P.M.; Hauser, M. J. Am. Chem. Soc. 1938, 60, 2581.

 2-Methyl-2-hexanol; C₇H₁₆O; [625-23-0] Water; H₂O; [7732-18-5] 	Ginnings, P.M.; Hauser, M.
[625-23-0]	
2) Water; H ₂ 0; [7732-18-5]	J. Am. Chem. Soc. <u>1938</u> , 60, 2581-2.
2	
RIABLES:	PREPARED BY:
emperature: 20-30 [°] C	A. Maczynski and Z. Maczynska
PERIMENTAL VALUES:	A
Mutual solubility of 2-methy	1-2-hexanol(1) and water(2)
t/ ⁰ C g(1)/100g sln	x_1 (compiler)
(2)-rich phase (1)-rich ph	ase (2)-rich phase (1)-rich phase
20 1.08 93.77	0.00169 0.7000
25 0.97 93.65	0.00152 0.6957
30 0.87 93.56	0.00134 0.6925
Relativ	e density, d_{μ}
	7
$t/{}^{\circ}$ C Water-rich pha	se Alcohol-rich phase
20 0.9967	0.8268
25 0.9958 30 0.9946	0.8233 0.8199
	INFORMATION
ETHOD /APPARATUS / PROCEDURE :	SOURCE AND PURITY OF MATERIALS:
The volumetric method was used as described in ref 1. Both components were introduced in known amounts into a two-bulb graduated and calibrated flask and shaken mechanically in a water-bath at constant temperature. After sufficient time the liquids were allowed to separate and the total volume was measured. Upon centrifugation, the phase separation line was read, and phase volumes were calculated. From the total weights of the components, the total volume individual phase volumes, and component concentrations in either phase were evaluated.	<pre>distilled from calcium oxide; b.p. range 143.0-143.2°C, d₄²⁵ 0.8093; purity not specified. (2) not specified.</pre>

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) 2-Methyl-2-hexanol; C ₇ H ₁₆ 0; [625-23-0]	Ratouis, M.; Dodé, M.
(1) Water; H ₂ 0; [[] 7732-18-5]	Bull. Soc. Chim. Fr. <u>1965</u> , 3318-22.
VARIABLES:	PREPARED BY:
One temperature: 30°C	S.C. Valvani; S.H. Yalkowsky; A.F.M. Barton
Ringer solution also studied	
EXPERIMENTAL VALUES:	

The proportion of 2-methyl-2-hexanol (1) in the water-rich phase at equilibrium at 30° C was reported to be 0.82 g(1)/100g sln.

The corresponding mole fraction solubility, calculated by the compilers, is $x_1 = 0.00128$.

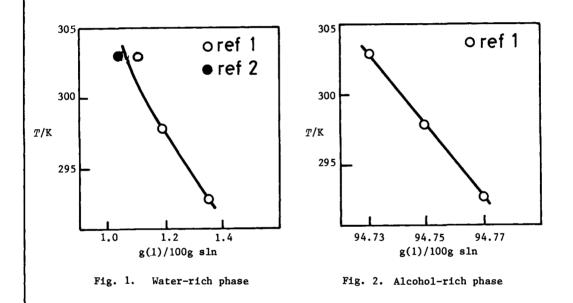
The proportion of (1) in the water-rich phase of a mixture with Ringer solution at 30° C was reported to be 0.78 g(1)/100g sln.

AUXILIARY	INFORMATION
METHOD/APPARATUS/PROCEDURE: In a round bottomed flask, 50 mL of water and a sufficient quantity of alcohol were introduced until two separate layers were formed. The flask assembly was equilibrated by agitation for at least 3h in a constant temperature bath. Equilibrium solubility as attained by first supersaturation at a slightly lower temperature (solubility of alcohols in water decreases with increasing temperature) and then equilibrating at the desired temperature. The aqueous layer was separated after an overnight storage in a bath. The alcohol content was determined by reacting the aqueous solution with potassium dichromate and titrating the excess dichromate with ferrous sulfate solution in the presence of phosphoric acid and diphenylamine barium sulfonate as an indicator.	<pre>SOURCE AND PURITY OF MATERIALS: (1) laboratory preparation; redistilled with 10:1 reflux ratio b.p. 143.6-143.7°C/765 mm Hg n²⁵ = 1.41614 (2) twice distilled from silica apparatus or ion-exchanged with Sagei A20 ESTIMATED ERROR: Solubility: relative error of 2 determinations less than 1% Temperature: ± 0.05°C REFERENCES:</pre>

COMPONENTS:	ORIGINAL MEASUREMENTS:	
(1) 2-Methyl-3-he x anol; C ₇ H ₁₆ 0; [617-29-8]	Ratouis, M.; Dodé, M.	
 (2) Water; H₂0; [7732-18-5] 	Bull. Soc. Chim. Fr. <u>1965</u> , 3318-22.	
(2) water; H_20 ; $L7732-10-53$		
VARIABLES:	PREPARED BY:	
Temperature: 25°C and 30°C	S.C. Valvani; S.H. Yalkowsky; A.F.M. Barte	
Ringer solution also studied	· · · · · · · · · · · · · · · · · · ·	
EXPERIMENTAL VALUES:		
Proportion of 2-methy1-3-h	exanol (1) in water-rich phase	
t/ ^o C g(1)/10	$\log \sin 10^4 x_1$ (compilers)	
25 0.	57 8.9	
30 0.	555 8.64	
AUXILIARY	INFORMATION	
	••••••••••••••••••••••••••••••••••••••	
	SOURCE AND PURITY OF MATERIALS:	
METHOD/APPARATUS/PROCEDURE: In a round bottomed flask, 50 mL of water and a sufficient quantity of alcohol were	SOURCE AND PURITY OF MATERIALS: (1) laboratory preparation; redistilled with 10:1 reflux ratio	
METHOD/APPARATUS/PROCEDURE: In a round bottomed flask, 50 mL of water and a sufficient quantity of alcohol were introduced until two separate layers were formed. The flask assembly was equilibrated	SOURCE AND PURITY OF MATERIALS: (1) laboratory preparation; redistilled with 10:1 reflux ratio b.p. 146-147 ⁰ C/755 mm Hg	
METHOD/APPARATUS/PROCEDURE: In a round bottomed flask, 50 mL of water and a sufficient quantity of alcohol were introduced until two separate layers were	<pre>SOURCE AND PURITY OF MATERIALS: (1) laboratory preparation; redistilled with 10:1 reflux ratio b.p. 146-147^oC/755 mm Hg n²⁵_D = 1.41942</pre>	
METHOD/APPARATUS/PROCEDURE: In a round bottomed flask, 50 mL of water and a sufficient quantity of alcohol were introduced until two separate layers were formed. The flask assembly was equilibrated by agitation for at least 3h in a constant	SOURCE AND PURITY OF MATERIALS: (1) laboratory preparation; redistilled with 10:1 reflux ratio b.p. 146-147 ⁰ C/755 mm Hg	
METHOD/APPARATUS/PROCEDURE: In a round bottomed flask, 50 mL of water and a sufficient quantity of alcohol were introduced until two separate layers were formed. The flask assembly was equilibrated by agitation for at least 3h in a constant temperature bath. Equilibrium solubility was attained by first supersaturation at a slightly lower temperature (solubility of alcohols in water decreases with	SOURCE AND PURITY OF MATERIALS: (1) laboratory preparation; redistilled with 10:1 reflux ratio b.p. $146-147^{\circ}C/755$ mm Hg $n_D^{25} = 1.41942$ (2) twice distilled from silica apparatus	
METHOD/APPARATUS/PROCEDURE: In a round bottomed flask, 50 mL of water and a sufficient quantity of alcohol were introduced until two separate layers were formed. The flask assembly was equilibrated by agitation for at least 3h in a constant temperature bath. Equilibrium solubility was attained by first supersaturation at a slightly lower temperature (solubility of alcohols in water decreases with increasing temperature) and then equilibrating at the desired temperature.	SOURCE AND PURITY OF MATERIALS: (1) laboratory preparation; redistilled with 10:1 reflux ratio b.p. 146-147°C/755 mm Hg $n_D^{25} = 1.41942$ (2) twice distilled from silica apparatus	
METHOD/APPARATUS/PROCEDURE: In a round bottomed flask, 50 mL of water and a sufficient quantity of alcohol were introduced until two separate layers were formed. The flask assembly was equilibrated by agitation for at least 3h in a constant temperature bath. Equilibrium solubility was attained by first supersaturation at a slightly lower temperature (solubility of alcohols in water decreases with increasing temperature) and then	SOURCE AND PURITY OF MATERIALS: (1) laboratory preparation; redistilled with 10:1 reflux ratio b.p. 146-147°C/755 mm Hg $n_D^{25} = 1.41942$ (2) twice distilled from silica apparatus	
METHOD/APPARATUS/PROCEDURE: In a round bottomed flask, 50 mL of water and a sufficient quantity of alcohol were introduced until two separate layers were formed. The flask assembly was equilibrated by agitation for at least 3h in a constant temperature bath. Equilibrium solubility was attained by first supersaturation at a slightly lower temperature (solubility of alcohols in water decreases with increasing temperature) and then equilibrating at the desired temperature. The aqueous layer was separated after an overnight storage in a bath. The alcohol content was determined by reacting the	 SOURCE AND PURITY OF MATERIALS: (1) laboratory preparation; redistilled with 10:1 reflux ratio b.p. 146-147°C/755 mm Hg n²⁵_D = 1.41942 (2) twice distilled from silica apparatus or ion-exchanged with Sagei A20 	
METHOD/APPARATUS/PROCEDURE: In a round bottomed flask, 50 mL of water and a sufficient quantity of alcohol were introduced until two separate layers were formed. The flask assembly was equilibrated by agitation for at least 3h in a constant temperature bath. Equilibrium solubility was attained by first supersaturation at a slightly lower temperature (solubility of alcohols in water decreases with increasing temperature) and then equilibrating at the desired temperature. The aqueous layer was separated after an overnight storage in a bath. The alcohol content was determined by reacting the aqueous solution with potassium dichromate and titrating the excess dichromate with	<pre>SOURCE AND PURITY OF MATERIALS: (1) laboratory preparation; redistilled with 10:1 reflux ratio b.p. 146-147^oC/755 mm Hg n²⁵_D = 1.41942 (2) twice distilled from silica apparatus or ion-exchanged with Sagei A20 ESTIMATED ERROR: Solubility: relative error of 2 determinations less than 1%.</pre>	
METHOD/APPARATUS/PROCEDURE: In a round bottomed flask, 50 mL of water and a sufficient quantity of alcohol were introduced until two separate layers were formed. The flask assembly was equilibrated by agitation for at least 3h in a constant temperature bath. Equilibrium solubility was attained by first supersaturation at a slightly lower temperature (solubility of alcohols in water decreases with increasing temperature) and then equilibrating at the desired temperature. The aqueous layer was separated after an overnight storage in a bath. The alcohol content was determined by reacting the aqueous solution with potassium dichromate and titrating the excess dichromate with ferrous sulfate solution in the presence of phosphoric acid and diphenylamine barium	<pre>SOURCE AND PURITY OF MATERIALS: (1) laboratory preparation; redistilled with 10:1 reflux ratio b.p. 146-147^oC/755 mm Hg n²⁵_D = 1.41942 (2) twice distilled from silica apparatus or ion-exchanged with Sagei A20</pre> ESTIMATED ERROR: Solubility: relative error of 2 determinations less than 1%. Temperature: ± 0.05 ^o C	
METHOD/APPARATUS/PROCEDURE: In a round bottomed flask, 50 mL of water and a sufficient quantity of alcohol were introduced until two separate layers were formed. The flask assembly was equilibrated by agitation for at least 3h in a constant temperature bath. Equilibrium solubility was attained by first supersaturation at a slightly lower temperature (solubility of alcohols in water decreases with increasing temperature) and then equilibrating at the desired temperature. The aqueous layer was separated after an overnight storage in a bath. The alcohol content was determined by reacting the aqueous solution with potassium dichromate and titrating the excess dichromate with ferrous sulfate solution in the presence of	<pre>SOURCE AND PURITY OF MATERIALS: (1) laboratory preparation; redistilled with 10:1 reflux ratio b.p. 146-147^oC/755 mm Hg n²⁵_D = 1.41942 (2) twice distilled from silica apparatus or ion-exchanged with Sagei A20 ESTIMATED ERROR: Solubility: relative error of 2 determinations less than 1%.</pre>	
METHOD/APPARATUS/PROCEDURE: In a round bottomed flask, 50 mL of water and a sufficient quantity of alcohol were introduced until two separate layers were formed. The flask assembly was equilibrated by agitation for at least 3h in a constant temperature bath. Equilibrium solubility was attained by first supersaturation at a slightly lower temperature (solubility of alcohols in water decreases with increasing temperature) and then equilibrating at the desired temperature. The aqueous layer was separated after an overnight storage in a bath. The alcohol content was determined by reacting the aqueous solution with potassium dichromate and titrating the excess dichromate with ferrous sulfate solution in the presence of phosphoric acid and diphenylamine barium	<pre>SOURCE AND PURITY OF MATERIALS: (1) laboratory preparation; redistilled with 10:1 reflux ratio b.p. 146-147^oC/755 mm Hg n²⁵_D = 1.41942 (2) twice distilled from silica apparatus or ion-exchanged with Sagei A20</pre> ESTIMATED ERROR: Solubility: relative error of 2 determinations less than 1%. Temperature: ± 0.05 ^o C	
METHOD/APPARATUS/PROCEDURE: In a round bottomed flask, 50 mL of water and a sufficient quantity of alcohol were introduced until two separate layers were formed. The flask assembly was equilibrated by agitation for at least 3h in a constant temperature bath. Equilibrium solubility was attained by first supersaturation at a slightly lower temperature (solubility of alcohols in water decreases with increasing temperature) and then equilibrating at the desired temperature. The aqueous layer was separated after an overnight storage in a bath. The alcohol content was determined by reacting the aqueous solution with potassium dichromate and titrating the excess dichromate with ferrous sulfate solution in the presence of phosphoric acid and diphenylamine barium	<pre>SOURCE AND PURITY OF MATERIALS: (1) laboratory preparation; redistilled with 10:1 reflux ratio b.p. 146-147^oC/755 mm Hg n²⁵_D = 1.41942 (2) twice distilled from silica apparatus or ion-exchanged with Sagei A20</pre> ESTIMATED ERROR: Solubility: relative error of 2 determinations less than 1%. Temperature: ± 0.05 ^o C	
METHOD/APPARATUS/PROCEDURE: In a round bottomed flask, 50 mL of water and a sufficient quantity of alcohol were introduced until two separate layers were formed. The flask assembly was equilibrated by agitation for at least 3h in a constant temperature bath. Equilibrium solubility was attained by first supersaturation at a slightly lower temperature (solubility of alcohols in water decreases with increasing temperature) and then equilibrating at the desired temperature. The aqueous layer was separated after an overnight storage in a bath. The alcohol content was determined by reacting the aqueous solution with potassium dichromate and titrating the excess dichromate with ferrous sulfate solution in the presence of phosphoric acid and diphenylamine barium	<pre>SOURCE AND PURITY OF MATERIALS: (1) laboratory preparation; redistilled with 10:1 reflux ratio b.p. 146-147°C/755 mm Hg n²⁵ = 1.41942 (2) twice distilled from silica apparatus or ion-exchanged with Sagei A20 ESTIMATED ERROR: Solubility: relative error of 2 determinations less than 1%. Temperature: ± 0.05°C</pre>	

COMPONENTS :	EVALUATOR:
(1) 3-Methy1-3-hexanol; C ₇ H ₁₆ 0; [597-96-6]	Z. Maczynska, Institute of Physical Chemistry of the Polish Academy of Sciences,
(2) Water; H ₂ 0; [7732-18-5]	Warsaw, Poland. November 1982

Solubilities in the system comprising 3-methyl-3-hexanol (1) and water (2) have been reported in two publications (Figures 1 and 2). Ginnings and Hauser (ref 1) carried out measurements of the mutual solubilities in the two phases at 293, 298 and 303 K by the volumetric method. Ratouis and Dode (ref 2) determined the solubility of (1) in the water-rich phase at one temperature (303 K) by an analytical method, their value of 1.05 g(1)/100g sln being in excellent agreement with that of 1.1 ± 0.1 g(1)/100g sln in ref 1. However, as the comparison involves a single point and as the other five points are derived from only one source, the data are regarded as being tentative.



Tentative values for the mutual solubilities of 3-methyl-3-hexanol (1) and water (2)

T/K	Water-rich phase		Alcohol-rich phase	
	g(1)/100g sln	$10^{3}x_{1}$	g(2)/100g sln	<i>*</i> 2
293	1.4	2.1	5.2	0.26
298	1.2	1.9	5.3	0.26
303	1.1	1.7	5.3	0.26

References

1. Ginnings, P.M.; Hauser, M. J. Am. Chem. Soc. 1938, 60, 2581.

<pre>(1) 3-Methy1-3-hexano1; C₇H₁₆O; [597-96-6] (2) Water; H₂O; [7732-18-5] ARIABLES: Temperature: 20-30^OC</pre>	Ginnings, P.M.; Hauser, M. J. Am. Chem. Soc. <u>1938</u> , 60, 2581-2. PREPARED BY: A. Maczynski and Z. Maczynska
[597-96-6] (2) Water; H ₂ 0; [7732-18-5] ARIABLES:	PREPARED BY: A. Maczynski and Z. Maczynska
ARIABLES:	A. Maczynski and Z. Maczynska
ARIABLES:	A. Maczynski and Z. Maczynska
	A. Maczynski and Z. Maczynska
Temperature: 20-30 [°] C	
	hy1-3-hexanol(1) and water(2)
XPERIMENTAL VALUES:	ny1-3-hexano1(1) and water(2)
Mutual solubility of 3-meth	
t/ ⁰ C g(1)/100g sln	$x_1(\text{compiler})$
(2)-rich phase (1)-rich p	ohase (2)-rich phase (1)-rich phase
20 1.35 94.	.77 0.00212 0.7374
25 1.19 94.	.75 0.00186 0.7366
30 1.07 94.	.73 0.00167 0.7359
Relati	we density, d_4
t/ ⁰ C Water-rich	phase Alcohol-rich phase
20 0.99	0.8348
25 0.99	0.8312
	Y INFORMATION
E THOD /APPARATUS / PROCEDURE :	SOURCE AND PURITY OF MATERIALS:
The volumetric method was used as described in ref 1. Both components were introduced in known amounts into a two-bulb graduated and calibrated flask and shaken mechanically i a water-bath at constant temperature. After sufficient time the liquids were allowed to separate and the total volume was measured. Upon centrifugation, the phase separation line was read, and phase volumes were calculated. From the total weights of the components, the total volum individual phase volumes, and component concentrations in either phase were evaluated.	distilled from calcium oxide; b.p. range 142.7-142.9°C, d_4^{25} 0.8202; purity not specified. (2) not specified. (2) not specified.

COMPONENTS :	ORIGINAL MEASUREMENTS:	
(1) 3-Methyl-3-hexanol; C ₇ H ₁₆ 0; [597-96-6] (2) Water; H ₂ 0; [7732-18-5]	Ratouis, M.: Dodé, M. Bull. Soc. Chim. Fr. <u>1965</u> , 3318-22	
VARIABLES: One temperature: 30 ⁰ C Ringer solution also studied	PREPARED BY: S.C. Valvani; S.H. Yalkowsky; A.F.M. Barton	
EXPERIMENTAL VALUES:		

The proportion of 3-methyl-3-hexanol (1) in the water-rich phase at equilibrium at 30° C was reported to be 1.05 g(1)/100g sln.

The corresponding mole fraction solubility calculated by the compilers is $x_1 = 0.00164$.

The proportion of (1) in the water-rich phase of a mixture with Ringer solution at 30° C was reported to be 0.97 g(1)/100g sln.

AUXILIARY	INFORMATION
In a round bottomed flask, 50 mL of water and a sufficient quantity of alcohol were introduced until two separate layers were formed. The flask assembly was equilibrated by agitation for at least 3h in a constant temperature bath. Equilibrium solubility was attained by first supersaturation at a slightly lower temperature (solubility of alcohols in water decreases with increasing temperature) and then equilibrating at the desired temperature. The aqueous layer was separated after an overnight storage in a	 SOURCE AND PURITY OF MATERIALS: (1) laboratory preparation; redistilled with 10:1 reflux ratio b.p. 75.5°C/60 mm Hg n²⁵ = 1.42076 (2) twice distilled from silica apparatus or ion-exchanged with Sagei A20 ESTIMATED ERROR: Solubility: relative error of 2
	determinations less than 1% Temperature: ± 0.05 [°] C REFERENCES:

	ORIGINAL MEASUREMENTS:	
(1) 5-Methyl-2-hexanol; C ₇ H ₁₆ 0; [627-59-8]	Ratouis, M.; Dodé, M.	
(2) Water; H ₂ 0; [7732-18-5]	Bull. Soc. Chim. Fr. <u>1965</u> , 3318-22.	
VARIABLES: PREPARED BY:		
Temperature: 25°C and 30°C	S.C. Valvani; S.H. Yalkowsky; A.F.M. Barto	
Ringer solution also studied		
EXPERIMENTAL VALUES:		
Proportion of 5-methy1-2	-hexanol (1) in water-rich phase	
t/ ^o C g(1)/100g	$10^4 x_1$ (compilers)	
25 0.49	7.6	
30 0.47	7.3	
1		
AUXILIAR	Y INFORMATION	
METHOD / APPARATUS / PROCEDURE :		
	SOURCE AND PURITY OF MATERIALS:	
In a round bottomed flask, 50 mL of water and a sufficient quantity of alcohol were introduced until two separate layers were formed. The flask assembly was equilibrate by agitation for at least 3h in a constant temperature bath. Equilibrium solubility was attained by first supersaturation at a slightly lower temperature (solubility of alcohols in water decreases with increasing temperature) and then equilibrating at the desired temperature. The aqueous layer was separated after an overnight storage in a bath. The alcohol content was determined b reacting the aqueous solution with potassiu dichromate and titrating the excess dichromate with ferrous sulfate solution in the presence of phosphoric acid and diphenylamine barium sulfonate as an indicator.	 (1) laboratory preparation; redistilled with 10:1 reflux ratio b.p. 152.6-153.5°C/760.5 mm Hg n²⁵_D = 1.41718 (2) twice distilled from silica apparatus or ion-exchanged with Sagei A20 ESTIMATED ERROR: Solubility: relative error of 2 determinations less than 1% 	

1-Heptanol

COMPONENTS:		EVALUATOR:	
(1) 1-Heptanol (n-heptyl alcohol)	; C ₇ H ₁₆ 0;	G.T. Hefter and A.F.M. Barton, Murdoch	
[111-70-6]		University, Perth, Western Australia.	
(2) Water; H ₂ 0; [7732-18-5]		June, 1983	
2			
CRITICAL EVALUATION:		<u></u>	
Solubilities in the 1-heptanol (1) - water (2	2) system have been repor	rted in the
following publications.			
Reference	T/K	Solubility	Method
Fuhner (ref 1)	343-403	(1) in (2)	synthetic
Butler et al. (ref 2)	298	(1) in (2)	interferometric
Addison (ref 3)	293	(1) in (2)	surface tension
Booth and Everson (ref 4)	298	(1) in (2)	titration
Harkins and Oppenheimer (ref 5)	-	(1) in (2)	turbidimetric
Donahue and Bartell (ref 6)	298	mutual	analytical
Erichsen (ref 7)	273-526	mutual	synthetic
Erichsen (ref 8)	273-323	(1) in (2)	synthetic
Kinoshita <i>et al</i> . (ref 9)	298	(1) in (2)	surface tension
Rao et al. (ref 10)	303	mutual	turbidity
Ratouis and Dode (ref 11)	303	(1) in (2)	analytical
Hanssens (ref 12)	298	(1) in (2)	refractometric
Krasnov and Gartseva (ref 13)	285,313	(2) in (1)	analytical
Ionin and Shanina (ref 14)	298	(2) in (1)	titration
Vochten and Petre (ref 15)	288-333	(1) in (2)	surface tension
Hill and White (ref 16)	279-308	(1) in (2)	interferometric
Korenman et al. (ref 17)	298	mutual	analytical
Nishino and Nakamura (ref 18)	280-350	mutual	synthetic
Tokunaga <i>et al</i> . (ref 19)	288-313	(2) in (1)	analytical

The original data are compiled in the data sheets immediately following this Critical Evaluation.

The l-heptanol-water system is interesting in that unlike most of the higher l-alkanols the data for the water-rich phase is more extensive and self-consistent than the data for the alcohol-rich phase.

In preparing this Critical Evaluation use has been made of the fact that the solubility of 1-heptanol in water is sufficiently low to enable weight/volume data (ref 6, 12, 15, 17) to be converted to weight/weight values by assuming the water-rich phase has the same density as pure water. The same is not true for the alcohol-rich phase and thus such data (ref 6, 12, 17) have been excluded from further consideration. The data of Booth and Everson (ref 4) given in volume/volume units and the graphical data of Nishino and Nakamura (ref 18) were also excluded.

In the water-rich phase the converted data of Korenman et al. (ref 17) and the data of Rao et al. (ref 10) disagree markedly with all other values and have therefore been rejected. The data of Harkins and Oppenheimer (ref 5) are also rejected as the temperature was not specified.

All other data are included in the Tables below.

(continued next page)

330	Seven-carbo	on Alcohols		
COMPONENTS	:	EVALUATOR:		
[111-	btanol (<i>n-heptyl alcohol);</i> C ₇ H ₁₆ O; 70-6] ; H ₂ O; [7732-18-5]	G.T. Hefter and A.F.M. Ba University, Perth, Wester June, 1983	-	
CRITICAL E	VALUATION (continued)			
data shee averaging statistic the sprea "Recommer	tained by the Evaluator by graphical ets are indicated by an asterisk(*). The uncertainty limits (σ_n) attact al significance and should be regarded d of reported values and not as error ded" data. Data are "Recommended" is easonable agreement ($\leq \pm$ 5% relative).	"Best" values have been ched to the "best" values ed only as a convenient r r limits. The letter (R)	obtained by s do not have epresentation o designates	imple of
For conve	nience the two phases will be further	r discussed separately.		
The solut	ility of 1-heptanol (1) in water (2)			
to be <i>Rec</i> ref 7).	nus data available are generally in ex commended over an unusually wide range Above 403 K, the data of Erichsen (1 puld be considered as <i>Tentative</i> . <u>Recommended (<i>R</i>) and tentative</u> <u>1-heptanol (1) in wa</u>	e of temperature (see par ref 7) are the only value ve solubilities of	ticularly ref	l and
Т/К	Sol	lubility, g(1)/100g sln		
	Reported values	"Bes		
	Reported varues	200	t" values (±σ)
273	0.34 (ref 7), 0.34 (ref 8)	205	t" values (±ơ _n 0.34)
273 283	0.34 (ref 7), 0.34 (ref 8)		11)
	-	(ref 16)	0.34) (<i>R</i>)
283	0.34 (ref 7), 0.34 (ref 8) 0.26 (ref 7), 0.30 (ref 8), 0.203* 0.172 (ref 3), 0.20 (ref 7), 0.20 (0.181 (ref 2), 0.180 (ref 6), 0.18*	(ref 16) (ref 8), 0.15 (ref 15), 0.175 (ref 16)	0.34 0.25 \pm 0.04 0.17 \pm 0.02	
283 293	0.34 (ref 7), 0.34 (ref 8) 0.26 (ref 7), 0.30 (ref 8), 0.203* 0.172 (ref 3), 0.20 (ref 7), 0.20 (0.181 (ref 2), 0.180 (ref 6), 0.18*	(ref 16) (ref 8), 0.15 (ref 15), 0.175 (ref 16) * (ref 7), 0.17 (ref 9), (ref 12), 0.168 (ref 16)	0.34 0.25 \pm 0.04 0.17 \pm 0.02	(<i>R</i>)
283 293 298	0.34 (ref 7), 0.34 (ref 8) 0.26 (ref 7), 0.30 (ref 8), 0.203 * 0.172 (ref 3), 0.20 (ref 7), 0.20 (0.181 (ref 2), 0.180 (ref 6), 0.18 0.17	<pre>(ref 16) (ref 8), 0.15 (ref 15),</pre>	$\begin{array}{c} 0.34 \\ 0.25 \pm 0.04 \\ 0.17 \pm 0.02 \\ 0.174 \pm 0.005 \end{array}$	(<i>R</i>) (<i>R</i>)
283 293 298 303	0.34 (ref 7), 0.34 (ref 8) 0.26 (ref 7), 0.30 (ref 8), 0.203* 0.172 (ref 3), 0.20 (ref 7), 0.20 (0.181 (ref 2), 0.180 (ref 6), 0.18 0.17 0.16 (ref 7), 0.16 (ref 8), 0.17 (r	<pre>(ref 16) (ref 8), 0.15 (ref 15),</pre>	$0.34 \\ 0.25 \pm 0.04 \\ 0.17 \pm 0.02 \\ 0.174 \pm 0.005 \\ 0.160 \pm 0.007 \\ 0.160 \pm 0.007 \\ 0.007 \\ 0.000 \\ 0$	(<i>R</i>) (<i>R</i>) (<i>R</i>)
283 293 298 303 313	0.34 (ref 7), 0.34 (ref 8) 0.26 (ref 7), 0.30 (ref 8), 0.203 * 0.172 (ref 3), 0.20 (ref 7), 0.20 (0.181 (ref 2), 0.180 (ref 6), 0.18 * 0.17 0.16 (ref 7), 0.16 (ref 8), 0.17 (1 0.13 (ref 7), 0.13 (ref 8), 0.13 (1	<pre>(ref 16) (ref 8), 0.15 (ref 15),</pre>	$\begin{array}{c} 0.34\\ 0.25 \pm 0.04\\ 0.17 \pm 0.02\\ 0.174 \pm 0.005\\ 0.160 \pm 0.007\\ 0.13\end{array}$	(R) (R) (R) (R)
283 293 298 303 313 323	0.34 (ref 7), 0.34 (ref 8) 0.26 (ref 7), 0.30 (ref 8), 0.203*(0.172 (ref 3), 0.20 (ref 7), 0.20 (0.181 (ref 2), 0.180 (ref 6), 0.18* 0.17 0.16 (ref 7), 0.16 (ref 8), 0.17 (r 0.13 (ref 7), 0.13 (ref 8), 0.13 (r 0.11 (ref 7), 0.12 (ref 8), 0.14 (r	<pre>(ref 16) (ref 8), 0.15 (ref 15),</pre>	$\begin{array}{c} 0.34\\ 0.25 \pm 0.04\\ 0.17 \pm 0.02\\ 0.174 \pm 0.005\\ 0.160 \pm 0.007\\ 0.13\\ 0.12 \pm 0.01\\ \end{array}$	(R) (R) (R) (R)
283 293 298 303 313 323 333	0.34 (ref 7), 0.34 (ref 8) 0.26 (ref 7), 0.30 (ref 8), 0.203*(0.172 (ref 3), 0.20 (ref 7), 0.20 (0.181 (ref 2), 0.180 (ref 6), 0.18 0.17 0.16 (ref 7), 0.16 (ref 8), 0.17 (ref 1) 0.13 (ref 7), 0.12 (ref 8), 0.14 (ref 1))	<pre>(ref 16) (ref 8), 0.15 (ref 15),</pre>	$0.34 0.25 \pm 0.04 0.17 \pm 0.02 0.174 \pm 0.005 0.160 \pm 0.007 0.13 0.12 \pm 0.01 0.13 \pm 0.02$	(R) (R) (R) (R) (R)
283 293 298 303 313 323 333 343	0.34 (ref 7), 0.34 (ref 8) 0.26 (ref 7), 0.30 (ref 8), 0.203 * 0.172 (ref 3), 0.20 (ref 7), 0.20 (0.181 (ref 2), 0.180 (ref 6), 0.18 * 0.17 0.16 (ref 7), 0.16 (ref 8), 0.17 (r 0.13 (ref 7), 0.13 (ref 8), 0.13 (r 0.11 (ref 7), 0.12 (ref 8), 0.14 (r 0.125 (ref 1), 0.15 (ref 7)	<pre>(ref 16) (ref 8), 0.15 (ref 15),</pre>	$\begin{array}{c} 0.34\\ 0.25 \pm 0.04\\ 0.17 \pm 0.02\\ 0.174 \pm 0.005\\ 0.160 \pm 0.007\\ 0.13\\ 0.12 \pm 0.01\\ 0.13 \pm 0.02\\ 0.14 \pm 0.01\\ \end{array}$	(R) (R) (R) (R) (R) (R)
283 293 298 303 313 323 333 343 353	0.34 (ref 7), 0.34 (ref 8) 0.26 (ref 7), 0.30 (ref 8), 0.203 * 0 0.172 (ref 3), 0.20 (ref 7), 0.20 (0.181 (ref 2), 0.180 (ref 6), 0.18 0 0.181 (ref 7), 0.180 (ref 6), 0.18 0 0.17 0.16 (ref 7), 0.16 (ref 8), 0.17 (ref 7), 0.16 (ref 8), 0.13 (ref 7), 0.13 (ref 8), 0.13 (ref 7), 0.13 (ref 7), 0.12 (ref 8), 0.14 (ref 7), 0.15 (ref 15) 0.125 (ref 1), 0.15 (ref 7) 0.17 (ref 1), 0.19 (ref 7)	<pre>(ref 16) (ref 8), 0.15 (ref 15),</pre>	$\begin{array}{c} 0.34\\ 0.25 \pm 0.04\\ 0.17 \pm 0.02\\ 0.174 \pm 0.005\\ 0.160 \pm 0.007\\ 0.13\\ 0.12 \pm 0.01\\ 0.13 \pm 0.02\\ 0.14 \pm 0.01\\ 0.18 \pm 0.01\\ \end{array}$	(R) (R) (R) (R) (R) (R) (R)
283 293 298 303 313 323 333 343 353 363	0.34 (ref 7), 0.34 (ref 8) 0.26 (ref 7), 0.30 (ref 8), 0.203 * 0 0.172 (ref 3), 0.20 (ref 7), 0.20 (0.181 (ref 2), 0.180 (ref 6), 0.18 0 0.181 (ref 7), 0.180 (ref 6), 0.18 0 0.17 0.16 (ref 7), 0.16 (ref 8), 0.17 (ref 7), 0.13 (ref 8), 0.13 (ref 7), 0.12 (ref 8), 0.14 (ref 7), 0.15 (ref 15), 0.125 (ref 1), 0.15 (ref 7), 0.15 (ref 7), 0.17 (ref 1), 0.19 (ref 7), 0.225 (ref 1), 0.23 (ref 7), 0.24 (ref 7), 0.25 (ref	<pre>(ref 16) (ref 8), 0.15 (ref 15),</pre>	$\begin{array}{c} 0.34\\ 0.25 \pm 0.04\\ 0.17 \pm 0.02\\ 0.174 \pm 0.005\\ 0.160 \pm 0.007\\ 0.13\\ 0.12 \pm 0.01\\ 0.13 \pm 0.02\\ 0.14 \pm 0.01\\ 0.18 \pm 0.01\\ 0.23\\ \end{array}$	 (R) (R)

0.52 ± 0.01

0.65

0.80

1.0

1.2

1.6

(R)

0.515 (ref 1), 0.53 (ref 7)

0.65 (ref 7)

0.80 (ref 7)

0.98 (ref 7)

1.23 (ref 7)

1.60 (ref 7)

403

413

423 433

443

453

COMPONENTS:	EVALUATOR:
<pre>(1) 1-Heptanol (n-heptyl alcohol); C₇H₁₆0; [111-70-6]</pre>	G.T. Hefter and A.F.M. Barton, Murdoch University, Perth, Western Australia.
(2) Water; H ₂ 0; [7732-18-5]	June, 1983

CRITICAL EVALUATION (continued)

T/K		Solubility, g(1)/100g sln	
		Reported values	"Best" values $(\pm \sigma_n)$
463	2.08 (ref 7)		2.1
473	2.64 (ref 7)		2.6
483	3.48 (ref 7)		3.5
493	4.68 (ref 7)		4.7
503	6.70 (ref 7)		6.7
513	10.10 (ref 7)		10.1

The solubility of water (2) in 1-heptanol (1)

Data for the alcohol-rich phase, unlike the water-rich phase considered above, is rather limited. Even those data which are available are not in good agreement and with the exception of the value at 35° C are regarded as *Tentative* only. This phase warrants thorough re-investigation.

Recommended (R) and tentative solubilities of water (2) in 1-heptanol (1)

T/K	Solubility, g(2)/100g sln		
	Reported values	"Best" values (±	σ n)
273	3.90 (ref 7)		
283	4.30 (ref 7)		
293	4.75 (ref 7), 5.82 (ref 19)	5.3 ± 0.5	
298	5.3 (ref 6), 5.0 [*] (ref 7), 5.8 (ref 14), 5.85 (ref 19)	5.4 ± 0.4	
303	5.20 (ref 7), 5.5 (ref 10), 5.90 (ref 19)	5.5 ± 0.3	
313	5.75 (ref 7), 5.90 (ref 13), 6.02 (ref 19)	5.9 ± 0.1	(<i>R</i>)
323	6.30 (ref 7)	6.3	
333	6.95 (ref 7)	7.0	
343	7.60 (ref 7)	7.6	
353	8.35 (ref 7)	8.4	
363	9.10 (ref 7)	9.1	
373	9.85 (ref 7)	9.9	
383	10.75 (ref 7)	10.8	
393	11.65 (ref 7)	11.7	
403	12.65 (ref 7)	12.7	
413	13.75 (ref 7)	13.8	
423	14.90 (ref 7)	14.9	
433	16.20 (ref 7)	16.2	
443	17.65 (ref 7)	17.7	
453	19.25 (ref 7)	19.3	
463	21.10 (ref 7) (continued next page	21.1	

COMPONENTS:	EVALUATOR:
 (1) 1-Heptanol (<i>n-heptyl alcohol</i>); C₇H₁₆0; [111-70-6] (2) Water; H₂0; [7732-18-5] 	G.T. Hefter and A.F.M. Barton, Murdoch University, Perth, Western Australia. June, 1983.

CRITICAL EVALUATION (continued)

π	/K	

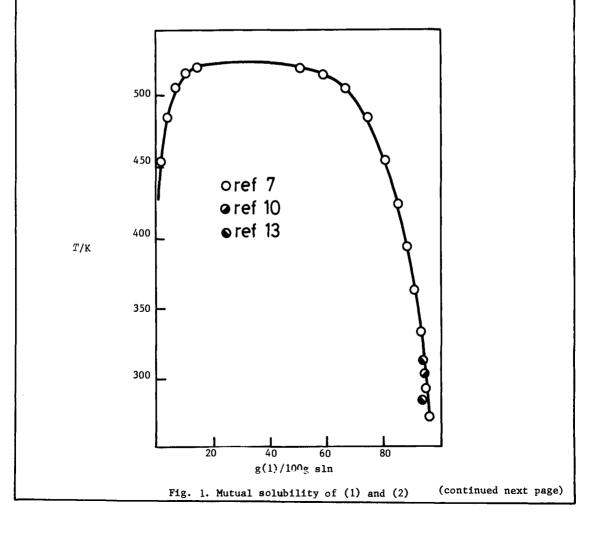
Solubility,	g(l)/100g	sln
-------------	-----------	-----

		Reported values	"Best" values $(\pm \sigma_n)$
473	23.20 (ref 7)		23.2
483	25.80 (ref 7)		25.8
4 9 3	29.15 (ref 7)		29.2
503	33.75 (ref 7)		33.8
513	41.50 (ref 7)		41.5

The upper critical solution temperature

The UCST appears to have been reported only by Erichsen (ref 7) who gave a value of 248.5° C (521.7 K).

Representative data for the mutual solubilities of 1-heptanol and water are plotted in Figure 1.



1-Heptanol

COMPONENTS:		EVALUATOR:
(1) 1-Heptanol ([111-70-6]	(n-heptyl alcohol); C ₇ H ₁₆ 0	University, Perth, Western Australia.
(2) Water; H ₂ 0;	[7732-18-5]	June, 1983.
CRITICAL EVALUAT	ION (continued)	I
References		
l. Fühner, H.	Ber. Dtsch. Chem. Ges. 19	124, 57, 510.
2. Butler, J.A	.V.; Thomson, D.W.; Maclen	nan, W.H. J. Chem Soc. <u>1933</u> , 674.
3. Addison, C.	C. J. Chem. Soc. <u>1945</u> , 98	l.
4. Booth, H.S.	; Everson, H.E. Ind. Eng.	Chem. <u>1948</u> , 40, 1491.
		. Chem. Soc. <u>1949</u> , 71, 808.
_	J.; Bartell, F.E. J. Phys	
	. von. Brennst. Chem. 195	
	. von. Naturwissenschafte	
		K. Bull. Chem. Soc. Jpn. <u>1958</u> , 31, 1081.
	; Dode, M. Bull. Soc. Chi	Sci. Ind. Res. <u>1961</u> , 20B, 283. m. Fr. 1965, 3318
		alcoholenen hun affiniteit voor water en
-	solventen, Doctoraatsproed	fschrift, Leuven, <u>1969</u> ; Huyskens, P.; <i>ll. Soc. Chim. Belg.</i> <u>1975</u> , 84, 253.
		Vysshykh Uchebn. Zavednii Khim. Tekhnol. <u>1970</u> ,
13, 952.	, -	,
14. Ionin, M.V. <u>1972</u> , <i>17</i> , 7		g. Khim. <u>1972</u> , 17, 1444; Russ. J. Inorg. Chem.
15. Vochten, R.	; Petre, G. J. Colloid In	nterface Sci. <u>1973</u> ,42, 320.
	.; White, L.R. Aust. J. (
17. Korenman, I	.M.; Gorokhov, A.A.; Polo:	zenko, G.N. Zhur. Fiz. Khim. <u>1974</u> , 48, 1010;
Russ. J. Ph	ys. Chem. <u>1974</u> , 48, 1065.	Zhur. Fiz. Khim. <u>1975</u> , 49, 1490; Russ. J. Phy
Chem. <u>1975</u> ,		
		n. Soc. Jpn. <u>1978</u> , 51, 1617; <u>1981</u> , 54, 545.
		Viihama Kogyo Koto Semmon Gakko Kiyo, Rikogaku
Hen (Memoir	es Niihama Technical Colleg	ge, Sci. and Eng.) <u>1980</u> , 16, 96.

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) 1-Heptanol; C _{7^H16} 0; [111-70-6]	Fühner, H.
	Ber.Dtsch. Chem. Ges.1924, 57, 510-5
(2) Water; H ₂ 0; [7732-18-5]	
VARIABLES:	PREPARED BY:
Temperature: 70-130 ⁰ C	A. Maczynski, Z. Maczynska and A. Szafranski
EXPERIMENTAL VALUES:	
Solubility of	1-heptanol(1) in water (2)
t/ ^o C g(1)/100	g sln x_1 (compiler)
70 0.12	5 0.000194
80 0.17	0.000264
90 0.22	
100 0.28	5 0.000443
110 0.33	5 0.000521
120 0.43	0.000669
130 0.51	5 0.000802
AUXI	LIARY INFORMATION
METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
Rothmund's synthetic method was used (1). Small amounts of (1) and (2) were seal a glass tube and heated with shaking i oil bath to complete dissolution. Th solution was cooled until a milky turb appeared and this temperature was adop as the equilibrium temperature.	specially purified, but no details provided. ed in n an e idity
	ESTIMATED ERROR:
	Not specified.
	REFERENCES :
	1. Rothmund, V. Z. physik. Chem. <u>1898</u> , 26, 433.

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) 1-Heptanol; C ₇ H ₁₆ O; [111-70-6] (2) Water; H ₂ O [7732-18-5]	Butler, J.A.V.; Thomson, D.W.; Maclennan, W.H. <i>J. Chem. Soc.</i> <u>1933</u> , 674-86
VARIABLES:	PREPARED BY:
One temperature: 25°C	S.H. Yalkowsky; S.C. Valvani; A.F.M. Barton

EXPERIMENTAL VALUES:

The proportion of 1-heptanol (1) in the water-rich phase at equilibrium at 25° C was reported to be 0.181 g(1)/100g sln, the mean of seven determinations (0.179, 0.184, 0.180, 0.182, 0.180, 0.178, 0.182 g(1)/100g sln).

The corresponding mole fraction solubility was reported as $x_1 = 0.000281$.

AUXILIARY INFORMATION		
METHOD/APPARATUS/PROCEDURE: An analytical method was used, with a U-tube apparatus having two internal stoppers. Suitable quantities of (1) and (2) were placed in one of the connected vessels and shaken in a thermostat for some hours. The liquid was allowed to separate into two layers, the heavier aqueous layer being separated by raising the stopper and allowing part of the liquid to run into the connected vessel. A weighed portion of the separated sln was diluted with about an equal quantity of (2) and the resulting sln	repeatedly fractionated in vacuum with a Hempel column, the middle fractions being refluxed with Ca and refractionated; b.p. 87.5 - 87.6°C/9 mm Hg, 175.6/760 mm Hg d^{25} 0.81960, n_D^{20} 1.42337 4	
compared with calibration slns in an interferometer. To avoid the possibility of reading the position of the wrong fringe, 2 cells (1 cm and 5 cm) were used. The method was unsuitable for analysis of alcohol-rich slns, as no stoppered interferometer cell	ESTIMATED ERROR: Solubility: the result is the mean of seven determinations agreeing within 0.003 g(1)/ 100g sln. Temperature: not stated (but in related experiments it was ± 0.03°C) REFERENCES:	
was available.		

COMPONENTS :	ORIGINAL MEASUREMENTS:
(1) 1-Heptanol; C ₇ H ₁₆ 0; [111-70-6] (2) Water; H ₂ 0; [7732-18-5]	Addison, C.C. J. Chem. Soc. <u>1945</u> , 98-106
VARIABLES:	PREPARED BY:
One temperature: 20°C	S.H. Yalkowsky; S.C. Valvani; A.F.M. Barton
EXPERIMENTAL VALUES:	· # · · · · · · · · · · · · · · · · · ·

The proportion of 1-heptanol (1) in the water-rich phase at equilibrium at 20° C was reported to be 0.172 g(1)/100g sln.

The corresponding mole fraction solubility, calculated by the compilers, is $x_1 = 0.000267$.

AUXILIARY METHOD/APPARATUS/PROCEDURE:	INFORMATION
METHOD/APPARATUS/PROCEDURE: The surface tension method was used. Sufficient excess of (1) was added to 100 mL of (2) in a stoppered flask to form a separate lens on the surface. The mixture was swirled gently, too vigorous an agitation being avoided as this gave a semi-permanent emulsion and incorrect readings. After settling, a small sample of the clear aqueous sln was withdrawn into a drop weight pipet and the surface tension determined. The swirling was continued until a constant value was obtained. The surface tension-concentration curve was known, and only a slight extrapolation (logarithmic scale) was necessary to find the concentration corresponding to the equilibrium value.	fraction from a distillation being redistilled; b.p. 176.5°C d_4^{20} 0.8220 n_D^{20} 1.4241 (2) not stated ESTIMATED ERROR:

1-Heptanol 33	
COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) 1-Heptanol; C ₇ H ₁₆ 0; [111-70-6]	Booth, H.S.; Everson, H.E.
(2) Water; H ₂ 0; [7732-18-5]	Ind. Eng. Chem. <u>1948</u> , 40, 1491-3.
(2) match, 120, 2002 2005	
VARIABLES:	PREPARED BY:
One temperature: 25 ⁰ C	S.H. Yalkowsky; S.C. Valvani; A.F.M. Barton
Sodium xylene sulfonate	
EXPERIMENTAL VALUES:	
It was reported that the solubility of 1-hep (2) at 25.0 [°] C.	tanol (1) in water (2) was 0.40 mL(1)/100mL
The solubility in 40% sodium xylene sulfonate solution as solvent was also studied. A gel began to form at 20 mL(1)/100mL sodium xylene sulfonate solution, and the amount of gel increased on successive additions. At 80 mL(1)/100mL sln the gel began to redissolv and at 120 mL(1)/100mL it completely disappeared.	
AUXILIARY	INFORMATION
METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
A known volume of (2) or aqueous solvent (usually 50mL) in a tightly stoppered	(1) "CP or highest grade commercial"
Babcock tube was thermostatted. Successive measured quantities of (1) were added and equilibrated until a slight excess of (1) remained. The solution was centrifuged, returned to the thermostat bath for 10 mins, and the volume of excess (1) measured directly. This was a modification of the method described in ref 1.	(2) distilled.
	ESTIMATED ERROR:
	Solubility: within 0.1 mL(1)/100mL (2)
	REFERENCES :
	 Hanslick, R.S. Dissertation, Columbia University, <u>1935</u>.

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) 1-Heptanol; C ₇ H ₁₆ 0; [111-70-6]	Harkins, W.D.; Oppenheimer, H.
(2) Water; H ₂ 0; [7732-18-5]	J. Am. Chem. Soc. <u>1949</u> , 71, 808–11.
VARIABLES:	PREPARED BY:
One temperature: assumed to be ambient	S.H. Yalkowsky, S.C. Valvani; A.F.M. Barton
EXPERIMENTAL VALUES:	
The solubility of 1-heptanol (1) in water was	s reported to be $0.0103 \text{ mol}(1)/\text{kg}(2)$.

Corresponding values calculated by the compilers are mass percentage 0.120 g(1)/100g sln and mole fraction $10^4 x_1 = 1.86$.

The temperature was not stated, but is assumed to be ambient.

AUXILIARY INFORMATION				
METHOD/APPARATUS/PROCEDURE: A turbidimetric method was used, with the aid of a photometer (turbidity increased rapidly in the presence of the emulsified second phase). The study was concerned with the effect of long-chain electrolytes (soaps) on solubility. The components were weighed into a glass ampoule, and shaken vigorously for at least 48h. Equilibrium was approached from both undersaturation and supersaturation.	 SOURCE AND PURITY OF MATERIALS: (1) Eastman Kodak Co; or Conneticut Hard Rubber Co; purified by fractional distillation. (2) not stated 			
	ESTIMATED ERROR: not stated REFERENCES:			

COMPONENTS:		ORIGINAL MEASU	JREMENTS:
(1) 1-Heptanol; C ₇ H ₁₆ 0; [111-70-6]		Donahue, D.J.; Bartell, F.E.	
(2) Water; H ₂ 0; [7732-18-5]]	J. Phys. Chem	a. <u>1952</u> , <i>56</i> , 480-4.
VARIABLES:		PREPARED BY:	··· · · · · · · · · · · · · · · ·
One temperature: 25 ⁰ C		A.F.M. Bartor	
one cemperature. 25 c		A.F.M. Dartor	1
EXPERIMENTAL VALUES:			· · · · · · · · · · · · · · · · · · ·
	Density		lubilities
	g mL ⁻¹	-	(1)/100g sln (compiler)
Alcohol-rich phase	0.8268	0.733	94.7
Water-rich phase	0.9967	0.000280 ^a	0.180
^a From ref 1.			
	AUXILIARY	INFORMATION	
		SOURCE AND PU	JRITY OF MATERIALS:
Mixtures were placed in gla		(1) "best re	eagent grade";
flasks and were shaken into at least 3 days in a water		fraction	al distillation
organic phase was analyzed	for water content	(2) purified	I
by the Karl Fischer method phase was analyzed interfer	rometrically.		
The solubility measurements a study of water-organic li			
tensions.	•		
		ESTIMATED ER	ROR:
		Temperature	: ± 0.1°C
		REFERENCES:	<u> </u>
			J.A.V.; Thomson, D.W.;
			an, W.H. J. Chem. Soc. <u>1933</u> , 674

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) 1-Heptanol; C ₇ H ₁₆ O; [111-70-6] (2) Water; H ₂ O; [7732-18-5]	Erichsen, L. von Brennst. Chem. <u>1952</u> , 33, 166-72.
(2) water, 20, [(),2 10 5]	
VARIABLES:	PREPARED BY:
Temperature: 0-245 [°] C	S.H. Yalkowsky and Z. Maczynska
EXPERIMENTAL VALUES: Mutual solubility of	1-heptanol and water
$t/{}^{0}C$ $(2)-rich phase$ $g(1)/100 sln$ x_{1} 0 0.34 0.0005 10 0.26 0.0004 20 0.20 0.0003 30 0.16 0.0002 40 0.13 0.0002 40 0.13 0.0002 50 0.11 0.0001 60 0.11 0.0001 60 0.19 0.0003 90 0.23 0.0003 100 0.29 0.0004 110 0.35 0.0005 120 0.43 0.0006 130 0.53 0.0008 140 0.65 0.0010 150 0.80 0.0012 160 0.98 0.0015 170 1.23 0.0019 180 1.60 0.98 0.0015 170 1.23 0.0019 180 1.60 0.0025 190 2.08 0.0032 200 2.64 0.0042 210 3.48 0.0056 220 4.68 0.0076 230 6.70 0.0110 0.0110 0.011	6 95.70 0.7753 1 95.25 0.7567 5 94.80 0.7387 0 94.25 0.7177 8 93.70 0.6977 8 93.05 0.6750 3 92.40 0.6535 0 91.65 0.6076 7 90.15 0.5868 5 89.25 0.5629 7 88.35 0.5405
245 13.96 0.0245 The UCST is 248.5°C	50.65 0.1373
AUXILIARY	INFORMATION
METHOD/APPARATUS/PROCEDURE: The synthetic method was used. The measurements were carried out in 2 ml glass ampules. These were placed in an aluminium block equipped with two glass windows. Cloud points were measured with a thermocouple wound up around the ampule. Each measurement was repeated twice.	 SOURCE AND PURITY OF MATERIALS: (1) Merck, or Ciba, or industrial product; distilled and chemically free from isomers; b.p. 175.9-176-0°C (758 mm Hg) n²⁰_D 1.4249. (2) not specified.
	ESTIMATED ERROR: Not specified.
	REFERENCES:

1-Heptanol

		1-110	pranor	
COMPONENTS:			ORIGINAL MEASUREMENTS:	
(1) l-Heptanol	; c ₇ H ₁₆ 0; [111-70-6]	Erichsen, L. von	
(2) Water; H ₂ 0; [7732-18-5]		-5]	Naturwissenschaften <u>1952</u> , 39, 41-2.	
VARIABLES:			PREPARED BY:	
Temperature: 0-50 [°] C			A. Maczynski and Z. Maczynska	
EXPERIMENTAL VAL	UES:		A	- <u>.</u> .
	s	Solubility of 1-h	eptanol (1) in water (2)	
	t/ ^o c	x_1	g(1)/100g sln (compiler)	
	0	0.00053	0.34	
	10	0.00046	0.30	
	20	0.00031	0.20	
	30	0.00025	0.16	
	40	0.00020	0.13	
	50	0.00018	0.12	
		AUXILIARY	INFORMATION	
METHOD/APPARATUS	5/PROCEDURE:	· · · · · ·	SOURCE AND PURITY OF MATERIALS:	
The synthetic	method was us	sed.	(1) not specified.	
No details reported in the paper.		paper.	(2) not specified.	
1				
			ESTIMATED ERROR:	
			Not specified.	
			REFERENCES :	
L			_L	-

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COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) 1-Heptanol; C ₇ H ₁₆ 0; [111-70-6]	Kinoshita, K.; Ishikawa, H.; Shinoda, K.
(2) Water; H ₂ 0; [7732-18-5]	Bull. Chem. Soc. Jpn. <u>1958</u> , 31, 1081-4.
VARIABLES:	PREPARED BY:
One temperature: 25 ⁰ C	S.H. Yalkowsky; S.C. Valvani; A.F.M. Barton

EXPERIMENTAL VALUES:

The equilibrium concentration of 1-heptanol (1) in the water-rich phase at 25° C was reported to be 0.0146 mol(1)/L, the mass percentage solubility was reported as 0.17 g(1)/100g sln, and the corresponding mole fraction solubility, calculated by the compiler, is $x_1 = 0.00026$.

AUXILIARY	INFORMATION
METHOD/APPARATUS/PROCEDURE: The surface tension in aqueous solutions of alcohols monotonously decreases up to their saturation cencentration and remains constant in the heterogeneous region (ref 1-4). Surface tension was measured by the drop weight method, using a tip 6 mm in diameter, the measurements being carried out in a water thermostat. From the (surface tension) - (logarithm of concentration) curves the saturation points were determined as the intersections of the curves with the horizontal straight lines passing through the lowest experimental points.	
	 ESTIMATED ERROR: Temperature: ± 0.05°C Solubility: within 4% REFERENCES: Motylewski, S. Z. Anorg. Chem. 1904, 38, 410. Taubamann, A. Z. physik. Chem. 1932, A161, 141. Zimmerman, H.K., Jr. Chem. Rev. 1952, 51, 25. Shinoda, K.; Yamanaka, T.; Kinoshita, K. J. Phys. Chem. 1959, 63, 648.

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) 1-Heptanol; C ₇ H ₁₆ 0; [111-70-6]	Rao, K.S.; Rao, M.V.R.; Rao, C.V.
(2) Water; H ₂ O; [7732-18-5]	J. Sci. Ind. Res. <u>1961</u> , 20B, 283-6.
VARIABLES:	PREPARED BY:
One temperature: 30°C	A. Maczynski
one temperature. 5000	R. Haczynski
EXPERIMENTAL VALUES:	
The solubility of 1-heptanol in water at 30°	C was reported to be 0.1 $g(1)/100 \text{sln}$.
The corresponding mole fraction, x_1 , calculation	
The corresponding more fraction, x_1 , careara	ted by the compiler is 0.0002.
The solubility of water in 1-heptanol at 30°	C was reported to be 5.5 g(2)/100g sln.
The corresponding mole fraction, $x_2^{}$, calcula	ted by the compiler is 0.27.
AUXILIARY	INFORMATION
METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
The method of appearance and disappearance	(1) British Drug House;
of turbidity described in ref 1 was used.	used as received;
No details were reported in the paper.	n^{30} 1.4193, d^{30} 0.8210 g/mL
	(2) distilled; free from carbon dioxide.
	ESTIMATED ERROR:
	Not specified.
	Not opportion.
	REFERENCES :
	1. Othmer, D.F.; White, R.E.; Trueger, E.
	Ind. Eng. Chem. <u>1941</u> , 33, 1240.

344 Seven-carbon Alcohols		
OMPONENTS: ORIGINAL MEASUREMENTS:		
(1) 1-Heptanol; C ₇ H ₁₆ 0; [111-70-6] (2) Water; H ₂ 0; [7732-18-5]	Ratouis, M.; Dodé, M. Bull. Soc. Chim. Fr. <u>1965</u> , 3318-22	
VARIABLES: One temperature: 30 ⁰ C	PREPARED BY: S.C. Valvani; S.H. Yalkowsky; A.F.M. Barton	
Ringer solution also studied		
EXPERIMENTAL VALUES:	I	
	ty, calculated by the compilers, is $x_1 = 0.00026$. phase of a mixture with Ringer solution at 30° C	
AUXIL	JARY INFORMATION	

METHOD/APPARATUS/PROCEDURE: In a round bottomed flask, 50 mL of water and a sufficient quantity of alcohol were introduced until two separate layers were formed. The flask assembly was equilibrated by agitation for at least 3h in a constant temperature bath. Equilibrium solubility was attained by first supersaturation at a slightly lower temperature (solubility of alcohols in water decrease with increasing temperature) and then equilibrating at the desired temperature. The aqueous layer was separated after an overnight storage in a bath. The alcohol content was determined by reacting the aqueous solution with potassium	<pre>2) twice distilled from silica apparatus or ion-exchanged with Sagei A20 ESTIMATED ERROR:</pre>
formed. The flask assembly was equilibrated by agitation for at least 3h in a constant	$n_{\rm D}^{25}$ = 1.42219 (2) twice distilled from silica apparatus
a slightly lower temperature (solubility of	or ion-exchanged with Sagei A20
desired temperature. The aqueous layer was	
	ESTIMATED ERROR:
reacting the aqueous solution with potassium dichromate and titrating the excess	
dichromate with ferrous sulfate solution in the presence of phosphoric acid and	Temperature: ± 0.05 ⁰ C
diphenylamine barium sulfonate as an indicator.	REFERENCES:

COMPONENTS:	ORIGINAL MEASUREMENTS:		
(1) 1-Heptanol; C ₇ H ₁₆ 0; [111-70-6]	Hanssens, I.		
(2) Water; H ₂ 0; [7732-18-5]	Associatie van normale alcoholen en hun		
	affiniteit voor water en organische solventen		
	Doctoraatsproefschrift, Leuven, 1969.		
	Huyskens, P.; Mullens, J.; Gomez, A.; Tack,J;		
	Bull. Soc. Chim. Bela. 1975. 84, 253-62.		
VARIABLES:	PREPARED BY:		
One temperature: 298 K	M.C. Haulait-Pirson; A.F.M. Barton		
EXPERIMENTAL VALUES:			
The concentration of 1-heptanol (1) in the	e water-rich phase was reported as		

0.01498 mol(1)/L sln, and the concentration of water (2) in the alcohol-rich phase was reported as 6.760 mol(2)/L sln.

The corresponding solubilities on a mass/volume basis, calculated by the compilers, are 1.7 g(1)/L sln, and 121.8 g(2)/L sln, respectively.

(The temperature was unspecified in the Thesis, but reported as 298 K in the 1975 published paper).

AUXILIARY INFORMATION			
METHOD/APPARATUS/PROCEDURE: (1) and (2) were equilibrated using a cell described in ref 1. The Rayleigh M75 interference refractometer with the cell M160 for liquids was used for the determina- tion of the concentrations. Cell thick- nesses were 1, 3 and 10 cm depending on the concentration range. Standard solutions covering the whole range of concentrations investigated were used for the calibration.	SOURCE AND PURITY OF MATERIALS: (1) Merck p.a. (2) distilled		
	ESTIMATED ERROR: Solubility ± 0.00036 - 0.05 mol(1)/L sln, depending on the concentration REFERENCES: 1. Meeussen, E.; Huyskens, P. J. Chim. Phys. <u>1966</u> , 63, 845.		

COMPONENTS:	ORIGINAL MEASUREMENTS:		
(1) 1-Heptanol; C ₇ H ₁₆ 0; [111-70-6]	Krasnov, K.S.; Gartseva, L.A.		
(2) Water; H_2^{0} ; [7732-18-5]	Izv. Vysshykh Uchebn. Zavedenii Khim. Khim. Tekhnol. <u>1970</u> , 13(7), 952-6.		
VARIABLES:	PREPARED BY:		
Temperature: 12 and 40 [°] C	A. Maczynski and Z. Maczynska		
EXPERIMENTAL VALUES:			
Solubility of wate	r in l-heptanol		
$t/^{0}$ C g(2)/100g slm	$x_2(\text{compiler})$		
12 5.75	0.282		
40 5.90	0.288		
	INFORMATION		
METHOD/APPARATUS/PROCEDURE: The analytical method was used. The saturated mixture of (1) and (2) was placed in a thermostat and phases were allowed to separate. Then (2) was determ- ined in the organic layer by Karl Fischer analysis.	<pre>SOURCE AND PURITY OF MATERIALS: (1) CP reagent; source not specified; distilled; no isomers by GLC; d²⁵₄ 0.8180. (2) not specified. (2) not specified. ESTIMATED ERROR: Temperature: ± 0.05°C Solubility: ± 0.05 wt %</pre>		
	<u> </u>		

COMPONENTS :	ORIGINAL MEASUREMENTS:	
(1) 1-Heptanol; C ₇ H ₁₆ 0; [111-70-6]	Ionin, M.V.; Shanina, P.I.	
(2) Water; H ₂ 0; [7732-18-5]	Zh. Neorg. Khim. <u>1972</u> , 17, 1444-9; * Russ. J. Inorg. Chem. <u>1972</u> , 17, 747-50.	
VARIABLES:	PREPARED BY:	
One temperature: 25 ⁰ C	A.F.M. Barton	
EXPERIMENTAL VALUES: The proportion of 1-heptanol (1) in the alco	-L	

94.2 g(1)/100g sln.

The corresponding mole fraction value, calculated by the compiler, is $x_1 = 0.716$.

AUXILIARY	INFORMATION

METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:	
The procedures and reagents described in ref 2 were used. The binodal curve of the hydrogen-chloride-water-l-heptanol ternary system was determined by isothermal titration. The value reported above is the zero hydrogen chloride point on this binodal curve.	(1) purified as recommended in ref 1. b.p. 175.5 - 176°C, d_4^{25} 0.8190 n_D^{25} 1.4203	
	ESTIMATED ERROR:	
	The binodal curve was determined with an accuracy of 0.5%	
	 REFERENCES: (1) Weissberger, A.; Proskauer, E.S.; Riddick, J.A.; Toops, E.E., Jr. Organic Solvents : Physical Properties and Method Methods of Purification, Russian edition, Inostr. Lt., Moscow, 1958. (2) Ionin, M.V.; Shanina, P.I. Zh. Obshch. Khim. <u>1967</u>, 37, 749; J. Gen. Chem. USSR. <u>1967</u>, 37, 708. 	

COMPONENTS :		ORIGINAL MEASUREMENTS:	
(1) 1-Heptanol: C_H0:	[111-70-6]	Vochten, R.; Petre, G.	
(1) 1-Heptanol; C ₇ H ₁₆ 0; [111-70-6]		J. Colloid Interface Sci. 1	973, 42, 320-7.
(2) Water; H ₂ 0; [7732-]	18-5.]		
VARIABLES:			
Temperature: 15-60°C		PREPARED BY: S.H. Yalkowsky; S.C. Valvan	i: A.F.M. Barton
		,,	- ,
EXPERIMENTAL VALUES:			
	Solubility of 1-h	eptanol (1) in water	
t∕°C	mol(l)/L sln	g(1)/100g sln	$10^{4}x_{1}$
<i>U</i> / U	mor(1)/L sin	(compilers) ^a	(compilers) ^a
		(compricis)	(compilers)
15	0.017	0.20	3.1
20	0.013	0.15	2.3
30	0.013	0.15	2.3
40	0.011	0.13	2.0
50	0.012	0.14	2.2
60	0.013	0.15	2.3
	AUXILIARY	INFORMATION	
METHOD/APPARATUS/PROCEDU	RE:	SOURCE AND PURITY OF MATERI	ALS:
The solubility was obta	ained from the	(1) purified by distillati	ion and
surface tension of sate measured by the static		preparative gas chroma	
(platinum plate). The	apparatus consisted	b.p. 175.8°C/760 mm Hg	5
of an electrobalance () with a high impedance of type 845 AR). An all- used.	null detector (Fluke	(2) triply distilled from solution	permanganate
		ESTIMATED ERROR:	
		Temperature: ± 0.1°C	
		Solubility (probably stand ± 0.001 mol(1	
		REFERENCES:	

1-Heptanol

COMPONENTS:		
COMPONENTS:	ORIGINAL MEASUREMENTS:	
(1) 1-Heptanol; C ₇ H ₁₆ 0; [111-70-6]	Hill, D.J.T.; White. L.R.	
(2) Water; H ₂ O; [7732-18-5]	Aust. J. Chem. <u>1974,</u> 27, 1905–16.	
VARIABLES:	PREPARED BY:	
Temperature: 279 - 308 K	A. Maczynski	
EXPERIMENTAL VALUES:		
Solubility of 1-he	eptanol in water	
<i>Т/</i> К <i>х</i> ₁	g(l)/100g sln (compiler)	
279.15 0.0003423 283.35 0.0003134 283.69 0.0003103 288.23 0.0002900 291.09 0.0002785 293.18 0.0002717 295.05 0.0002662 297.11 0.0002615 298.14 0.0002602 298.22 0.0002585 299.19* 0.0002565 301.17 0.0002544 303.29 0.0002519 303.31 0.0002522 306.05 0.0002491 * Based on one determination only	0.2204 0.2020 0.1998 0.1868 0.1794 0.1750 0.1715 0.1685 0.1676 0.1665 0.1652 0.1639 0.1623 0.1623 0.1625 0.1610 0.1605	
AUXILIARY	INFORMATION	
METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:	
The interferometric method was used. The saturated solutions of (1) were prepared in an equilibrium flask and solution concentrations were determined from their refractive index using a Zeiss inter- ferometer and appropriate calibration curves Duplicate determinations were always within the error limits calculated from the curve fit to the calibration measurements (0.5% at the 95% confidence level).	$n_{\rm D}$ 1.4213.	
Numerous technical details were reported in the paper.	ESTIMATED ERROR: Temperature: ± 0.02°C Solubility: < 0.5% (accuracy at 95% confidence level) REFERENCES:	

COMPONENTS :	ORIGINAL MEASUREMENTS:		
(1) 1-Heptanol; C ₇ H ₁₆ 0; [111-70-6] (2) Water; H ₂ 0; [7732-18-5]	Korenman, I.M.; Gorokhov, A.A.; Polozenko, G.N. Zhur. Fiz. Khim. <u>1974</u> , 48, 1010-2; Russ. J. Phys. Chem. <u>1974</u> , 48, 1065-7; Zhur. Fiz. Khim. <u>1975</u> , 49, 1490-3; Russ. J. Phys. Chem. <u>1975</u> , 49, 877-8.		
VARIABLES:	PREPARED BY:		
One temperature: 25 ⁰ C	A.F.M. Barton		

The equilibrium concentration of 1-heptanol (1) in the water-rich phase at 25.0° C was reported to be 0.058 mol(1)/L sln, and the concentration of water (2) in the alcohol-rich phase was reported to be 3.59 mol(2)/L sln.

The corresponding solubilities on a mass/volume basis, calculated by the compiler, are 6.7 g(1)/L sln, and 64.7 g(2)/L sln, respectively.

AUXILIARY INFORMATION			
METHOD/APPARATUS/PROCEDURE: The two liquids were shaken in a closed vessel at 25.0 \pm 0.1°C until equilibrium was established. The soly of (1) in the aqueous phase was determined in a Tsvet-1 chromatograph with a flame-ionisation detector. The sorbent was a polythethylene glycol adipate deposited on Polychrom-1 (10% of the mass of the carrier). The lm column had an internal diameter 4mm, its temperature was 140°C, and the flow of the carrier gas (nitrogen) was 50 mL min ⁻ . The soly of water in the alcohol was deter- mined on a UKh-2 universal chromatograph under isothermal conditions (150°C) with a heat-conductivity detector. The lm by 6 mm column was filled with Polysorb1The carrier gas was helium (50 mL min ⁻). The study formed part of an investigation of salting-out by alkali halides of higher alcohol-water systems.			

COMPONENTS:	ORIGINAL MEASUREMENTS:	
(1) 1-Heptanol; C ₇ H ₁₆ 0; [111-70-6] (2) Water; H ₂ 0; [7732-18-5]	Tokunaga, S.; Manabe, M.; Koda, M. Niihama Kogyo Koto Semmon Gakko Kiyo, Rikogaku Hen (Memoirs Niihama Technical College, Sci. and Eng.) <u>1980</u> , 16, 96-101.	
VARIABLES: Temperature: 15-40 [°] C	PREPARED BY: A.F.M. Barton	

Solubility of water (2) in the alcohol-rich phase

t∕°c	g(2)/100g sln	<i>x</i> ₂	mol(1)/mol(2)
15	5.73	0.282	2.54
20	5.82	0.285	2.52
25	5.85	0.286	2.49
30	5.90	0.288	2.46
35	6.01	0.292	2.44
40	6.02	0.293	2.41

AUXILIARY INFORMATION	
METHOD/APPARATUS/PROCEDURE: The mixtures of 1-heptanol (~5 mL) and water (~10 mL) were stirred magnetically in a stoppered vessel and allowed to stand for 10-12 h in a water thermostat. The alcohol-rich phase was analyzed for water by Karl Fischer titration.	 SOURCE AND PURITY OF MATERIALS: (1) distilled; no impurities detectable by gas chromatography. (2) deionized; distilled prior to use.
	ESTIMATED ERROR: Temperature: ± 0.1°C Solubility: each result is the mean of three determinations. REFERENCES:

COMPONENTS:	ODICINAL ACTINEMENTS -
	ORIGINAL MEASUREMENTS:
(1) 2-Heptanol; (n-pentylmethylcarbinol)	Ratouis, M.; Dodé, M.
C ₇ H ₁₆ 0; [543-49-7]	Bull. Soc. Chim. Fr. <u>1965</u> , 3318-22.
(2) Water; H ₂ 0; [7732-18-5]	
_	
VARIABLES:	PREPARED BY:
One temperature: 30 ⁰ C	S.C. Valvani; S.H. Yalkowsky; A.F.M. Barton
EXPERIMENTAL VALUES: The proportion of 2-heptanol (1) in the wat reported to be 0.33 g(1)/100g sln.	er-rich phase at equilibrium at 30 ⁰ C was
The corresponding mole fraction solubility,	calculated by the compiler, is $x_1 = 0.00051$.

	INFORMATION
METHOD/APPARATUS/PROCEDURE: In a round bottomed flask, 50 mL of water and a sufficient quantity of alcohol were introduced until two separate layers were formed. The flask assembly was equilibrated by agitation for at least 3h in a constant temperature bath. Equilibrium solubility was attained by first supersaturation at a slightly lower temperature (solubility of alcohols in water decreases with increasing temperature) and then equilibrating at the desired temperature. The aqueous layer was separated after an overnight storage in a bath. The alcohol content was determined by reacting the aqueous solution with potassium dichromate and titrating the excess dichromate with ferrous sulfate solution in the presence of phosphoric acid and diphenylamine barium sulfonate as an indicator.	<pre>SOURCE AND PURITY OF MATERIALS: (1) laboratory preparation; redistilled with 10:1 reflux ratio b.p. 68-69°C/22 mm Hg n²⁵ = 1.41888 (2) twice distilled from silica apparatus or ion-exchanged with Sagei A20 ESTIMATED ERROR: Solubility: relative error of 2 determinations less than 1% Temperature: ± 0.05°C REFERENCES:</pre>

2-Heptanol 3	
COMPONENTS:	ORIGINAL MEASUREMENTS:
 (1) 2-Heptanol (n-pentylmethylcarbinol); C₇H₁₆⁰; [543-49-7] (2) Water; H₂⁰; [7732-18-5] 	Nishino, N.; Nakamura, M. Bull. Chem. Soc. Jpn. <u>1978</u> , 51, 1617-20; <u>1981</u> , 54, 545-8.
VARIABLES: Temperature: 275-360 K	PREPARED BY: G.T. Hefter
EXPERIMENTAL VALUES:	
The mutual solubility of (1) and (2) in mole temperature range in graphical form. Graph: heat of evaporation of (1).	
AUXTLIARY	INFORMATION
	······································
METHOD/APPARATUS/PROCEDURE: The turbidimetric method was used. Twenty to thirty glass ampoules containing aqueous solutions of ca . 5 cm ³ of various concentra- tions near the solubility at room temperature were immersed in a water theromostat. The distinction between clear and turbid ampoules was made after equil- ibrium was established (ca . 2h). The smooth curve drawn to separate the clear and turbid regions was regarded as the solubility curve.	(2) Deionized, refluxed for 15 h with
	ESTIMATED ERROR: Not stated
	REFERENCES:

COMPONENTS :	EVALUATOR:
(1) 3-Heptanol; C ₇ H ₁₆ 0; [589-82-2]	A. Maczynski, Institute of Physical
(2) Water; H ₂ 0 [7732-18-5]	Chemistry of the Polish Academy of Sciences,
(-)	Warsaw, Poland.
	November 1982
CRITICAL EVALUATION:	
Solubilities in the system comprising 3-hept	anol (1) and water (2) have been reported
in two publications: Crittenden and Hixon (ref 1) determined the mutual solubility	
at 298 K, presumably by the titration method; and Ratouis and Dode determined the	
proportion of 3-heptanol in the aqueous phase	e at 298 K and 303 K by an analytical method.
The value 0.4 g(1)/100g sln at 298 K in ref	l is in good agreement with the value
0.43 g(1)/100g sln given in ref 2.	
	luce for the colubility of
Recommended and tentative values for the solubility of	
<u>3-heptanol (1) in the wa</u>	
T/K g(1)/100g sln	10 ⁴ x ₁
298 0.43 (rec	commended) 6.7
303 0.41 (t	centative) 6.4
Since there is only one value available for	the propertion of water in the alashel-wish
Since there is only one value available for phase, the value of ref l is regarded as ten	
The tentative value for the solubility of wa	
is 3 g(2)/100g sln or $x_2 = 0.17$.	
References	
1. Crittenden, E.D., Jr.; Hixon, A.N. Ind.	Eng. Chem. 1954, 46, 265.
2. Ratouis, M., Dode, M. Bull. Soc. Chim.	Fr. <u>1965</u> , 3318.

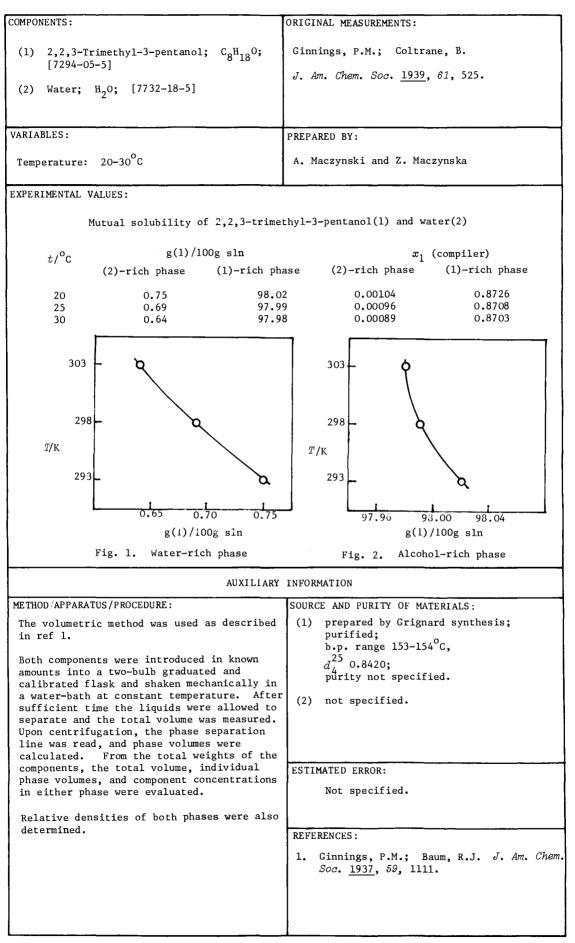
3-Heptanol

COMPONENTS:	
COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) 3-Heptanol; C ₇ H ₁₆ ⁰ ; [589-82-2]	Crittenden, E.D., Jr.; Hixon, A.N.
(2) Matome H O [7722 19 5]	Ind. Eng. Chem. <u>1954</u> , 46, 265–8.
(2) Water; H ₂ 0 [7732-18-5]	
	PREPARED BY:
One temperature: 25 [°] C	A. Maczynski
EXPERIMENTAL VALUES:	
The solubility of 3-heptanol in water at 25°C	C was reported to be 0.4 g(1)/100 sln.
The corresponding mole fraction, x_1 , calculat	
The corresponding more fraction, w ₁ , calculat	
The solubility of water in 3-heptanol at 25 ⁰ 0	
The corresponding mole fraction, x_2 , calculat	ed by the compiler is 0.17.
AUXILIARY	INFORMATION
METHOD / APPARATUS / PROCEDURE :	SOURCE AND PURITY OF MATERIALS:
Presumably the titration method described	(1) source not specified;
for ternary systems containing HCl was used. In this method the solubility was determined	purified; purity not specified.
by bringing 100-mL samples of (1) or (2) to a temperature of 25.0 ± 0.1°C and the	(2) not specified.
second component was then added from a calibrated buret, with vigorous stirring,	
until the solution became permanently cloudy.	
1	ESTIMATED ERROR:
	Temperature: ± 0.10 [°] C.
	REFERENCES:

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Seven-carb	on Alcohois	
COMPONENTS :	ORIGINAL MEAS	SUREMENTS :
(1) 3-Heptanol; C ₇ H ₁₆ 0; [589-82-2]	Ratouis, M.;	Dodé, M.
(2) Water; H ₂ 0; [7732-18-5]	Bull. Soc. C	Chim. Fr. <u>1965</u> , 3318-22.
VARIABLES:	PREPARED BY:	· · · · · · · · · · · · · · · · · · ·
Temperature: 25°C and 30°C	S.C. Valvani	l; S.H. Yalkowsky; A.F.M. Barton
EXPERIMENTAL VALUES:	<u> </u>	
Proportion of 3-hep	anol (l) in wa	ater-rich phase.
t/ ^o c g()/100g sln	$10^4 x_1$ (compiler)
25	0.43	6.7
30	0.41	6.4
AUXILIAR	Y INFORMATION	
AUXILIAR METHOD/APPARATUS/PROCEDURE:		URITY OF MATERIALS:
METHOD/APPARATUS/PROCEDURE: In a round bottomed flask, 50 mL of water	SOURCE AND P	URITY OF MATERIALS: 11ed with 10:1 reflux ratio
METHOD/APPARATUS/PROCEDURE: In a round bottomed flask, 50 mL of water and a sufficient quantity of alcohol were introduced until two separate layers were	SOURCE AND P (1) redisti b.p. 15	lled with 10:1 reflux ratio 8.5–158.6 ⁰ C/768.8 mm Hg
METHOD/APPARATUS/PROCEDURE: In a round bottomed flask, 50 mL of water and a sufficient quantity of alcohol were introduced until two separate layers were formed. The flask assembly was	SOURCE AND P (1) redisti	lled with 10:1 reflux ratio 8.5-158.6 ⁰ C/768.8 mm Hg
METHOD/APPARATUS/PROCEDURE: In a round bottomed flask, 50 mL of water and a sufficient quantity of alcohol were introduced until two separate layers were formed. The flask assembly was equilibrated by agitation for at least 3h in a constant temperature bath. Equilibrium solubility was attained by first	SOURCE AND P (1) redisti b.p. 15 $n_{\rm D}^{25} = 1$ (2) twice d	lled with 10:1 reflux ratio 8.5–158.6 ⁰ C/768.8 mm Hg
METHOD/APPARATUS/PROCEDURE: In a round bottomed flask, 50 mL of water and a sufficient quantity of alcohol were introduced until two separate layers were formed. The flask assembly was equilibrated by agitation for at least 3h in a constant temperature bath. Equilibrium solubility was attained by first supersaturation at a slightly lower temperature (solubility of alcohols in wate decrease with increased temperature) and	SOURCE AND P (1) redisti b.p. 15 $n_{D}^{25} = 1$ (2) twice di or ion-	lled with 10:1 reflux ratio 8.5-158.6 ⁰ C/768.8 mm Hg .41978 istilled from silica apparatus
METHOD/APPARATUS/PROCEDURE: In a round bottomed flask, 50 mL of water and a sufficient quantity of alcohol were introduced until two separate layers were formed. The flask assembly was equilibrated by agitation for at least 3h in a constant temperature bath. Equilibrium solubility was attained by first supersaturation at a slightly lower temperature (solubility of alcohols in wate decrease with increased temperature) and then equilibrating at the desired temperature. The aqueous layer was	SOURCE AND P (1) redisti b.p. 15: $n_{D}^{25} = 1$ (2) twice d: or ion-o	lled with 10:1 reflux ratio 8.5-158.6 ⁰ C/768.8 mm Hg .41978 istilled from silica apparatus exchanged with Sagei A20
METHOD/APPARATUS/PROCEDURE: In a round bottomed flask, 50 mL of water and a sufficient quantity of alcohol were introduced until two separate layers were formed. The flask assembly was equilibrated by agitation for at least 3h in a constant temperature bath. Equilibrium solubility was attained by first supersaturation at a slightly lower temperature (solubility of alcohols in wate decrease with increased temperature) and then equilibrating at the desired	SOURCE AND P (1) redisti b.p. 15 $n^{25}_{D} = 1$ (2) twice d or ion-	lled with 10:1 reflux ratio 8.5-158.6 ^o C/768.8 mm Hg .41978 istilled from silica apparatus exchanged with Sagei A20
METHOD/APPARATUS/PROCEDURE: In a round bottomed flask, 50 mL of water and a sufficient quantity of alcohol were introduced until two separate layers were formed. The flask assembly was equilibrated by agitation for at least 3h in a constant temperature bath. Equilibrium solubility was attained by first supersaturation at a slightly lower temperature (solubility of alcohols in wate decrease with increased temperature) and then equilibrating at the desired temperature. The aqueous layer was separated after an overnight storage in a bath. The alcohol content was determined b reacting the aqueous solution with potassiu	SOURCE AND P (1) redisti b.p. 15 $n^{25}_{D} = 1$ (2) twice d or ion-or ESTIMATED EF	lled with 10:1 reflux ratio 8.5-158.6 ⁰ C/768.8 mm Hg .41978 istilled from silica apparatus exchanged with Sagei A20
METHOD/APPARATUS/PROCEDURE: In a round bottomed flask, 50 mL of water and a sufficient quantity of alcohol were introduced until two separate layers were formed. The flask assembly was equilibrated by agitation for at least 3h in a constant temperature bath. Equilibrium solubility was attained by first supersaturation at a slightly lower temperature (solubility of alcohols in wate decrease with increased temperature) and then equilibrating at the desired temperature. The aqueous layer was separated after an overnight storage in a bath. The alcohol content was determined b reacting the aqueous solution with potassiu dichromate and titrating the excess dichromate with ferrous sulfate solution in	SOURCE AND P (1) redisti b.p. 15 n ²⁵ = 1 (2) twice d or ion-o ESTIMATED EF Solubility: Temperature	<pre>1led with 10:1 reflux ratio 8.5-158.6^oC/768.8 mm Hg .41978 istilled from silica apparatus exchanged with Sagei A20 RROR: relative error of 2 determinations less than 1%</pre>
METHOD/APPARATUS/PROCEDURE: In a round bottomed flask, 50 mL of water and a sufficient quantity of alcohol were introduced until two separate layers were formed. The flask assembly was equilibrated by agitation for at least 3h in a constant temperature bath. Equilibrium solubility was attained by first supersaturation at a slightly lower temperature (solubility of alcohols in wate decrease with increased temperature) and then equilibrating at the desired temperature. The aqueous layer was separated after an overnight storage in a bath. The alcohol content was determined b reacting the aqueous solution with potassiu dichromate and titrating the excess	SOURCE AND P (1) redisti b.p. 15 $n^{25}_{D} = 1$ (2) twice d or ion- r ESTIMATED EF Solubility:	<pre>1led with 10:1 reflux ratio 8.5-158.6^oC/768.8 mm Hg .41978 istilled from silica apparatus exchanged with Sagei A20 RROR: relative error of 2 determinations less than 1%</pre>
METHOD/APPARATUS/PROCEDURE: In a round bottomed flask, 50 mL of water and a sufficient quantity of alcohol were introduced until two separate layers were formed. The flask assembly was equilibrated by agitation for at least 3h in a constant temperature bath. Equilibrium solubility was attained by first supersaturation at a slightly lower temperature (solubility of alcohols in wate decrease with increased temperature) and then equilibrating at the desired temperature. The aqueous layer was separated after an overnight storage in a bath. The alcohol content was determined b reacting the aqueous solution with potassiu dichromate and titrating the excess dichromate with ferrous sulfate solution in the presence of phosphoric acid and diphenylamine barium sulfonate as an	SOURCE AND P (1) redisti b.p. 15 n ²⁵ = 1 (2) twice d or ion-o ESTIMATED EF Solubility: Temperature	<pre>1led with 10:1 reflux ratio 8.5-158.6^oC/768.8 mm Hg .41978 istilled from silica apparatus exchanged with Sagei A20 RROR: relative error of 2 determinations less than 1%</pre>
METHOD/APPARATUS/PROCEDURE: In a round bottomed flask, 50 mL of water and a sufficient quantity of alcohol were introduced until two separate layers were formed. The flask assembly was equilibrated by agitation for at least 3h in a constant temperature bath. Equilibrium solubility was attained by first supersaturation at a slightly lower temperature (solubility of alcohols in wate decrease with increased temperature) and then equilibrating at the desired temperature. The aqueous layer was separated after an overnight storage in a bath. The alcohol content was determined b reacting the aqueous solution with potassiu dichromate and titrating the excess dichromate with ferrous sulfate solution in the presence of phosphoric acid and diphenylamine barium sulfonate as an	SOURCE AND P (1) redisti b.p. 15 n ²⁵ = 1 (2) twice d or ion-o ESTIMATED EF Solubility: Temperature	<pre>1led with 10:1 reflux ratio 8.5-158.6^oC/768.8 mm Hg .41978 istilled from silica apparatus exchanged with Sagei A20 RROR: relative error of 2 determinations less than 1%</pre>

OMPONENTS:	ORIGINAL MEASUREMENTS:
(1) 4-Heptanol; C ₇ H ₁₆ 0; [589-55-9]	Ratouis, M.; Dodé, M.
(2) Water; H ₂ 0; [7732-18-5]	Bull. Soc. Chim. Fr. 1965, 3318-22.
ARIABLES:	PREPARED BY:
Temperature: 25 ^o C and 30 ^o C	S.C. Valvani; S.H. Yalkowsky; A.F.M. Barton
Ringer solution also studied	
XPERIMENTAL VALUES:	
Proportion of 4-heptano	l (l) in water-rich phase.
t/ ^o C g(1)/100g	sln $10^4 x_1$ (compiler)
25 0.47	7.3
30 0.45	7.0
AUXILIARY	INFORMATION
AUXILIARY METHOD/APPARATUS/PROCEDURE:	INFORMATION SOURCE AND PURITY OF MATERIALS:
TETHOD/APPARATUS/PROCEDURE: In a round bottomed flask, 50 mL of water	
TETHOD/APPARATUS/PROCEDURE: In a round bottomed flask, 50 mL of water and a sufficient quantity of alcohol were introduced until two separate layers were	SOURCE AND PURITY OF MATERIALS: (1) redistilled with 10:1 reflux ratio b.p. 154.8-154.9 ^o C/760.7 mm Hg
AETHOD/APPARATUS/PROCEDURE: In a round bottomed flask, 50 mL of water and a sufficient quantity of alcohol were introduced until two separate layers were formed. The flask assembly was equilibrated	SOURCE AND PURITY OF MATERIALS: (1) redistilled with 10:1 reflux ratio
ÆTHOD/APPARATUS/PROCEDURE: In a round bottomed flask, 50 mL of water and a sufficient quantity of alcohol were introduced until two separate layers were formed. The flask assembly was equilibrated by agitation for at least 3h in a constant temperature bath. Equilibrium solubility	SOURCE AND PURITY OF MATERIALS: (1) redistilled with 10:1 reflux ratio b.p. 154.8-154.9 ^o C/760.7 mm Hg
ÆTHOD/APPARATUS/PROCEDURE: In a round bottomed flask, 50 mL of water and a sufficient quantity of alcohol were introduced until two separate layers were formed. The flask assembly was equilibrated by agitation for at least 3h in a constant temperature bath. Equilibrium solubility was attained by first supersaturation at a slightly lower temperature (solubility of	SOURCE AND PURITY OF MATERIALS: (1) redistilled with 10:1 reflux ratio b.p. 154.8-154.9°C/760.7 mm Hg $n_{\rm D}^{25}$ = 1.41780
ÆTHOD/APPARATUS/PROCEDURE: In a round bottomed flask, 50 mL of water and a sufficient quantity of alcohol were introduced until two separate layers were formed. The flask assembly was equilibrated by agitation for at least 3h in a constant temperature bath. Equilibrium solubility was attained by first supersaturation at a slightly lower temperature (solubility of alcohols in water decreases with increasing temperature) and then equilibrating at the	SOURCE AND PURITY OF MATERIALS: (1) redistilled with 10:1 reflux ratio b.p. 154.8-154.9°C/760.7 mm Hg $n_D^{25} = 1.41780$ (2) twice distilled from silica apparatus
ÆTHOD/APPARATUS/PROCEDURE: In a round bottomed flask, 50 mL of water and a sufficient quantity of alcohol were introduced until two separate layers were formed. The flask assembly was equilibrated by agitation for at least 3h in a constant temperature bath. Equilibrium solubility was attained by first supersaturation at a slightly lower temperature (solubility of alcohols in water decreases with increasing	 SOURCE AND PURITY OF MATERIALS: (1) redistilled with 10:1 reflux ratio b.p. 154.8-154.9°C/760.7 mm Hg n²⁵_D = 1.41780 (2) twice distilled from silica apparatus or ion-exchanged with Sagei A20
AETHOD/APPARATUS/PROCEDURE: In a round bottomed flask, 50 mL of water and a sufficient quantity of alcohol were introduced until two separate layers were formed. The flask assembly was equilibrated by agitation for at least 3h in a constant temperature bath. Equilibrium solubility was attained by first supersaturation at a slightly lower temperature (solubility of alcohols in water decreases with increasing temperature) and then equilibrating at the desired temperature. The aqueous layer was separated after an overnight storage in a bath. The alcohol content was determined by	 SOURCE AND PURITY OF MATERIALS: (1) redistilled with 10:1 reflux ratio b.p. 154.8-154.9°C/760.7 mm Hg n²⁵_D = 1.41780 (2) twice distilled from silica apparatus or ion-exchanged with Sagei A20 ESTIMATED ERROR:
ÆTHOD/APPARATUS/PROCEDURE: In a round bottomed flask, 50 mL of water and a sufficient quantity of alcohol were introduced until two separate layers were formed. The flask assembly was equilibrated by agitation for at least 3h in a constant temperature bath. Equilibrium solubility was attained by first supersaturation at a slightly lower temperature (solubility of alcohols in water decreases with increasing temperature) and then equilibrating at the desired temperature. The aqueous layer was separated after an overnight storage in a bath. The alcohol content was determined by reacting the aqueous solution with potassium dichromate and titrating the excess	 SOURCE AND PURITY OF MATERIALS: (1) redistilled with 10:1 reflux ratio b.p. 154.8-154.9°C/760.7 mm Hg n²⁵_D = 1.41780 (2) twice distilled from silica apparatus or ion-exchanged with Sagei A20
ÆTHOD/APPARATUS/PROCEDURE: In a round bottomed flask, 50 mL of water and a sufficient quantity of alcohol were introduced until two separate layers were formed. The flask assembly was equilibrated by agitation for at least 3h in a constant temperature bath. Equilibrium solubility was attained by first supersaturation at a slightly lower temperature (solubility of alcohols in water decreases with increasing temperature) and then equilibrating at the desired temperature. The aqueous layer was separated after an overnight storage in a bath. The alcohol content was determined by reacting the aqueous solution with potassium dichromate and titrating the excess dichromate with ferrous sulfate solution in the presence of phosphoric acid and	 SOURCE AND PURITY OF MATERIALS: (1) redistilled with 10:1 reflux ratio b.p. 154.8-154.9°C/760.7 mm Hg n²⁵ = 1.41780 (2) twice distilled from silica apparatus or ion-exchanged with Sagei A20 ESTIMATED ERROR: Solubility: relative error of 2 determinations less than 1% Temperature: ± 0.05°C
ÆTHOD/APPARATUS/PROCEDURE: In a round bottomed flask, 50 mL of water and a sufficient quantity of alcohol were introduced until two separate layers were formed. The flask assembly was equilibrated by agitation for at least 3h in a constant temperature bath. Equilibrium solubility was attained by first supersaturation at a slightly lower temperature (solubility of alcohols in water decreases with increasing temperature) and then equilibrating at the desired temperature. The aqueous layer was separated after an overnight storage in a bath. The alcohol content was determined by reacting the aqueous solution with potassium dichromate and titrating the excess dichromate with ferrous sulfate solution in	 SOURCE AND PURITY OF MATERIALS: (1) redistilled with 10:1 reflux ratio b.p. 154.8-154.9°C/760.7 mm Hg n²⁵_D = 1.41780 (2) twice distilled from silica apparatus or ion-exchanged with Sagei A20 ESTIMATED ERROR: Solubility: relative error of 2 determinations less than 1%
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COMPONENTS:	EVALUATOR:
(1) 2-Ethy1-1-hexanol; C ₈ H ₁₈ ⁰ ; [104-76-7]	A.F.M. Barton, Murdoch University, Perth, Western Australia
(2) Water; H ₂ 0; [7732-18-5]	November 1982.
CRITICAL EVALUATION:	
Only one determination of each of the phases	
reported (ref. 1 and 2) so the values can be	
The tentative value for the solubility of 2-ethyl-1-hexanol (1) in the water-rich	
phase at 298 K is $0.01 \text{ g}(1)/100 \text{ g sln}$ or 10	-
The tentative value for the solubility of wa 298 K is 0.02 g(2)/100 g sln or $x_2 = 0.001$	
References:	
	a Cham 1946 38 642
1. McBain, J.W.; Richards, P.H. Ind. En	<i>y. chem.</i> <u>1740</u> , <i>30</i> , 042.
2. Hlavaty, K.; Linek, J. Collect. Czec	h. Chem. Commun. <u>1973</u> , 38, 374.

COMPONENTS:	ORIGINAL MEASUREMENTS:
<pre>(1) 2-Ethyl-l-hexanol; C₈H₁₈0; [104-76-7] (2) Water; H₂0; [7732-18-5]</pre>	McBain, J.W.; Richards, P.H. Ind. Eng. Chem. <u>1946</u> , 38, 642-6.
VARIABLES: One temperature : 25 ⁰ C	PREPARED BY: M.C. Haulait-Pirson; A.F.M. Barton
EXPERIMENTAL VALUES:	

The solubility of 2-ethyl-l-hexanol in water at 25° C was reported to be 0.013 g(1)/100 g(2). The corresponding mole fraction solubility calculated by the compilers is $10^{5}x_{1} = 1.7$.

AUXILIARY INFORMATION	
METHOD/APPARATUS/PROCEDURE: 10 mL of (2) was measured into glass bottles with plastic caps and known amounts of (1) were added from a microburet reading to 0.001 mL. They were placed on a gentle shaker in an air thermostat overnight. The turbidity was measured in a Barnes turbidimeter (ref. 1), the turbidity rising sharply in the presence of emulsified droplets. The measurements formed part of a study of solubilization by detergents.	SOURCE AND PURITY OF MATERIALS: (1) "purest obtainable". (2) unspecified
	ESTIMATED ERROR: unspecified REFERENCES: 1. McBain, J.W.; Stamberg, O.E. Rept. to Master Brewers' Assoc. of Am., <u>1942</u> .

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) 2-Ethyl-1-hexanol; C ₈ H ₁₈ 0; [104-76-7] (2) Water; H ₂ 0; [7732-18-5]	Hlavaty, K.; Linek, J. Collect. Czech. Chem. Commun. <u>1973</u> , 38, 374-8.
VARIABLES: One temperature: 24.6 ⁰ C	PREPARED BY: A. Maczynski

The solubility of water in 2-ethyl-1-hexanol at 24.6° C was reported to be 0.020 g(2)/100g sln.

The corresponding mole fraction, x_2 , calculated by the compiler, is 0.0014.

AUXILIARY	INFORMATION
	••••••••••••••••••••••••••••••••••••••
ME THOD / AP PARATUS / PROCEDURE :	SOURCE AND PURITY OF MATERIALS:
The titration method was used. The measurements were performed in a titration	(1) not specified
wessel according to Mertl, ref 1, which can be thermostatted during the titration. Both the vessel and the buret were thermostatted to $24.6 \pm 0.1^{\circ}$ C. The mixture was agitated vigorously by a magnetic stirrer during the titration,	(2) not specified
	ESTIMATED ERROR:
	Solubility: better than ± 0.3 wt %
	Temperature: ± 0.1°C
	REFERENCES:
	 Mertl, I. Thesis, Institute of Chemical Process Fundamentals, Czechoslovak Academy of Sciences, Prague <u>1969</u>.

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) 2-Methyl-2-heptanol; C ₈ H ₁₈ 0; [625-25-2]	Ratouis, M.; Dode, M.;
(2) Water; H ₂ 0; [7732-18-5]	Bull. Soc. Chim. Fr. 1965, 3318-22.
VARIABLES:	PREPARED BY:
One temperature: 30 ⁰ C	S.C. Valvani; S.H. Yalkowsky; A.F.M. Barton
EXPERIMENTAL VALUES:	

The proportion of 2-methyl-2-heptanol (1) in the water-rich phase at equilibrium at 30° C was reported to be 0.25 g(1)/100 g sln.

The corresponding mole fraction solubility, calculated by the compilers, is $10^4 x_1 = 3.5$.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

In a round bottomed flask, 50 mL of water and a sufficient quantity of alcohol were introduced until two separate layers were formed. The flask assembly was equilibrated by agitation for at least 3 h in a constant temperature bath. Equilibrium solubility was attained by first supersaturation at a slightly lower temperature (solubility of alcohols in water decreases with increasing temperature) and then equilibrating at the desired temperature. The aqueous layer was separated after an overnight storage in a bath. The alcohol content was determined by reacting the aqueous solution with potassium dichromate and titrating the excess dichromate with ferrous sulfate solution in the presence of phosphoric acid and diphenylamine barium sulfonate as an indicator.

SOURCE AND PURITY OF MATERIALS:

- (1) laboratory preparation; redistilled with 10:1 reflux ratio, b.p. 63.1-63.2°C/15mm Hg $n_{\rm D}^{25}$ = 1.42110
- (2) twice distilled from silica apparatus or ion-exchanged with Sagei A20.

ESTIMATED ERROR:

Solubility: relative error of 2 determinations less than 1%.

Temperature: $\pm 0.05^{\circ}C$

REFERENCES:

COMPONENTS:	ORIGINAL MEASUREMENTS:
<pre>(1) 3-Methyl-3-heptanol; C₈H₁₈0;</pre>	Ratouis, M.; Dode, M.;
[598-06-1]	Bull. Soc. Chim. Fr. <u>1965</u> , 3318-22
	<u></u> ;
(2) Water; H ₂ 0; [7732-18-5]	
VARIABLES:	PREPARED BY:
One temperature: 30 [°] C	S.C. Valvani; S.H. Yalkowsky; A.F.M. Barton
Ringer solution also studied	
EXPERIMENTAL VALUES:	
The proportion of 3-methyl-3-heptanol (1) in	the water-rich phase at equilibrium at
30° C was reported to be 0.325 g(1)/100g sln.	
The corresponding mole fraction solubility, c	alculated by the compilers, is
4.5×10^{-4} .	arculated by the compilers, 15
The proportion of (1) in the water-rich phase	
at equilibrium at 30° C was reported to be 0.2	9 g(1)/100g sln.
AUXILIARY	INFORMATION
METHOD/APPARATUS/PROCEDURE: SOURCE AND PURITY OF MATERIALS:	
In a round bottomed glask, 50 mL of water	(1) laboratory preparation;
and a sufficient quantity of alcohol were	redistilled with 10:1 reflux ratio;
introduced until two separate layers were formed. The flask assembly was equilibrated	ь.р. 68.8-69.2 [°] С/24mm Нg
by agitation for at least 3 h in a constant	$n_{\rm D}^{25} = 1.42670$
temperature bath. Equilibrium solubility	
was attained by first supersaturation at a slightly lower temperature (solubility of	(2) twice distilled from silica apparatus or ion-exchanged with Sagei A20.
alcohols in water decreases with increasing	of ion-exchanged with Sager A20.
temperature) and then equilibrating at the	
desired temperature. The aqueous layer was separated after an overnight storage in	
a bath. The alcohol content was determined	ESTIMATED ERROR:
by reacting the aqueous solution with potassium dichromate and titrating the excess	Solubility: relative error of 2 determina-
dichromate with ferrous sulfate solution in	tions less than 1%.
the presence of phosphoric acid and diphonylaming barium sulfonate as an	Temperature: ± 0.05°C
diphenylamine barium sulfonate as an indicator.	REFERENCES :
L	

COMPONENTS: (1) 1-Octanol (1-octyl alcohol, capryl alcohol); C ₈ H ₁₈ 0; [111-87-5] (2) Water; H ₂ 0; [7732-18-5]		ter, Murdoch Univ Australia.	versity, Perth,
CRITICAL EVALUATION:	· - A	······	
Solubilities in the system comprising 1-o the following publications:	ctanol (1) and	l water (2) have	been reported in
Reference	T/K	Solubility	Method
Butler et al. (ref 1)	298	(1) in (2)	interferometric
Sobotka and Glick (ref 2)	303	(1) in (2)	not stated
Addison (ref 3)	293	(1) in (2)	surface tension
McBain and Richards (ref 4)	298	(1) in (2)	titration
Erichsen (ref 5)	273-523	(2) in (1)	synthetic
Crittenden and Hixon (ref 6)	298	mutual	titration
Kinoshita <i>et al</i> . (ref 7)	298	(1) in (2)	surface tension
Shinoda et al. (ref 8)	298	(1) in (2)	surface tension
Ababi and Popa (ref 9)	298	(2) in (1)	turbidimetric
Rao et al. (ref 10)	303	mutual	turbidimetric
Vochten and Petre (ref 11)	288	(1) in (2)	surface tension
Lavrova and Lesteva (ref 12)	313,333	mutual	titration
Zhuravleva <i>et al</i> . (ref 13)	280-388	mutual	polythermic
Tokunaga et al. (ref 14)	288-313	(2) in (1)	analytical

The original data are compiled in the data sheets immediately following this Critical Evaluation.

Considering its widespread use in solvent extraction there is surprisingly little information available on the mutual solubilities of 1-octanol and water especially for the water-rich phase. Insufficient data have been reported to define the upper critical solution temperature. It will be clear from the following Tables and discussion that this system warrants a thorough reinvestigation.

In preparing this Critical Evaluation use has been made of the fact that the solubility of 1-octanol in water is sufficiently low to enable weight/volume (ref 11) and volume/volume (ref 2) solubilities to be converted to weight/weight values by assuming the water-rich phase has the same density as pure water. Values obtained by the Evaluator by graphical interpolation or extrapolation from the data sheets are indicated by an asterisk (*). "Best" values have been obtained by simple averaging. The uncertainty limits (σ_n) attached to the "best" values do not have statistical significance and should be regarded only as a convenient representation of the spread of reported values and not as error limits. The letter (*R*) designates "Recommended" data Data are "Recommended" if two or more apparently reliable studies are in reasonable agreement ($\leq \pm 5\%$ relative).

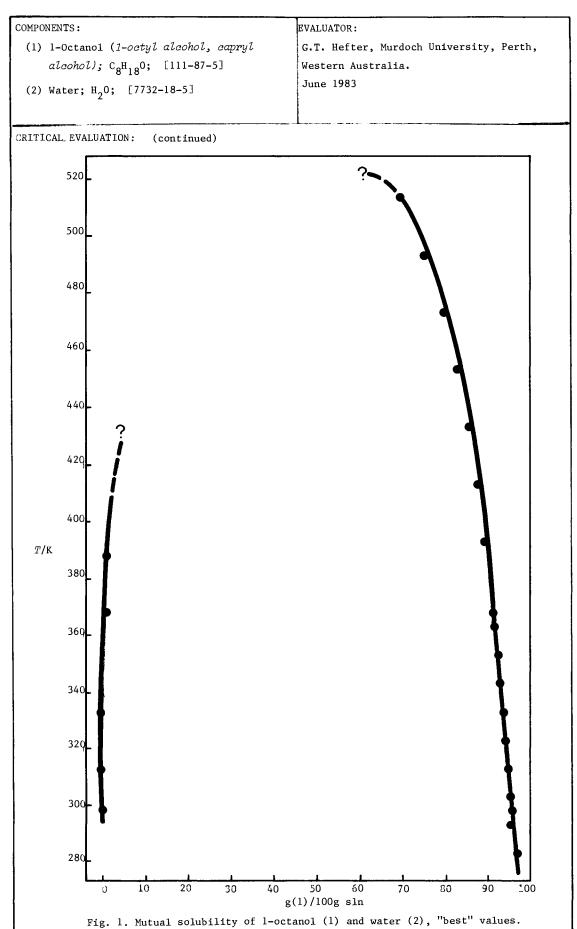
For convenience the two phases will be further discussed separately.

(continued next page)

1-Octanol

COMPONENTS:	EVALUATOR:		
(1) 1-Octanol (1-octyl alcohol, capryl	G.T. Hefter, Murdoch University, Perth,		
alcohol); C ₈ H ₁₈ 0; [111-87-5]	Western Australia.		
(2) Water; H ₂ 0; [7732-18-5]	June 1983.		
CRITICAL EVALUATION (continued)			
Water-rich phase			
All the available data are summarized in	n the Table below. With the exception of the		
value at 298 K most of the data are mutu	ally inconsistent and should therefore be		
regarded as very tentative.			
Tentative and Recommend	ded (R) values for the solubility		
of l-octanol (1)	in water (2)		
Т/К	Solubility, g(1)/100g sln		
	ed values "Best" values (±σ_)		
- 288 0.053 (ref 11)	n		
293 0.042 (ref 3)			
), 0.05 (ref 6), 0.049 (ref 7) $0.054 \pm 0.005(R)$		
298 0.0586 (ref 1), 0.059 (ref 4), 0.05 (ref 6), 0.049 (ref 7) 0.054 ± 0.005(R 303 0.076 (ref 2), 0.1 (ref 10) 0.09 ± 0.01			
$303 0.076 (ref 2), 0.1 (ref 10) 0.09 \pm 0.01$ 313 0.06 (ref 12)			
368 1.0 (ref 13)	333 0.06 (ref 12) 368 1.0 (ref 13)		
388 0.5 (ref 13)			
	value at 298 K is slightly higher than the		
value 0.046 g(1)/100g sln predicted by a	the equation given in the Editor's Preface.		
Alcohol-rich phase			
Sufficient data are available for the se	olubility of water in l-octanol for a realistic		
Evaluation to be made.			
The data of Crittenden and Hixon (ref 6) and Zhuravleva et al. (ref 13) are consistently		
	erefore been rejected. All other data are		
included in the Table below. With the	exception of the values otherwise indicated all		
data are regarded as Tentative and, as a	may be seen from the Table, are largely the		
values of Erichsen (ref 5).			
Tentative and Recommended (R) values for the solubility			
of water (2) in l-octanol (1)		
T/K	Solubility, g(2)/100g sln		
Repo	rted values "Best" values $(\pm \sigma_n)$		
273 3.40 (ref 5)	3.4		
283 3.85 (ref 5), 4.62 [*] (ref 14)	4.2 ± 0.4		
293 4.30 (ref 5), 4.75 (ref 14)	4.5 ± 0.2 (R)		
	.78 (ref 14) 4.6 ± 0.1 (R)		
298 4.45 [*] (ref 5), 4.7 (ref 9), 4			
298 4.45 (ref 5), 4.7 (ref 9), 4 303 4.75 (ref 5), 4.6 (ref 10),			

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COMPONENTS:
                                               EVALUATOR:
                                                G.T. Hefter, Murdoch University, Perth,
 (1) 1-Octanol (1-octyl alcohol, capryl
     alcohol); C<sub>8</sub>H<sub>18</sub>0; [111-87-5]
                                                Western Australia.
                                                June 1983.
 (2) Water; H<sub>2</sub>0: [7732-18-5]
CRITICAL EVALUATION (continued)
   T/K
                                                 Solubility, g(2)/100g sln
                                                                       "Best" values (±σ_)
                                Reported values
                                                                            5.9
   323
           5.90 (ref 5)
   333
           6.45 (ref 5), 6.0 (ref 12)
                                                                            6.2 \pm 0.2 (R)
           7.10 (ref 5)
                                                                            7.1
   343
                                                                            7.7
   353
           7.70 (ref 5)
   363
           8.35 (ref 5)
                                                                            8.4
                                                                           9.1
   373
         9.10 (ref 5)
                                                                          10.7
   393
         10.65 (ref 5)
   413
          12.45 (ref 5)
                                                                          12.5
         14.60 (ref 5)
                                                                          14.6
   433
                                                                          17.1
   453
         17.10 (ref 5)
                                                                          20.1
   473
          20.10 (ref 5)
                                                                          23.9
   493
          23.90 (ref 5)
          29.95 (ref 5)
                                                                          30.0
   513
 The "best" values of the mutual solubility of 1-octanol and water are plotted in
 Figure 1 (see following page).
 References
 1. Butler, J.A.V.; Thomson, D.W.; Maclennan, W.H. J. Chem. Soc. 1933, 674.
 2. Sobotka, H.; Glick, D. J. Biol. Chem. 1934, 105, 199.
 3. Addison, C.C. J. Chem. Soc. 1945, 98.
 4. McBain, J.W.; Richards, P.H. Ind. Eng. Chem. 1946, 38, 642.
 5. Erichsen, L.von Brennst. Chem. 1952, 33, 166.
 6. Crittenden, E.D., Jr.; Hixon, A.N. Ind. Eng. Chem. 1954, 46, 265.
 7. Kinoshita, K.; Ishikawa H.; Shinoda, K. Bull. Chem. Soc. Jpn. 1958, 31,1081.
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     3818-75.
 13. Zhuravleva, I.K.; Zhuravlev, E.F.; Lomakina, N.G. Zh. Fiz. Khim. 1977, 51, 1700.
 14. Tokunaga, S.; Manabe, M.; Koda, M. Niihama Kogyo Koto Semmon Gakko Kiyo, Rikagaku
     Hen (Memoirs Niihama Technical College, Sci. and Eng.) 1980, 16, 96.
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COMPONENTS:	ORIGINAL MEASUREMENTS:
 (1) 1-Octanol (<i>capryl alcohol</i>); C₈H₁₈O; [111-87-5] (2) Water; H₂O; [7732-18-5] 	Butler, J.A.V.; Thomson, D.W.; Maclennan, W.H. <i>J. Chem. Soc.</i> <u>1933</u> , 674-86.
VARIABLES: One temperature: 25 ⁰ C	PREPARED BY: S.H. Yalkowsky; S.C. Valvani; A.F.M. Barton

The proportion of 1-octanol (1) in the water-rich phase at equilibrium at 25° C was reported to be 0.0586 g(1)/100g sln, the mean of six determinations (0.0571, 0.0606, 0.0590, 0.0587, 0.0582, 0.0580 g(1)/100g sln).

The corresponding mole fraction solubility was reported as $10^5 x_1 = 8.11$.

AUXILIARY	INFORMATION
METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
An analytical method was used, with a U-tube apparatus having two internal stoppers. Suitable quantities of (1) and (2) were placed in one of the connected vessels and shaken in a thermostat for some hours. The liquid was allowed to separate into two layers, the heavier aqueous layer being separated by raising the stopper and allow- ing part of the liquid to run into the connected vessel. A weighed portion of the separated sln was diluted with about an equal quantity of (2) and the resulting sln compared with calibration slns in an interferometer. To avoid the possibility of reading the position of the wrong fringe, l cells (1 cm and 5 cm) were used. The method was unsuitable for analysis of alcohol-rich slns, as no stoppered inter- ferometer cell was available.	(1) B.D.H; repeated fractionated in vacuum with a Hempel column, the middle fractionation being refluxed with Ca and refraction- ated; b.p. 94.80-94.85°C/8 mm Hg, 194.5°C/760 mm Hg d_4^{25} 0.82238 n_D^{20} 1.42937 (2) not stated ESTIMATED ERROR: Solubility: the result is the mean of six determinations agreeing within 0.002 g(1)/100g sln. Temperature: not stated (but in related experiment is was \pm 0.03°C). REFERENCES

1-Octanol

COMPONENTS :	ORIGINAL MEASUREMENTS:
(1) 1-Octanol (<i>capryl alcohol</i>); C ₈ H ₁₈ 0;	Sobotka, H.; Glick, D.
	J. Biol. Chem. <u>1934</u> , 105, 199–219.
(2) Water; H ₂ ⁰ ; [7732-18-5]	
VARIABLES:	
One temperature: 30°C	PREPARED BY: S.H. Yalkowsky; S.C. Valvani; A.F.M. Barton
Effect of enzyme solutions also studied	bin fullowory, bio fullouil, herens barcon
EXPERIMENTAL VALUES:	
The solubility of 1-octanol (1) in water at 30	$D^{O}C$ was reported to be 0.093 mL(1)/100mL (2).
The corresponding mass percentage and mole fra	action solubilities, calculated by the
compiler using a density of 0.82 g mL ^{-1} , are (0.076 g(1)/100g sln and $10^4 x_1 = 1.05$.
The solubility of (1) in pancreas globulin so	Ĩ
0.111 mL(1)/100mL sln.	
The solubility of (1) in liver albumin solution	on (total solids U.50 mg/100mL) was 0.104
mL(1)/100mL sln.	
	· · · · · · · · · · · · · · · · · · ·
AUXILIARY	INFORMATION
ME THOD /APPARATUS / PROCEDURE :	SOURCE AND PURITY OF MATERIALS:
The method was described in ref l. A few	(1) Not stated
mL of (1) was stained with a minute quantity of Sudan IV, a water-insoluble lipoid-	
soluble dye. It was then added dropwise	(2) Distilled
from a microburet with a capillary tip to 100, 250 or 500 mL of (2) of constant	
temperature in a narrow-mouthed glass-	
stoppered stock bottle, which was shaken after each addition. While the added (1)	
was dissolved, the Sudan dye was wholly or	
partly dissolved, imparting a pink tinge to the aqueous sln. When the water was	
saturated with (1), the second phase con-	ESTIMATED ERROR:
sisted of transparent droplets. The end point could be improved by adding the	Solubility: ± 0.001 mL(1)/100mL (2)
Sudan IV (1-5 mg) to the water, and the alcohol added dropwise. When saturation	
was reached, one additional drop converted	
the floating, jagged indicator particles into dark transparent droplets.	REFERENCES: 1. Sobotka, H.; Kahn, J.
	J. Am. Chem. Soc. <u>1931</u> , 53, 2935.
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COMPONENTS:	ORIGINAL MEASUREMENTS:
 (1) 1-Octanol (capryl alcohol); C₈H₁₈O;	Addison, C.C.
[111-87-5] (2) Water; H₂O; [7732-18-5]	J. Chem. Soc. <u>1945</u> , 98-106.
VARIABLES:	PREPARED BY:
One temperature: 20 ⁰ C	S.H. Yalkowsky; S.C. Valvani; A.F.M. Barton

The proportion of 1-octanol (1) in the water-rich phase at equilibrium at 20° C was reported to be 0.042 g(1)/100g sln.

The corresponding mole fraction solubility, calculated by the compilers is $10^5 x_1 = 5.8$.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE: The surface tension method was used. Sufficient excess of (1) was added to 100 mL of (2) in a stoppered flask to form a separate lens on the surface. The mixture was swirled gently, too vigorous an agita- tion being avoided as this gave a semi- permanent emulsion and incorrect readings. After settling, a small sample of the clear aqueous sln was withdrawn into a drop weight pipet and the surface tension determined. The swirling was continued until a constant value was obtained. The surface tension-concentration curve was known, and only a slight extrapolation (logarithmic scale) was necessary to find the concentration corresponding to the equilibrium value.	<pre>SOURCE AND PURITY OF MATERIALS: (1) impure alcohols were purified by fractional distillation, the middle fraction from a distillation being redistilled; b.p. 194.5°C d²⁰₄ 0.8244 n²⁰_D 1.4291 (2) not stated ESTIMATED ERROR: Solubility: ± 0.5%</pre>
	REFERENCES :

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) 1-Octanol (capryl alcohol); C ₈ H ₁₈ 0;	McBain, J.W.; Richards, P.H.
[111-87-5]	Ind. Eng. Chem. <u>1946</u> , 38, 642-6.
(2) Water; H ₂ 0; [7732-18-5]	
VARIABLES:	PREPARED BY:
One temperature: 25 [°] C	S.H. Yalkowsky; S.C. Valvani; A.F.M. Barton
EXPERIMENTAL VALUES:	
The proportion of 1-octanol (1) in the wat reported to be $0.059 \text{ g(1)}/100 \text{g(2)}$.	er-rich phase at equilibrium at 25 ⁰ C was
The corresponding mole fraction solubility $10^5 x_1 = 8.1$.	, calculated by the compilers, is
AUXILIA	RY INFORMATION
METHOD / APPARATUS / PROCEDURE :	SOURCE AND PURITY OF MATERIALS;
10 mL of (2) were measured into glass	(1) "purest obtainable"
	ng Le (2) not specified The
turbidity was measured in a Barnes Turbid imeter (ref 1), the turbidity rising	-
sharply in the presence of emulsified droplets. The measurements formed part o	f
a study of solubilization by detergents.	
	ESTIMATED ERROR:
	Not specified
	REFERENCES :
	 McBain, J.W.; Stamberg, O.E. <i>Rept. to Master Brewers' Assoc. of Am.</i>, 1942.
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Eight-carbon Alcohols

COMPONENTS:	ORIGINAL MEASUREMENTS:		
(1) 1-Octanol (capryl alcohol); C ₈ H ₁₈ 0;	Erichsen, L. von		
[111-87-5]	Brennst. Chem. <u>1952</u> , 33, 166–72.		
(2) Water; H ₂ 0; [7732-18-5]	Diennet. (nem. <u>1992</u> , 55, 100-72.		
2			
VARIABLES:	PREPARED BY:		
Temperature: 0-260 [°] C	S.H. Yalkowsky and Z. Maczynska		
EXPERIMENTAL VALUES:			
Proportion of 1-octano	l (l) in alcohol-rich phase		
t/ ^o C g(1)/100	Og sln x ₁		
0 96.			
10			
20 95. 30 95.			
40 94.			
50 94.	10 0.6882		
60 93.			
70 92.			
80 92. 90 91.			
100 90.			
110 90.			
120 89.			
130 88.			
140 87. 150 86.	. –		
160 85.			
170 84.			
180 82.			
190 81.			
200 79. 210 78.			
220 76.			
230 73.			
240 70.			
250 65.	50 0.2081		
AUXILIARY	INFORMATION		
METHOD / APPARATUS / PROCEDURE :	SOURCE AND PURITY OF MATERIALS:		
The synthetic method was used.	(1) Merck, or Ciba, or industrial product;		
-	distilled and chemically free from		
The measurements were carried out in 2 mL	isomers;		
glass ampules. These were placed in an	b.p. 195.7-195.8 [°] C (759 mm Hg),		
aluminium block equipped with two glass windows. Cloud points were measured with	$n_{\rm D}^{20}$ 1.4292.		
a thermocouple wound up around the ampule.	(2) not exception		
Each measurement was repeated twice.	(2) not specified.		
	ESTIMATED ERROR:		
	Not specified.		
	REFERENCES :		
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COMPONENTS:	ORIGINAL MEASUREMENTS:
 (1) 1-Octanol (capryl alcohol); C₈H₁₈O; [111-87-5] (2) Water; H₂O; [7732-18-5] 	Crittenden, E.D., Jr.; Hixon, A.N. Ind. Eng. Chem. <u>1954</u> , 46, 265-8.
VARIABLES:	PREPARED BY:
One temperature: 25 ⁰ C	A. Maczynski
Une temperature: 25 C	A. Maczynski
EXPERIMENTAL VALUES:	
The solubility of 1-octanol in water at 25°C	
The corresponding mole fraction, x_1 , calculat	ed by the compiler is 0.0007.
The solubility of water in 1-octanol at 25°C	was reported to be 1.7 g(2)/100g sln.
The corresponding mole fraction, $x_2^{}$, calculat	ed by the compiler is 0.111.
AUXILIARY	INFORMATION
METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
Presumably the titration method described for ternary systems containing HCl was used.	 source not specified; purified;
In this method the solubility was determined by bringing 100 mL samples of (1) or (2)	purity not specified.
to a temperature $25.0 \pm 0.1^{\circ}C$ and the second component was then added from a calibrated	(2) not specified.
buret with vigorous stirring, until the	
solution became permanently cloudy.	
	ESTIMATED ERROR:
	Temperature: ± 0.10 [°] C.
	REFERENCES:

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) 1-Octanol (capryl alcohol); C ₈ H ₁₈ O;	Kinoshita, K.; Ishikawa, H.; Shinoda, K;
[111-87-5]	Bull. Chem. Soc. Jpn. <u>1958</u> , 31, 1081-4.
(2) Water; H ₂ 0; [7732-18-5]	
VARIABLES:	PREPARED BY:
One temperature: 25°C	S.H. Yalkowsky; S.C. Valvani; A.F.M. Barton
one cemperature. 25 C	Sine raikowsky, See varvani, mirin Sarton
EXPERIMENTAL VALUES:	
The equilibrium of 1-octanol (1) in the water	-rich phase at 25.0°C was reported
to be 0.0038 mol(1)/L ⁻¹ and the mass percent	
	age solubility was reported as
0.049 g(1)/100g sln.	
	5
The corresponding mole fraction solubility, c	alculated by the compilers, is $10^{5}x_{1} = 6.7$.
AUXILIARY	INFORMATION
METHOD / APPARATUS / PROCEDURE :	SOURCE AND PURITY OF MATERIALS:
HE THOD/AF FARATOS/FROCEDORE.	
The surface tension in aqueous solutions of	(1) purified by vacuum distillation through
alcohols monotonously decreases up to their	50-100 cm column;
saturation concentration and remains con-	b.p. 96 ⁰ С/16mm Нg
stant in the heterogeneous region (ref 1-4). Surface tension was measured by the drop	
weight method, using a tip 6 mm in diameter,	(2) not stated
the measurements being carried out in a	
water thermostat. From the (surface ten-	
sion)-(logarithm of concentration) curves the saturation points were determined as the	
intersections of the curves with the	
horizontal straight lines passing through	
the lowest experimental points.	ESTIMATED ERROR:
	Temperature: ± 0.05°C
	Solubility: within 4%
	REFERENCES:
	1. Motylewski, S. Z. Anorg. Chem. 1904,
	38, 410.
	2. Taubamann, A. Z. physick. Chem. 1932,
	A161, 141.
	3. Zimmerman, H.K. Jr. Chem. Rev. <u>1952</u> , 51, 25.
	4. Shinoda, K.; Yamanaka, T.; Kinoshita, K.
	J. Phys. Chem. 1959, 63, 648.

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) 1-Octanol (capryl alcohol); C ₈ H ₁₈ 0;	Shinoda, K.; Yamanaka, T.; Kinoshita, K.
[111-87-5]	J. Phys. Chem. <u>1959</u> , 63, 648-50
(2) <u>Wate</u> r; H ₂ 0; [7732-18-5]	
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VARIABLES:	PREPARED BY:
One temperature: 25 ⁰ C	A.F.M. Barton
EXPERIMENTAL VALUES:	
The equilibrium concentration of 1-octanol (1) in the water-rich phase at 25 ⁰ C
was reported to be 0.0038 mol(1)/L sln.	
AUXILIARY	INFORMATION
METHOD /APPARATUS / PROCEDURE :	SOURCE AND PURITY OF MATERIALS:
Surface tension was measured by the drop weight method, with a tip 0.249 cm in	(1) Kao Soap Co. fractional distillation in 100 cm
diameter, in an air thermostat. Solubility	
was determined by the turbidity change and/or the break in the (surface tension)-	b.p. 96 ⁰ C/16 mm Hg
(logarithm of concentration) plot.	(2) not stated
	ESTIMATED ERROR:
	Temperature: $\pm 0.2^{\circ}C$
	REFERENCES :

COMPONENTS:	ORIGINAL MEASUREMENTS:		
<pre>(1) 1-Octanol (capryl alcohol); C₈H₁₈O; [111-87-5] (2) Water; H₂O; [7732-18-5]</pre>	Ababi, V.; Popa, A. An. Stiint. Univ. "Al. I. Cuza" Iasi. <u>1960</u> , 6, 929-42.		
VARIABLES: One temperature: 25 [°] C	PREPARED BY: A. Maczynski		
EXPERIMENTAL VALUES:			
The solubility of water in 1-octanol at 25° C was reported to be 4.7 g(2)/100g sln.			
The corresponding mole fraction, $x_2^{}$, calculated by the compiler is 0.26.			

	INFORMATION
METHOD/APPARATUS/PROCEDURE: The turbidimetric method was used. Ternary solubilities were described in the paper but nothing reported on binary solubilities.	<pre>SOURCE AND PURITY OF MATERIALS: (1) Merck analytical reagent; used as received, (2) not specified. ESTIMATED ERROR: Not specified. REFERENCES: </pre>

(1) 1-Octanol (ampryl alcohol); C _{gB1g} O; (1) Water; H ₂ O; [7732-18-5] Rao, K.S.; Rao, M.V.R.; Rao, C.V. <i>X</i> . Soi. Ind. Res. 1961, 203, 283-6. VARIABLES: Case temperature: 30°C PREPARED BY: A. Macrymski EXPERIMENTAL VALUES: PREPARED BY: A. Macrymski The solubility of 1-octanol in water at 30°C was reported to be 0.1 g(1)/100g sin. The corresponding mole fraction, x ₁ , calculated by the compiler is 0.0001. The solubility of water in 1-octanol at 30°C was reported to be 4.6 g(2)/100g sin. The corresponding mole fraction, x ₂ , calculated by the compiler is 0.268. METHOD/APPARATUS/FROCEDURE: The method of appearance and disappearance of turbidity described in ref 1 was used. No details were reported in the paper. SOURCE AND PURITY OF MATERIALS: Not specified. (2) distilied; Free from carbon dioxide. ESTIMATED ERROR: Not specified. REFERENCES: 1. Othmer, D.F.; White, R.E.; Trueger, E. Ind. Eng. Chem. 1941, 33, 1240.	COMPONENTS:	ORIGINAL MEASUREMENTS:
Ill-87-51 J. Sai. Ind. Res. 1961, 208, 283-6. (2) Water; H_0; [7732-18-5] J. Sai. Ind. Res. 1961, 208, 283-6. VARIABLES: PREPARED BY: One temperature: 30°C A. Maczynski EXPERIMENTAL VALUES: A. Maczynski The solubility of l-octanol in water at 30°C was reported to be 0.1 g(1)/100g sln. The corresponding mole fraction, x_1 , calculated by the compiler is 0.0001. The solubility of water in 1-octanol at 30°C was reported to be 4.6 g(2)/100g sln. The corresponding mole fraction, x_2 , calculated by the compiler is 0.268. METHOD/APPARATUS/PROCEDURE: SOURCE AND PURITY OF MATERIALS: The method of appearance and disappearance of turbidity described in ref 1 was used. No details were reported in the paper. SOURCE AND PURITY OF MATERIALS: (1) Marden and Co.; used as recived; m ³⁰ 0.4245, d ³⁰ 0.8215 g/mL. (2) distilled free from carbon dioxide. ESTIMATED ERBOR: Not specified. Not specified. EFEFRENCES: 1. Othmer, D.F.; White, R.E.; Trueger, E.		
(2) Water; H ₂ O; [7732-18-5] VARIABLES: Due temperature: 30° C The solubility of 1-octanol in water at 30° C was reported to be 0.1 g(1)/100g sln. The corresponding mole fraction, x_1 , calculated by the compiler is 0.0001. The solubility of water in 1-octanol at 30° C was reported to be 4.6 g(2)/100g sln. The corresponding mole fraction, x_2 , calculated by the compiler is 0.268. AUXILIARY INFORMATION METHOD/APPARATUS/PROCEDURE: The method of appearance and disappearance of turbidity described in ref 1 was used. No details were reported in the paper. SUBCE AND PURITY OF MATERIALS: (1) Marden and Co.; used as recived; π^{30} 1.4245, d^{30} 0.8215 g/mL. (2) distilled; free from carbon dioxide. ESTIMATED ERROR: Not specified.	(1) 1-Octanol (capryl alcohol); C ₈ H ₁₈ 0;	Rao, K.S.; Rao, M.V.R.; Rao, C.V.
VARIABLES: PREPARED EV: One temperature: $30^{\circ}C$ A. Maczynski EXPERIMENTAL VALUES: The solubility of 1-octanol in water at $30^{\circ}C$ was reported to be 0.1 g(1)/100g sln. The corresponding mole fraction, x_1 , calculated by the compiler is 0.0001. The solubility of water in 1-octanol at $30^{\circ}C$ was reported to be 4.6 g(2)/100g sln. The corresponding mole fraction, x_2 , cslculated by the compiler is 0.268. AUXILIARY INFORMATION METHOD/APPARATUS/FROCEDURE: The method of appearance and disappearance of turbidity described in ref 1 was used. No details were reported in the paper. SOURCE AND PURITY OF MATERIALS: (1) Maardon and Co.; used as recived; n^{20} 1.4245, d^{20} 0.8215 g/mL. (2) distilled; Free from carbon dioxide. ESTIMATED ERROR: Not specified. REFERENCES: 1. Othmer, D.F.; White, R.E.; Trueger, E.		J. Sci. Ind. Res. <u>1961</u> , 20B, 283-6.
One temperature: 30°C A. Maczynski EXPERIMENTAL VALUES: The solubility of 1-octanol in water at 30°C was reported to be 0.1 g(1)/100g sln. The corresponding mole fraction, x1, calculated by the compiler is 0.0001. The solubility of water in 1-octanol at 30°C was reported to be 4.6 g(2)/100g sln. The corresponding mole fraction, x2, calculated by the compiler is 0.268. METHOD/APPARATUS/PROCEDURE: The method of appearance and disappearance of turbidity described in ref 1 was used. No details were reported in the paper. Source And PURITY OF MATERIALS: (1) Naerden and Co.; used as recived; n°0 1,4245, d°0 0,8215 g/mL. (2) distilled; free from carbon dioxide. ESTIMATED ERROR: Not specified. REPERENCES: 1. Othmer, D.P.; White, R.E.; Trueger, E.	(2) Water; H ₂ O; [7732-18-5]	
One temperature: 30°C A. Maczynski EXPERIMENTAL VALUES: The solubility of 1-octanol in water at 30°C was reported to be 0.1 g(1)/100g sln. The corresponding mole fraction, x1, calculated by the compiler is 0.0001. The solubility of water in 1-octanol at 30°C was reported to be 4.6 g(2)/100g sln. The corresponding mole fraction, x2, calculated by the compiler is 0.268. METHOD/APPARATUS/PROCEDURE: The method of appearance and disappearance of turbidity described in ref 1 was used. No details were reported in the paper. Source And PURITY OF MATERIALS: (1) Naerden and Co.; used as recived; n°0 1,4245, d°0 0,8215 g/mL. (2) distilled; free from carbon dioxide. ESTIMATED ERROR: Not specified. REPERENCES: 1. Othmer, D.P.; White, R.E.; Trueger, E.		
EXPERIMENTAL VALUES: The solubility of 1-octanol in water at 30°C was reported to be 0.1 g(1)/100g sin. The corresponding mole fraction, x_1 , calculated by the compiler is 0.0001. The solubility of water in 1-octanol at 30°C was reported to be 4.6 g(2)/100g sin. The corresponding mole fraction, x_2 , calculated by the compiler is 0.268. METHOD/APPARATUS/PROCEDURE: The method of appearance and disappearance of turbidity described in ref 1 was used. No details were reported in the paper. No details were reported in the paper. ESTIMATED ERROR: Not specified. REFERENCES: 1. Othmer, D.F.; White, R.E.; Trueger, E.	VARIABLES:	PREPARED BY:
The solubility of 1-octanol in water at 30° C was reported to be 0.1 g(1)/100g sln. The corresponding mole fraction, x_1 , calculated by the compiler is 0.0001. The solubility of water in 1-octanol at 30° C was reported to be 4.6 g(2)/100g sln. The corresponding mole fraction, x_2 , calculated by the compiler is 0.268. METHOD/APPARATUS/PROCEDURE: The method of appearance and disappearance of turbidity described in ref 1 was used. No details were reported in the paper. SURCE AND PURITY OF MATERIALS: (1) Naarden and Co.; used as recived; π^{30} 1.4245, d^{30} 0.8215 g/mL. (2) distilled; free from carbon dioxide. ESTIMATED ERROR: Not specified. REFERENCES: 1. Othmer, D.F.; White, R.E.; Trueger, E.	One temperature: 30°C	A. Maczynski
The solubility of 1-octanol in water at 30° C was reported to be 0.1 g(1)/100g sln. The corresponding mole fraction, x_1 , calculated by the compiler is 0.0001. The solubility of water in 1-octanol at 30° C was reported to be 4.6 g(2)/100g sln. The corresponding mole fraction, x_2 , calculated by the compiler is 0.268. METHOD/APPARATUS/PROCEDURE: The method of appearance and disappearance of turbidity described in ref 1 was used. No details were reported in the paper. SURCE AND PURITY OF MATERIALS: (1) Naarden and Co.; used as recived; π^{30} 1.4245, d^{30} 0.8215 g/mL. (2) distilled; free from carbon dioxide. ESTIMATED ERROR: Not specified. REFERENCES: 1. Othmer, D.F.; White, R.E.; Trueger, E.		
The corresponding mole fraction, x_1 , calculated by the compiler is 0.0001. The solubility of water in 1-octanol at 30°C was reported to be 4.6 g(2)/100g sln. The corresponding mole fraction, x_2 , calculated by the compiler is 0.268. METHOD/APPARATUS/PROCEDURE: The method of appearance and disappearance of turbidity described in ref 1 was used. No details were reported in the paper. SOURCE AND PURITY OF MATERIALS: (1) Naarden and Co.; urbidity described in ref 1 was used. No details were reported in the paper. (2) distilled; free from carbon dioxide. ESTIMATED ERROR: Not specified. REFERENCES: 1. Othmer, D.F.; White, R.E.; Trueger, E.	EXPERIMENTAL VALUES:	
AUXILIARY INFORMATION METHOD/APPARATUS/PROCEDURE: The method of appearance and disappearance of turbidity described in ref 1 was used. No details were reported in the paper. SOURCE AND PURITY OF MATERIALS: (1) Naarden and Co.; x^{30} 1.4245, d^{30} 0.8215 g/mL. (2) distilled; free from carbon dioxide. ESTIMATED ERROR: Not specified. REFERENCES: 1. Othmer, D.F.; White, R.E.; Trueger, E.	The solubility of 1-octanol in water at 30° C	was reported to be 0.1 $g(1)/100g \ sln$.
AUXILIARY INFORMATION METHOD/APPARATUS/PROCEDURE: The method of appearance and disappearance of turbidity described in ref 1 was used. No details were reported in the paper. SOURCE AND PURITY OF MATERIALS: (1) Naarden and Co.; x^{30} 1.4245, d^{30} 0.8215 g/mL. (2) distilled; free from carbon dioxide. ESTIMATED ERROR: Not specified. REFERENCES: 1. Othmer, D.F.; White, R.E.; Trueger, E.	The corresponding mole fraction, x_1 , calcula	ted by the compiler is 0.0001.
AUXILIARY INFORMATION METHOD/APPARATUS/PROCEDURE: The method of appearance and disappearance of turbidity described in ref 1 was used. No details were reported in the paper. SURCE AND PURITY OF MATERIALS: (1) Naarden and Co.; used as recived; n ³⁰ 1.4245, d ³⁰ 0.8215 g/mL. (2) distilled; free from carbon dioxide. ESTIMATED ERROR: Not specified. REFERENCES: 1. Othmer, D.F.; White, R.E.; Trueger, E.	1 · · · ·	
AUXILIARY INFORMATION METHOD/APPARATUS/PROCEDURE: The method of appearance and disappearance of turbidity described in ref 1 was used. No details were reported in the paper. SURCE AND PURITY OF MATERIALS: (1) Naarden and Co.; used as recived; n ³⁰ 1.4245, d ³⁰ 0.8215 g/mL. (2) distilled; free from carbon dioxide. ESTIMATED ERROR: Not specified. REFERENCES: 1. Othmer, D.F.; White, R.E.; Trueger, E.		
AUXILIARY INFORMATION METHOD/APPARATUS/PROCEDURE: The method of appearance and disappearance of turbidity described in ref 1 was used. No details were reported in the paper. Source AND PURITY OF MATERIALS: (1) Naarden and Co.; used as recived; n ³⁰ 1.4245, d ³⁰ 0.8215 g/mL. (2) distilled; free from carbon dioxide. ESTIMATED ERROR: Not specified. REFERENCES: 1. Othmer, D.F.; White, R.E.; Trueger, E.	The solubility of water in 1-octanol at 30 C	was reported to be 4.6 g(2)/100g sin.
METHOD/APPARATUS/PROCEDURE: SOURCE AND PURITY OF MATERIALS: The method of appearance and disappearance of turbidity described in ref 1 was used. No details were reported in the paper. No details were reported in the paper. (1) Naarden and Co.; used as recived; n ³⁰ 1.4245, d ³⁰ 0.8215 g/mL. (2) distilled; free from carbon dioxide. ESTIMATED ERROR: Not specified. REFERENCES: 1. Othmer, D.F.; White, R.E.; Trueger, E.	The corresponding mole fraction, x_2 , calcula	ted by the compiler is 0.268.
METHOD/APPARATUS/PROCEDURE: SOURCE AND PURITY OF MATERIALS: The method of appearance and disappearance of turbidity described in ref 1 was used. No details were reported in the paper. No details were reported in the paper. (1) Naarden and Co.; used as recived; n ³⁰ 1.4245, d ³⁰ 0.8215 g/mL. (2) distilled; free from carbon dioxide. ESTIMATED ERROR: Not specified. REFERENCES: 1. Othmer, D.F.; White, R.E.; Trueger, E.		
METHOD/APPARATUS/PROCEDURE: SOURCE AND PURITY OF MATERIALS: The method of appearance and disappearance of turbidity described in ref 1 was used. No details were reported in the paper. No details were reported in the paper. (1) Naarden and Co.; used as recived; n ³⁰ 1.4245, d ³⁰ 0.8215 g/mL. (2) distilled; free from carbon dioxide. ESTIMATED ERROR: Not specified. REFERENCES: 1. Othmer, D.F.; White, R.E.; Trueger, E.		
METHOD/APPARATUS/PROCEDURE: SOURCE AND PURITY OF MATERIALS: The method of appearance and disappearance of turbidity described in ref 1 was used. No details were reported in the paper. No details were reported in the paper. (1) Naarden and Co.; used as recived; n ³⁰ 1.4245, d ³⁰ 0.8215 g/mL. (2) distilled; free from carbon dioxide. ESTIMATED ERROR: Not specified. REFERENCES: 1. Othmer, D.F.; White, R.E.; Trueger, E.		
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METHOD/APPARATUS/PROCEDURE: SOURCE AND PURITY OF MATERIALS: The method of appearance and disappearance of turbidity described in ref 1 was used. No details were reported in the paper. No details were reported in the paper. (1) Naarden and Co.; used as recived; n ³⁰ 1.4245, d ³⁰ 0.8215 g/mL. (2) distilled; free from carbon dioxide. ESTIMATED ERROR: Not specified. REFERENCES: 1. Othmer, D.F.; White, R.E.; Trueger, E.		
METHOD/APPARATUS/PROCEDURE: SOURCE AND PURITY OF MATERIALS: The method of appearance and disappearance of turbidity described in ref 1 was used. No details were reported in the paper. No details were reported in the paper. (1) Naarden and Co.; used as recived; n ³⁰ 1.4245, d ³⁰ 0.8215 g/mL. (2) distilled; free from carbon dioxide. ESTIMATED ERROR: Not specified. REFERENCES: 1. Othmer, D.F.; White, R.E.; Trueger, E.		
METHOD/APPARATUS/PROCEDURE: SOURCE AND PURITY OF MATERIALS: The method of appearance and disappearance of turbidity described in ref 1 was used. No details were reported in the paper. No details were reported in the paper. (1) Naarden and Co.; used as recived; n ³⁰ 1.4245, d ³⁰ 0.8215 g/mL. (2) distilled; free from carbon dioxide. ESTIMATED ERROR: Not specified. REFERENCES: 1. Othmer, D.F.; White, R.E.; Trueger, E.		
METHOD/APPARATUS/PROCEDURE: SOURCE AND PURITY OF MATERIALS: The method of appearance and disappearance of turbidity described in ref 1 was used. No details were reported in the paper. No details were reported in the paper. (1) Naarden and Co.; used as recived; n ³⁰ 1.4245, d ³⁰ 0.8215 g/mL. (2) distilled; free from carbon dioxide. ESTIMATED ERROR: Not specified. REFERENCES: 1. Othmer, D.F.; White, R.E.; Trueger, E.		
METHOD/APPARATUS/PROCEDURE: SOURCE AND PURITY OF MATERIALS: The method of appearance and disappearance of turbidity described in ref 1 was used. No details were reported in the paper. No details were reported in the paper. (1) Naarden and Co.; used as recived; n ³⁰ 1.4245, d ³⁰ 0.8215 g/mL. (2) distilled; free from carbon dioxide. ESTIMATED ERROR: Not specified. REFERENCES: 1. Othmer, D.F.; White, R.E.; Trueger, E.		
METHOD/APPARATUS/PROCEDURE: SOURCE AND PURITY OF MATERIALS: The method of appearance and disappearance of turbidity described in ref 1 was used. No details were reported in the paper. No details were reported in the paper. (1) Naarden and Co.; used as recived; n ³⁰ 1.4245, d ³⁰ 0.8215 g/mL. (2) distilled; free from carbon dioxide. ESTIMATED ERROR: Not specified. REFERENCES: 1. Othmer, D.F.; White, R.E.; Trueger, E.		
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METHOD/APPARATUS/PROCEDURE: SOURCE AND PURITY OF MATERIALS: The method of appearance and disappearance of turbidity described in ref 1 was used. No details were reported in the paper. No details were reported in the paper. (1) Naarden and Co.; used as recived; n ³⁰ 1.4245, d ³⁰ 0.8215 g/mL. (2) distilled; free from carbon dioxide. ESTIMATED ERROR: Not specified. REFERENCES: 1. Othmer, D.F.; White, R.E.; Trueger, E.	······································	
The method of appearance and disappearance of turbidity described in ref 1 was used. No details were reported in the paper. (1) Naarden and Co.; used as recived; n^{30} 1.4245, d^{30} 0.8215 g/mL. (2) distilled; free from carbon dioxide. ESTIMATED ERROR: Not specified. REFERENCES: 1. Othmer, D.F.; White, R.E.; Trueger, E.	AUXILIARY	INFORMATION
of turbidity described in ref 1 was used. No details were reported in the paper. (2) distilled; free from carbon dioxide. ESTIMATED ERROR: Not specified. REFERENCES: 1. Othmer, D.F.; White, R.E.; Trueger, E.	METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
No details were reported in the paper. (2) distilled; free from carbon dioxide. ESTIMATED ERROR: Not specified. REFERENCES: 1. Othmer, D.F.; White, R.E.; Trueger, E.		
<pre>(2) distilled; free from carbon dioxide.</pre> (2) distilled; free from carbon dioxide. ESTIMATED ERROR: Not specified. REFERENCES: 1. Othmer, D.F.; White, R.E.; Trueger, E.	of turbidity described in fer 1 was used.	
free from carbon dioxide. ESTIMATED ERROR: Not specified. REFERENCES: 1. Othmer, D.F.; White, R.E.; Trueger, E.	No details were reported in the paper.	
ESTIMATED ERROR: Not specified. REFERENCES: 1. Othmer, D.F.; White, R.E.; Trueger, E.		
Not specified. REFERENCES: 1. Othmer, D.F.; White, R.E.; Trueger, E.		
Not specified. REFERENCES: 1. Othmer, D.F.; White, R.E.; Trueger, E.		
Not specified. REFERENCES: 1. Othmer, D.F.; White, R.E.; Trueger, E.		
Not specified. REFERENCES: 1. Othmer, D.F.; White, R.E.; Trueger, E.		ESTIMATED EDDOD.
REFERENCES: 1. Othmer, D.F.; White, R.E.; Trueger, E.		
1. Othmer, D.F.; White, R.E.; Trueger, E.		Not specified.
1. Othmer, D.F.; White, R.E.; Trueger, E.		
		REFERENCES:
1741. Ery, Orteni, <u>1741</u> , 55, 1240.		
		1741. Dray. Orkent. <u>1741</u> , 00, 1240.

COMPONENTS:	ORIGINAL MEASUREMENTS:
 (1) 1-Octanol (<i>capryl alcohol</i>); C₈H₁₈O; [111-87-5] (2) Water; H₂O; [7732-18-5] 	Vochten, R.; Petre, G. J. Colloid Interface Sci. <u>1973</u> , 42, 320-7
VARIABLES:	PREPARED BY:
One temperature: 15°C	S.H. Yalkowsky; S.C. Valvani; A.F.M. Barton

The equilibrium concentration of 1-octanol (1) in the water-rich phase at 15° C was reported to be 0.0041 mol(1)/L.

The corresponding mass percentage solubility, calculated by the compilers with the assumption of a solution density equal to that of water, is 0.053 g(1)/100g sln, and the mole fraction solubility is $10^5 x_1 = 7.3$.

AUXILIARY	INFORMATION
METHOD/APPARATUS/PROCEDURE: The solubility was obtained from the surface tension of saturated solutions, measured by the static method of Wilhelmy (platinum plate). The apparatus consisted of an electrobalance (R.G. Cahn) connected with a high impedance null detector (Fluke type 845 AR). An all-Pyrex vessel was used.	 SOURCE AND PURITY OF MATERIALS: (1) purified by distillation and preparative gas chromatography; b.p. 195.0°C/760 mm Hg (2) triply distilled from permanganate solution.
	ESTIMATED ERROR: Temperature: ± 0.1°C Solubility: (probably standard deviation) ± 0.0001 mol(1) L ⁻¹ sln. REFERENCES:

COMPONENTS:			ORIGIN	AL MEASUREMENTS:	
(1) 1-Octanol (capryl alcohol); C ₈ H ₁₈ 0;		Lavro	va, O.A.; Lesteva	, T.M.	
[111-87-	-5]	8"18",	Zh. F	iz. Khim., 1976, 5	60, 1617; Dep. Doc.
(2) Water;	H ₂ 0; [7732-18-5]			I, 3813-75.	
VARIABLES:	······································		PREPAR	RED BY:	
Temperature:	40 and 60 ⁰ C		A. Ma	czynski	
EXPERIMENTAL					
	Mutual	solubility of	l-octa	nol (1) and water	(2)
t/°c	g(1)/10	00g sln		x_1 (compiler)
	(2)-rich phase	(1)-rich pha	se	(2)-rich phase	(1)-rich phase
40	0.06	94.90		0.00008	0.720
60	0.06	94.0		0.00008	0.685
					•
		AUXILIARY	INFORM	ATION	
METHOD/APPARA	ATUS/PROCEDURE:		SOURC	E AND PURITY OF MA	TERIALS:
The titrati	on method was used.		(1)		
N- 1-5-41-				distilled with he	eptane; %, 0.03 wt % of water,
No details	were reported in th	e paper.	i		
				$n_{\rm D}^{20}$ 1.4291, d_4^{20}	0.8148
				b.p. 195.0°C.	
				-	
			(2)	not specified.	
ļ					
			ESTIN	ATED ERROR:	
				Not specified.	
			REFE	RENCES :	<u></u>
1			1		

COMPONENTS:	ORIGINAL MEASUREMENTS:
<pre>(1) 1-Octanol (capryl alcohol); C₈H₁₈0; [111-87-5]</pre>	Zhuravleva, I.K.; Zhuravlev, E.F.; Lomakina, N.G.
(2) Water; H ₂ O; [7732-18-5]	*Zh. Fiz. Khim. <u>1977</u> , 51, 1700-7;
	Russ. J. Phys. Chem. <u>1977</u> , 51, 994–8.
VARIABLES:	PREPARED BY:
Temperature: 7-115 ⁰ C	A. Maczynski
EXPERIMENTAL VALUES:	
Solubility of wa	ter (2) in l-octanol (1)
t/ ^o C g(2)/100g s1	n $x_2(\text{compiler})$
7.0 2.5	0.15
23.0 3.5	0.21
35.0 4.0	0.23
52.0 5.0	0.28
74.0 6.0	0.32
Solubility of 1-	octanol(l) in water (2)
	2
95.0 1.0 115.0 0.5	0.001
AUXILIARY	INFORMATION
METHOD / APPARATUS / PROCEDURE :	SOURCE AND PURITY OF MATERIALS:
The "polythermic" method (ref 1) was used. No details were reported in the paper. The results formed part of a report on the ternary system including nitromethane.	 source not specified; purity not specified, n_D²⁰ 1.4395, d²⁰ 0.8240 n_D²⁰ 1.333.
	ESTIMATED ERROR: Not specified. REFERENCES: 1. Alekseev, W.F. Zh. russk. khim. o-va, <u>1876</u> , 8, 249.

		OPTOTNAL MEAG	UDEMENTO .			
COMPONENTS: (1) 1-Octanol (<i>capryl alcohol)</i> ; C ₈ H ₁₈ O; [111-87-5] (2) Water; H ₂ O; [7732-18-5] VARIABLES: Temperature: 15-40 [°] C		Tokunaga, S. Niihama Kogy Rikogaku Hen	ORIGINAL MEASUREMENTS: Tokunaga, S.; Manabe, M.; Koda, M. Niihama Kogyo Koto Semmon Gakko Kiyo, Rikogaku Hen (Memoirs Niihama Technical College, Sci. and Eng.) <u>1980</u> , 16, 96-101. PREPARED BY: A.F.M. Barton			
		PREPARED BY:				
		A.F.M. Bart				
EXPERIMENTAL VA	LUES:		···· · · · · · · · · · · · · · · · · ·			
	Proportion of water (2)	in the alcohol-	-rich phase			
t∕°c	g(2)/100g sln	<i>x</i> 2	mol(1)/mol(2)			
15	4.68	0.262	2.82			
20	4.75	0.265	2.78			
25	4.78	0.266	2.75			
30	4.81	0.267	2.72			
35 40	4.88 4.93	0.271 0.273	2.70 2.67			
	AUXILIA	Y INFORMATION				
METHOD /APPARAT			PURITY OF MATERIALS;			
The mixtures (~10 mL) wer stoppered ves 10-12 h in a	US/PROCEDURE: of 1-octanol (~5 mL) and wat e stirred magnetically in a sel and allowed to stand for water thermostat. The phase was analyzed for water	SOURCE AND F er (1) distill no impu chromot (2) deioniz	.ed; mities detectable by gas cography			

COMPONENTS:	EVALUATOR:
(1) 2-Octanol; C ₈ H ₁₈ O; [123-96-6]	A.Maczynski, Institute of Physical Chemistry
(2) Water; H ₂ 0; [7732-18-5]	of the Polish Academy of Sciences, Warsaw,
.,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,	Poland; A.F.M. Barton, Murdoch University,
	Perth, Western Australia.
	November 1982

CRITICAL EVALUATION:

The proportion of 2-octanol (1) in the water-rich phase has been reported in three publications: Mitchell (ref 1) at 288 K and 298 K by an interferometric method; Addison (ref 2) at 293 K from surface tension measurements; and Crittenden and Hixon (ref 3) at 298 K, presumably by a titration method. The values in refs 1 and 2 are in reasonable agreement, but about one-third of those reported in ref 3. Since the data of Crittenden and Hixon (ref 3) is the most recent, because their results for other systems appear reliable, and because the earlier works identified the alcohol only as "sec-octyl alcohol", the measurement at 298 K of ref 3 is selected as the tentative value.

The tentative value for the solubility of 2-octanol in water at 298 K is 0.4 g(1)/100g sln $x_1 = 6 \times 10^{-4}$

The proportion of water (2) in the alcohol-rich phase has been measured only by Crittenden and Hixon (ref 3).

The tentative value for the solubility of water in 2-octanol at 298 K is 3.7 g(2)/100g sln or $x_2 = 0.22$.

References

- 1. Mitchell, S. J. Chem. Soc. <u>1926</u>, 1333.
- 2. Addison, C.C. J. Chem. Soc. 1945, 98.
- 3. Crittenden, E.D., Jr.; Hixon, A.N. Ind. Eng. Chem. 1954, 46, 265.

2-Octanol

COMPONENTS :		ORIGINAL MEASUREMENTS:	
(1) 2-Octanol; C ₈ H ₁₈ O;	[123-96-6]	Mitchell S.;	
(identified in thi	s publication only	J. Chem. Soc. <u>1926</u> , 133	3-6.
as sec-octyl alcoh			
(2) Water; H ₂ 0; [7732			
2			
VARIABLES:		PREPARED BY:	
Temperature: 15°C and 25°C		S.H. Yalkowsky; S.C. Va	lvni; A.F.M. Barton
EXPERIMENTAL VALUES:		L	
S	olubility of <i>sec</i> -octyl	alcohol (1) in water-ric	h phase
t/ ^o c	g(1)/L sln	10 ³ mol (1) (compilers)	g(1)/100 g sln (compilers) ^a
15	1.508	11.6	0.15
25	1.280	9.8	0.13
	AUXILIAR	· INFORMATION	
METHOD/APPARATUS/PROCE		INFORMATION SOURCE AND PURITY OF MA	TERIALS:
METHOD/APPARATUS/PROCEI An interferometric me of % saturation agains was linear, and the co saturated solution cou extrapolation.	DURE: thod was used. A plo t compensator reading mposition of the	SOURCE AND PURITY OF MA	TERIALS :
An interferometric me of % saturation agains was linear, and the co saturated solution cou	DURE: thod was used. A plo t compensator reading mposition of the	SOURCE AND PURITY OF MA	TERIALS:
An interferometric me of % saturation agains was linear, and the co saturated solution cou	DURE: thod was used. A plo t compensator reading mposition of the	SOURCE AND PURITY OF MA	TERIALS :
An interferometric me of % saturation agains was linear, and the co saturated solution cou	DURE: thod was used. A plo t compensator reading mposition of the	SOURCE AND PURITY OF MA	TERIALS :
An interferometric me of % saturation agains was linear, and the co saturated solution cou	DURE: thod was used. A plo t compensator reading mposition of the	SOURCE AND PURITY OF MA Not stated ESTIMATED ERROR:	TERIALS :
An interferometric me of % saturation agains was linear, and the co saturated solution cou	DURE: thod was used. A plo t compensator reading mposition of the	SOURCE AND PURITY OF MA Not stated ESTIMATED ERROR:	TERIALS :
An interferometric me of % saturation agains was linear, and the co saturated solution cou	DURE: thod was used. A plo t compensator reading mposition of the	SOURCE AND PURITY OF MA Not stated ESTIMATED ERROR: Not stated	TERIALS :
An interferometric me of % saturation agains was linear, and the co saturated solution cou	DURE: thod was used. A plo t compensator reading mposition of the	SOURCE AND PURITY OF MA Not stated ESTIMATED ERROR: Not stated	TERIALS :

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) 2-Octanol; C ₈ H ₁₈ 0; [123-96-6]	Addison, C.C.
(identified in this publication only as	J. Chem. Soc. <u>1945</u> , 98-106.
sec-octyl alcohol)	
(2) Water; H ₂ 0; [7732-18-5]	
2	
VARIABLES:	PREPARED BY:
0	
One temperature: 20 [°] C	S.H. Yalkowsky; S.C. Valvani; A.F.M. Barton
EXPERIMENTAL VALUES:	
The proportion of sec-octyl alcohol (1) in th	e water-rich phase at equilibrium at
20° C was reported to be 0.106 g(1)/100g sln.	
The corresponding mole fraction solubility, c	alculated by the compilers, is 10 $x_1 = 1.46$.
	INFORMATION
METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
The surface tension method was used,	(1) impure alcohols were purified by
Sufficient excess of (1) was added to 100 mL	fractional distillation, the middle fraction from a distillation being
of (2) in a stoppered flask to form a separate lens on the surface. The mixture	redistilled;
was swirled gently, too vigorous an agitation	b.p. 178.0°C d_{L}^{20} 0.8200
being avoided as this gave a semi-permanent emulsion and incorrect readings. After	
settling, a small sample of the clear	$n_{\rm D}^{20}$ 1.4255
aqueous sln was withdrawn into a drop weight pipet and the surface tension determined.	
The swirling was continued until a constant	(2) not stated
value was obtained. The surface tension- concentration curve was known, and only a	ESTIMATED ERROR:
slight extrapolation (logarithmic scale) was	c_{-1} b_{-1} b
necessary to find the concentration corresponding to the equilibrium value.	Solubility: ± 0.5%
	REFERENCES :
L	

2-Octanol

COMPONENTS:	ORIGINAL MEASUREMENTS:
	CRICIAL FERBULFERIS.
(1) 2-Octanol; C ₈ H ₁₈ 0; [123-96-6]	Crittenden, E.D., Jr.; Hixon, A.N.;
	Ind. Eng. Chem. <u>1954</u> , 46, 265–8.
(2) Water; H ₂ 0; [7732-18-5]	
VARIABLES:	PREPARED BY:
One temperature: 25 [°] C	A. Maczynski
	-
EXPERIMENTAL VALUES:	
The solubility of 2-octanol in water at 25 [°] C	was reported to be 0.4 g(1)/100g sln.
The corresponding mole fraction, x_1 , calcula	
The corresponding more fraction, x_1 , carcula	ted by the compiler is 0.0000.
The solubility of water in 2-octanol at 25 ⁰ C	was reported to be 3.7 g(2)/100 sln.
The corresponding mole fraction, x_2 , calcula	ted by the compiler is 0.22.
_	
	INFORMATION
	· · · · · · · · · · · · · · · · · · ·
METHOD / APPARATUS / PROCEDURE :	SOURCE AND PURITY OF MATERIALS:
Presumably the titration method described for ternary systems containing HCl was used.	(1) source not specified; purified;
In this method the solubility was determined	
by bringing 100-mL samples of (1) or (2) to a temperature of $25.0 \pm 0.1^{\circ}$ C and the second	(2) not specified.
component was then added from a calibrated	
buret, with vigorous stirring, until the solution became permanently cloudy.	
	ESTIMATED ERROR:
	Temperature: ± 0.10
	REFERENCES:
	ALL DALADED.

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COMPONENTS:	ORIGINAL MEASUREMENTS:
<pre>(1) 2,2-Diethyl-1-pentanol; C₉H₂₀0; [14202-62-1] (2) Water; H₂0; [7732-18-5]</pre>	Vochten, R.; Petre, G. J. Colloid Interface Sci. <u>1973</u> , 42, 320-7.
VARIABLES:	PREPARED BY:
One temperature: 15 ⁰ C	S.H. Yalkowsky; S.C. Valvani; A.F.M. Barton

The equilibrium concentration of 2,2-diethyl-1-pentanol (1) in the water-rich phase at 15° C was reported to be 0.0038 mol(1)/L sln.

The corresponding mass percentage solubility, calculated by the compilers with the assumption of a solution density equal to that of water, is 0.055 g(1)/100g sln, and the mole fraction solubility is $10^5 x_1 = 6.8$.

AUXILIARY	INFORMATION
METHOD/APPARATUS/PROCEDURE: The solubility was obtained from the surface tension of saturated solutions, measured by the static method of Wilhelmy (platinum plate). The apparatus consisted of an electrobalance (R.G. Cahn) connected with a high impedance null detector (Fluke type AR). An all-Pyrex vessel was used.	 SOURCE AND PURITY OF MATERIALS: (1) purified by distillation and preparative gas chromatography; b.p. 192.0°C/760 mm Hg (2) triply distilled from permanganate solution
	ESTIMATED ERROR: Temperature: ± 0.1 ^o C Solubility: (probably standard deviation) ± 0.0001 mol(1)/L sln. REFERENCES:

COMPONENTS:	EVALUATOR:		
 2,6-Dimethyl-4-heptanol; C₉H₂₀0; 	A. Maczynski, Institute of Physical Chemistry		
[108-82-7]	of the Polish Academy of Sciences, Warsaw,		
(2) Water; H ₂ 0; [7732-18-5]	Poland.		
(2) water, "2°, [7752 10 5]	November 1982		

CRITICAL EVALUATION:

The solubilities of 2,6-dimethyl-4-heptanol (1) and water (2) have been reported in two publications. Crittenden and Hixon (ref 1) determined the mutual solubilities at 298 K, presumably by the titration method, Vochten and Petre (ref 2) determined the proportion of (1) in the water-rich phase at 288 K from surface tension measurements. Data from the two references cannot be compared directly, and the information should be regarded as very tentative.

Tentative	values	of	the	mut	ual		Lubilit	ies:	of
2,6-dime	ethy1-4	-her	otand	51 ((1)	and	water	(2)	

T/K	g(1)/100g sln		<i>x</i> ₁	
	water-rich phase	alcohol-rich phase	water-rich phase	alcohol-rich phase
288	0.05	-	0.00006	-
298	0.1	99.0	0.0001	0.93

References

1. Crittenden, E.D., Jr.; Hixon, A.N. Ind. Eng. Chem. 1954, 46, 265.

2. Vochten, R.; Petre, G. J. Colloid Interface Sci. 1973, 42, 320.

COMPONENTS:	ORIGINAL MEASUREMENTS:
CONFORCEMENTS.	ORIGINAL FERSOREFENIS.
(1) 2,6-Dimethyl-4-heptanol; C ₉ H ₂₀ O;	Crittenden, E.D., Jr., Hixon, A.N.
[108-82-7]	Ind. Eng. Chem. <u>1954</u> , 46, 265-8.
	Ind. Ing. Onem. <u>1754</u> , 1 0, 205-0.
(2) Water; H ₂ O; [7732-18-5]	
VARIABLES:	PREPARED BY:
One temperature: 25 [°] C	A. Maczynski
EXPERIMENTAL VALUES:	
The solubility of 2,6-dimethyl-4-heptanol in	water at 25° C was reported to be 0.1 g(1)/
100 sln.	
The corresponding mole fraction, x_1 , calcula	ted by the compiler is 0.0001.
The solubility of water in 2,6-dimethyl-4-he	ptanol at 25 ⁰ C was reported to be
1.0 g(2)/100g sln.	
The corresponding mole fraction, x_{2} , calcula	ted by the compiler is 0.07.
2	
AUXILIARY	INFORMATION
METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS;
Presumably the titration method described	(1) source not specified;
for ternary systems containing HCl was used. In this method the solubility was determined	purified; purity not specified.
by bringing 100-ml samples of (1) or (2) to a temperature of 25.0 ± 0.1 C and the second	(2) not specified.
component was then added from a calibrated	
buret, with vigorous stirring, until the solution became permanently cloudy.	
	ESTIMATED ERROR:
	Temperature: ± 0.10 [°]
	REFERENCES :

COMPONENTS:	ORIGINAL MEASUREMENTS:
 (1) 2,6-Dimethyl-4-heptanol; C₉H₂₀O; [108-82-7] (2) Water; H₂O; [7732-18-5] 	Vochten, R.; Petre, G. J. Colloid Interface Sci. <u>1973</u> , 42, 320-7.
VARIABLES:	PREPARED BY:
One temperature: 15 [°] C	S.H. Yalkowsky; S.C. Valvani; A.F.M. Barton

The equilibrium concentration of 2,6-dimethyl-4-heptanol (1) in the water-rich phase at 15° C was reported to be 0.0031 mol(1)/L sln.

The corresponding mass percentage solubility, calculated by the compilers, with the assumption of a solution density equal to that of water, is 0.045 g(1)/100g sln, and the mole fraction solubility is $x_1 = 5.6 \times 10^{-5}$.

AUXILIARY	AUXILIARY INFORMATION		
METHOD/APPARATUS/PROCEDURE: The solubility was obtained from the surface tension of saturated solutions, measured by the static method of Wilhelmy (platinum plate). The apparatus consisted of an electrobalance (R.G. Cahn) connected with a high impedance null detector (Fluke type 845 AR). An all-Pyrex vessel was used.	 SOURCE AND PURITY OF MATERIALS: (1) purified by distillation and preparative gas chromatography; b.p. 178.0°C/760 mm Hg (2) triply distilled from permanganate solution 		
	ESTIMATED ERROR: Temperature: ± 0.1 [°] C Solubility: (probably standard deviation) ± 0.0001 mol(1)/L sln. REFERENCES:		

COMPONENTS:	ORIGINAL MEASUREMENTS:
 (1) 3,5-Dimethyl-4-heptanol; C₉H₂₀0;	Vochten, R.; Petre, G.
19549-79-2 (2) Water; H₂0; 7732-18-5	J. Colloid Interface Sci. <u>1973</u> , 42, 320-7.
VARIABLES:	PREPARED BY:
One temperature: 15 [°] C	S.H. Yalkowsky; S.C. Valvani; A.F.M. Barton

The equilibrium concentration of 3,5-dimethyl-4-heptanol (1) in the water-rich phase at 15° C was reported to be 0.0050 mol(1)/L sln.

The corresponding mass percentage solubility, calculated by the compilers with the assumption of a solution density equal to that of water, is 0.072 g(1)/100g sln, and the mole fraction solubility is $x_1 = 8.9 \times 10^{-5}$.

ATIVELEADV	INFORMATION
AUAILIARI	INFURMATION

SOURCE AND PURITY OF MATERIALS:
 purified by distillation and preparative gas chromatography; b.p. 171.0^oC/760 mm Hg triply distilled from permanganate solution
ESTIMATED ERROR:
Temperature: ± 0.1 [°] C
Solubility: (probably standard deviation) ± 0.0001 mol(1)/L sln.
REFERENCES :

COMPONENTS:	ORIGINAL MEASUREMENTS:	
 7-Methyl-1-octanol; C₉H₂₀0; 	Vochten, R.; Petre, G.	
[2430-22-0]	J. Colloid Interface Sci. <u>1973</u> , 42, 320-7.	
(2) Water; H ₂ 0; [7732-18-5]		
VARIABLES:	PREPARED BY:	
One temperature: 15 ⁰ C	S.H. Yalkowsky; S.C. Valvani; A.F.M. Barton	
EXPERIMENTAL VALUES:		
The equilibrium concentration of 7-methyl-l-octanol (1) in the water-rich phase at 15° C was reported to be 0.0032 mol(1)/L sln.		
The corresponding mass percentage solubility calculated by the compilers with the		
assumption of a solution density equal to that of water, is 0.046 g(1)/100g sln, and the mole fraction solubility is $x_1 = 5.7 \times 10^{-5}$.		

AUXILIARY INFORMATION		
SOURCE AND PURITY OF MATERIALS:		
<pre>gas chromatography; b.p. 206.0^oC/760 mm Hg</pre>		
ESTIMATED ERROR:		
Temperature: $\pm 0.1^{\circ}C$		
Solubility: (probably standard deviation) ± 0.0001 mol(1)/L sln.		
REFERENCES :		

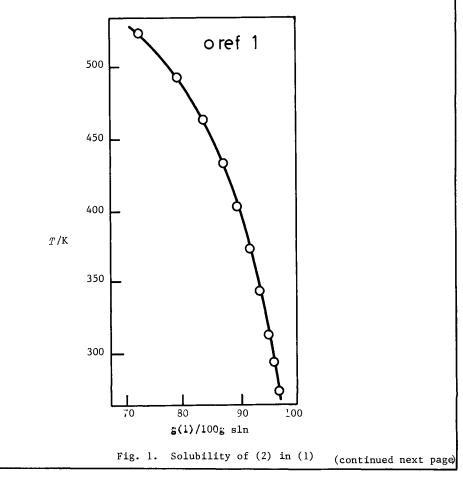
COMPONENTS:	EVALUATOR:
(1) 1-Nonanol (<i>n-nonyl alcohol</i>) C ₉ H ₂₀ O;	A.Maczynski, Institute of Physical Chemistry
[143-08-8]	of the Polish Academy of Sciences, Warsaw,
(2) Water; H ₂ 0; [7732-18-5]	Poland; A.F.M. Barton, Murdoch University,
	Perth, Western Australia
	November 1982

CRITICAL EVALUATION:

The proportion of 1-nonanol (1) in the water-rich phase was determined by Kinoshita *et al.* (ref 2) at 298 K and by Vochten and Petre (ref 3) at 288 K, both from surface tension measurements. The two values are consistent and the former agrees with that calculated from the equation correlating the solubilities at 298 K of normal aliphatic alcohols (equation 5 in the Editor's Preface), $\log (c/mol(1)/L \sin = 2.722 - 0.6988n + 0.006418n^2$, where *n* is the number of carbon atoms in the alcohol. This equation predicts for 1-nonanol 0.00090 mol(1)/L sln or 0.013 g(1)/100g sln.

The recommended value for the solubility of 1-nonanol in water at 298K is $1.0 \times 10^{-3} \text{ mol}(1)/\text{L}$ sln or 0.014 g(1)/100g sln.

The proportion of water (2) in the alcohol-rich phase has been reported by Erichsen (ref 1) over a large temperature range. The temperature dependence of these results in the 290-310 K range does not agree with the more recent work of Tokunaga *et al.* (ref 6), although the values agree at 293 K. Sazonov and Chernysheva (ref 4) provided only graphical data of the binary system, and details of the report of Zhuravleva *et al.* (ref 5) were unavailable to the evaluator. Erichsen's values form the basis of the tentative values (Figure 1).



1-Nonanol

COMPONENTS:	EVALUATOR:
 (1) 1-Nonanol (<i>n-nonyl alcohol</i>) C₉H₂₀0; [143-08-8] (2) Water; H₂0; [7732-18-5] 	A. Maczynski, Institute of Physical Chemistry of the Polish Academy of Sciences, Warsaw, Poland; A.F.M. Barton, Murdoch University, Perth, Western Australia. November 1982
CRITICAL EVALUATION: (continued)	
Tentative values of the solubility of water (2) in the 1-nonanol-rich phase	

<i>Т</i> /К	g(2)/100g sln	<i>x</i> 2
273	2.9	0.20
293	3.8	0.24
298	4.0	0,25
303	4.3	0.26
313	4.9	0.29
343	6.5	0.35
373	8.2	0.42
403	10.4	0.48
433	13	0.55
463	17	0.61
493	21	0.68
523	28	0.76

References

- 1. Erichsen, L. von Brennst. Chem. 1952, 33, 166.
- 2. Kinoshita, K.; Ishikawa, H.; Shinoda, K. Bull. Chem. Soc. Jpn. <u>1958</u>, 31, 1081.
- 3. Vochten, R.; Petre, G. J. Colloid Interface Sci. 1973, 42, 320.
- 4. Sazonov, V.P.; Chernysheva, M.F. Zh. Obshch. Khim. 1976, 46, 993.
- 5. Zhuravleva, I.K.; Zhuravlev, E.F.; Khotkovskaya, T.L. Zhur. Prikl. Khim. <u>1976</u>, 49, 2586; Dep. Doc. VINITI 1951-76.
- Tokunaga, S.; Manabe, M.; Koda, M. Niihama Kogyo Koto Semmon Gakko Kiyo, Rikogaku Hen (Memoirs Niihama Technical College, Sci and Eng.) <u>1980</u>, 16, 96.

COMPONENTS :	ORIGINAL MEASUREMENTS:
COM CADALD .	ONCOLNED PERSONEPENIS.
(1) 1-Nonanol; C ₉ H ₂₀ O; [143-08-8]	Erichsen, L. von
	Brennst. Chem. 1952, 33, 166-72.
(2) Water; H ₂ 0; [7732-18-5]	510/m/b/d 0/10/m 100/100 / 20
2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2	
VARIABLES:	PREPARED BY:
Temperature: 0-250°C	C. H. Vollesseler and Z. Massurale
Temperature: 0-250 C	S.H. Yalkowsky and Z. Maczynska
EXPERIMENTAL VALUES:	1 (1) in alcohol-rich phase
-	I (I) IN diconol lich phase
t/ ^o C g(1)/100g	$sln x_1$
0 97 05	0.8045
0 97.05 10 96.65	
20 96.20	
30 95.75	0.7370
40 95.10	
50 94.75	
60 94.25	
70 93.55 80 93.10	
90 92.50	
100 91.85	
110 90.95	
120 90.40	0.5410
130 89.65	
150 87.90 160 86.95	
170 85.90	
180 84.75	
190 83.50	
200 82.15	0.3650
210 80.80	
220 79.00	
230 77.10 240 74.95	
250 72.00	
AUXILIARY	INFORMATION
METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
The synthetic method was used.	(1) Merck, or Ciba, or industrial product;
The synthetic method was used.	distilled and chemical free from
The measurements were carried out in 2 mL	isomers;
glass ampules. These were placed in an	b.p. 214.7-214.8°C (762 mm Hg)
aluminium block equipped with two glass	$n_{\rm D}^{20}$ 1.4334.
windows. Cloud points were measured with	
a thermocouple wound up around the ampule. Each measurement was repeated twice.	(2) not specified.
Lach measurement was repeated twice.	
	ESTIMATED ERROR:
	Not specified.
l	
	DEFEDENCIA
	REFERENCES :
	1

COMPONENTS:	ORIGINAL MEASUREMENTS:	
(1) 1-Nonanol; C ₉ H ₂₀ 0; [143-08-8] (2) Water; H ₂ 0; [7732-18-5]	Kinoshita, K.; Ishikawa, H.; Shinoda, K. Bull. Chem. Soc. Jpn. <u>1958</u> , 31, 1081-4.	
VARIABLES:	PREPARED BY:	
One temperature: 25 [°] C	S.H. Yalkowsky; S.C. Valvani; A.F.M. Barton	
EXPERIMENTAL VALUES:		
The equilibrium concentration of 1-nonanol (1) in the water-rich phase at 25.0° C was reported to be 0.00097 mol(1)/L sln and the mass percentage solubility was reported		

The corresponding mole fraction solubility, calculated by the compilers, is $x_1 = 1.7 \times 10^{-5}$.

as 0.014 g(1)/100g sln.

AUXILIARY INFORMATION		
<pre>SOURCE AND PURITY OF MATERIALS: (1) laboratory preparation from nonanoic acid; purified by vacuum distillation through 50-100 cm column; b.p. 113-114.5°C/20 mm Hg (2) not stated (2) not stated ESTIMATED ERROR: Temperature: ± 0.05°C Solubility: within 4% REFERENCES: 1. Motylewski, S. Z. Anorg. Chem. 1904, 38, 410 2. Taubamann, A. Z Physik. Chem. 1932, A161, 141. 3. Zimmerman H.K., Jr. Chem. Rev. 1952, 51, 25.</pre>		

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) 1-Nonano1; C ₉ H ₂₀ 0; [143-08-8]	Vochten, R.; Petre, G. J. Colloid Interface Sci. 1973, 42, 320-7.
(2) Water; H ₂ 0; [7732-18-5]	J. COLLULA INCELJACE DEL. <u>1975</u> , 42, 520-7.
VARIABLES:	PREPARED BY:
One temperature; 15°C	S.H. Yalkowsky; S.C. Valvani; A.F.M. Barton
EXPERIMENTAL VALUES: The equilibrium concentration of 1-nonan reported to be 0.0010 mol(1)/L sln.	ol (1) in the water-rich phase at 15 ⁰ C was
	lity, calculated by the compilers with the so that of water, is $0.014 \text{ g}(1)/100 \text{g sln}$, 1.7×10^{-5} .

AUXILIARY	INFORMATION
METHOD/APPARATUS/PROCEDURE: The solubility was obtained from the surface tension of saturated solutions, measured by the static method of Wilhelmy (platinum plate). The apparatus consisted of an electrobalance (R.G. Cahn) connected with a high impedance null detector (Fluke type 845 AR). An all-Pyrex vessel was used.	<pre>SOURCE AND PURITY OF MATERIALS: (1) purified by distillation and preparative gas chromatography; b.p. 212.0°C/760 mm Hg (2) triply distilled from permangante solutions</pre>
	ESTIMATED ERROR: Temperature: ± 0.1°C Solubility (probably standard deviation) ± 0.0001 mol(1)/L sln. REFERENCES:

COMPONENTS:		ORIGINAL MEAS	UREMENTS:
(1) 1-Nonanol;	C ₉ H ₂₀ 0; [143-08-8]	Tokunaga, S.	; Manabe, M.; Koda, M.
(2) Water; H ₂ 0		Niihama Kogy	o Koto Semmon Gakko Kiyo,
Z			(Memoirs Niihama Technical
		College, Sci	. and Eng.) <u>1980</u> , 16, 96-101.
VARIABLES:		PREPARED BY:	
Temperature: 1	5-40 [°] C.	A.F.M. Bart	on
EXPERIMENTAL VAI	LUES :	<u></u> ,	
	Proportion of water (2) in	the alcohol-	rich phase
t∕°c	g(2)/100g sln	<i>x</i> ₂	mo1(1)/mo1(2)
15	4.25	0.262	2.81
20	4.27	0.263	2.80
25	4.31	0.265	2.78
30	4.32	0.265	2.77
35	4.36	0.267	2.76
40	4.32	0.265	2.75
	AUXILIARY	INFORMATION	
ME THOD / APPARATU	S/PROCEDURE:	SOURCE AND P	URITY OF MATERIALS:
	f l-nonanol (~ 5 mL) and water		
stoppered vesse	stirred magnetically in a 1 and allowed to stand for		urities detectable by gas tography
rich phase was	ter thermostat. The alcohol- analyzed for water by Karl	(2) deioni	
Fischer titrati	on.	distil	led prior to use
		ESTIMATED EN	
			e: $\pm 0.1^{\circ}$ C
		Solubility	: each result is the mean of three determinations
		REFERENCES:	
1		1	

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) 2-Nonanol; C ₉ H ₂₀ O; [628-99-9]	Vochten, R.; Petre, G.
(2) Water; H ₂ O; [7732-18-5]	J. Colloid Interface Sci. <u>1973</u> , 42, 320-7.
VARIABLES:	PREPARED BY:
One temperature: 15 [°] C	S.H. Yalkowsky; S.C. Valvani; A.F.M. Barton

The equilibrium concentration of 2-nonanol (1) in the water-rich phase at 15° C was reported to be 0.0018 mol(1)/L sln.

The corresponding mass percentage solubility, calculated by the compilers with the assumption of a solution density equal to that of water, is 0.026 g(1)/100g sln, and the mole fraction solubility is $x_1 = 3.2 \times 10^{-5}$.

AUXILIARY	INFORMATION
METHOD/APPARATUS/PROCEDURE: The solubility was obtained from the surface tension of saturated solutions, measured by the static method of Wilhelmy (platinum plate). The apparatus consisted of an electrobalance (R.G. Cahn) connected with a high impedance null detector (Fluke type 845 AR). An all-Pyrex vessel was used.	 SOURCE AND PURITY OF MATERIALS: (1) purified by distillation and preparative gas chromatography; b.p. 193.0°C/760mm Hg (2) triply distilled from permanganate solution
	ESTIMATED ERROR: Temperature: ± 0.1 ^o C Solubility (probably standard deviation): ± 0.0001 mol(1)/L sln . REFERENCES:

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) 3-Nonanol; C ₉ H ₂₀ 0; [624-51-1]	Vochten, R.; Petre, G.
(2) Water; H ₂ 0; [7732-18-5]	J. Colloid Interface Sci. <u>1973</u> , 42, 320-7.
VARIABLES:	PREPARED BY:
One temperature: 15 [°] C	S.H. Yalkowsky; S.C. Valvani; A.F.M. Barton
EXPERIMENTAL VALUES:	1
The equilibrium concentration of 3-nonanol (reported to be $0.0022 \text{ mol}(1)/L \text{ sln}$.	1) in the water-rich phase at 15 ⁰ C was
The corresponding mass percentage solubility, calculated by the compilers with the	

assumption of a solution density	y equal to that of water, is $0.032 g(1)/100g s$	1n,
and the mole fraction solubility	y is $x_1 = 3.9 \times 10^{-5}$.	

AUXILIARY	INFORMATION
METHOD/APPARATUS/PROCEDURE: The solubility was obtained from the surface tension of saturated solutions, measured by the static method of Wilhelmy (platinum plate). The apparatus consisted of an electrobalance (R.G. Cahn) connected with a high impedance null detector (Fluke type 845 AR). An all-Pyrex vessel was used.	 SOURCE AND PURITY OF MATERIALS: (1) purified by distillation and preparative gas chromatography; b.p. 194.5°C/760 mm Hg (2) triply distilled from permanganate solution
	ESTIMATED ERROR:
	Temperature: \pm 0.1°C Solubility (probably standard deviation): \pm 0.0001 mol(1)/L sln.
	REFERENCES :

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) 4-Nonanol; C ₉ H ₂₀ O; [5932-79-6]	Vochten, R.; Petre, G.
(2) Water; H ₂ O; [7732-18-5]	J. Colloid Interface Sci. <u>1973</u> , 42, 320-7.
VARIABLES:	PREPARED BY:
One temperature: 15 ⁰ C	S.H. Yalkowsky; S.C. Valvani; A.F.M. Barton

The equilibrium concentration of 4-nonanol (1) in the water-rich phase at 15° C was reported to be 0.0026 mol(1)/L sln.

The corresponding mass percentage solubility, calculated by the compilers with the assumption of a solution density equal to that of water, is 0.038 g(1)/100g sln, and the mole fraction solubility is $x_1 = 4.7 \times 10^{-5}$.

AUXILIARY	INFORMATION
METHOD/APPARATUS/PROCEDURE: The solubility was obtained from the surface tension of saturated solutions, measured by the static method of Wilhelmy (platinum plate). The apparatus consisted of an electrobalance (R.G. Cahn) connected with a high impedance null detector (Fluke type 845 AR). An all-Pyrex vessel was used.	 SOURCE AND PURITY OF MATERIALS: (1) purified by distillation and preparative gas chromatography; b.p. 192.0°C/760 mm Hg (2) triply distilled from permanganate solution
	ESTIMATED ERROR: Temperature: [±] 0.1 ^o C Solubility (probably standard deviation): <u>±</u> 0.0001 mol(1)/L sln. REFERENCES:

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) 5-Nonanol; ^C 9 ^H 20 ⁰ ; [623-93-8] (2) Water; H ₂ 0; [7732-18-5]	Vochten, R.; Petre, G. J. Colloid Interface Sci. <u>1973</u> , 42, 320-7.
VARIABLES:	PREPARED BY:
One temperature: 15 [°] C	S.H. Yalkowsky; S.C. Valvani; A.F.M. Barton
EXPERIMENTAL VALUES:	

The equilibrium concentration of 5-nonanol (1) in the water-rich phase at 15° C was reported to be 0.0032 mol(1)/L sln.

The corresponding mass percentage solubility, calculated by the compilers with the assumption of a solution density equal to that of water, is 0.046 g(1)/100g sln, and the mole fraction solubility is $x_1 = 5.7 \times 10^{-5}$.

	INFORMATION
METHOD/APPARATUS/PROCEDURE: The solubility was obtained from the surface tension of saturated solutions, measured by the static method of Wilhelmy (platinum plate). The apparatus consisted of an electrobalance (R.G. Cahn) connected with a high impedance null detector (Fluke type 845 AR). An all-Pyrex vessel was used.	 SOURCE AND PURITY OF MATERIALS: (1) purified by distillation and preparative gas chromatography; b.p. 193^oC/760 mm Hg (2) triply distilled from permanganate solution
	ESTIMATED ERROR: Temperature: ± 0.1°C
	Solubility (probably standard deviation): ± 0.0001 mol(1)/L sln.
	REFERENCES:

<u> </u>			
COMPONENTS:		EVALUATOR:	
(1) 1-Decanol; C ₁₀ H ₂₂ O; [112-30	-1]	. ,	itute of Physical Chem-
(2) Water; H ₂ 0; [7732-18-5]			h Academy of Sciences,
			nd A.F.M. Barton, Murdoch
		University, Perth,	western Australia.
		November 1982	
CRITICAL EVALUATION:			
The proportion of 1-decanol (1) in	the meter	rich phase has been	reported in air
publications:	the water	Tich phase has been h	reported in Six
Reference	Т/К	g(1)/100g sln	Method
Stearns et al. (ref 1)	298	0.005	turbidimetric
Addison and Hutchinson (ref 2)	293	0.0036	surface tension
Harkins and Oppenheimer (ref 3)	-	0.005	turbidimetric
Kinoshita et al.(ref 5)	298	0.0037	surface tension
Vochten and Petre (ref 6)	288	0.0032	surface tension
Zhuravleva et al. (ref 7)	375	1.0	polythermic
	394	0.8	1
	n the Edit - 0.6988n toms in th or 0.003 mutual agr for recomm only.	ors's Preface) is + 0.006418 n ² e alochol. This equa 8 g(1)/100g sln. eement, conform with s ended values. The har values of the solubil:	ation predicts for the results for other igher temperature values
T/K g(1)/	100g s1n		x_1
288 0	.0032	(recommended)	3.0×10^{-6}
293 0	.0036	(recommended)	3.8×10^{-6}
298 0	.0037	(recommended)	4.2×10^{-6}
375 1		(tentative)	1×10^{-3}
393 0	.8	(tentative)	9×10^{-4}
The proportion of water (2) in the phase has been reported in three p			ium with the water-rich
Reference	<i>Т</i> /К	Me	ethod
Erichsen (ref 4)	273-533	SVI	nthetic
Zhuravleva <i>et al.</i> (ref 7)		•	lythermic
Tokunaga et al. (ref 8)	288-313	-	alytical
The data of ref 4 span a wide temp three temperatures of ref 7 (alth been used as the basis for the fol	ough they	are not very consisten	-

(continued next page)

1-Decanol

COMPONENTS:	EVALUATOR:
(1) 1-Decanol; C ₁₀ H ₂₂ 0; [112-30-1]	A. Maczynski, Institute of Physical Chemistry of the Polisy Academy of Sciences,
(2) Water; H ₂ 0; [7732-18-5]	Warsaw, Poland; and A.F.M. Barton, Murdoch
	University, Perth, Western Australia.
	November 1982
CRITICAL EVALUATION: (continued)	

	Tentative values of the solubility of	water (2)
	in l-decanol-rich phase	
<i>Т</i> /К	g(2)/100g sln	<i>x</i> 2
273	2.6	0.19
293	3.4	0.24
298	3.6	0.25
313	4.2	0.28
333	5.1	0.33
353	6.1	0.37
373	7.3	0.41
393	8.6	0.45
413	10	0.50
433	12	0.54
453	14	0.58
473	16	0.63
493	19	0.67
513	23	0.72
523	25	0.75
533	28	0.77

References

- Stearns, R.S.; Oppenheimer, H.; Simon, E.; Harkins, W.D. J. Chem. Phys. <u>1947</u>, 15, 496.
- 2. Addison, C.C.; Hutchinson, S.K. J. Chem. Soc. 1949, 3387.
- 3. Harkins, W.D.; Oppenheimer, H. J. Am. Chem. Soc. <u>1949</u>, 71, 808.
- 4. Erichsen, L. von Brennst. Chem. 1952, 33, 166.
- 5. Kinoshita, K.; Ishikawa, H.; Shinoda, K. Bull. Chem. Soc. Jpn. <u>1958</u>, 31, 1081.
- 6. Vochten, R.; Petre, G. J. Colloid Interface Sci. 1973, 42, 320.
- 7. Zhuravleva, I.K.; Zhuravlev, E.F.; Lomakina, N.G. Zh. Fiz. Khim. 1977, 51, 1700.
- Tokunaga, S.; Manabe, M.; Koda, M. Niihama Kogyokota Semmon Gakko Kiyo, Rikogaku Hen (Memoirs Niihama Technical College, Sci. and Eng.) <u>1980</u>, 16, 96.

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) 1-Decanol; C ₁₀ H ₂₂ 0; [112-30-1]	Stearns, R.S.; Oppenheimer, H.; Simon, E.; Harkins, W.D.
(2) Water; H ₂ 0; [7732-18-5]	J. Chem. Phys. <u>1947</u> , 15, 496–507.
VARIABLES:	PREPARED BY:
One temperature: 25 [°] C	A. Maczynski
EXPERIMENTAL VALUES:	
The solubility of 1-decanol in water at 25 ± 3 The corresponding mole fraction, x_1 , calculate	
AUXILIARY	INFORMATION
METHOD / APPARATUS / PROCEDURE :	SOURCE AND PURITY OF MATERIALS:
The turbidimetric method was used. (A turbidimetric method in which a photometer	(1) not specified.
was used to determine turbidity in a soap solution was described in the paper but nothing was reported regarding the turbidity in water).	(2) not specified.
	ESTIMATED ERROR:
	Temperature $\pm 3^{\circ}$ C
	REFERENCES:

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) 1-Decanol; C ₁₀ H ₂₂ 0; [112-30-1]	Addison, C.C.; Hutchinson, S.K.
(2) Water; H ₂ 0; [7732-18-5]	J. Chem. Soc. <u>1949</u> , 3387-95.
Ζ	
VARIABLES:	PREPARED BY:
One temperature: 20°C	FREFARED DI:
	A.F.M. Barton
EXPERIMENTAL VALUES:	
	0
The proportion of 1-decanol (1) in the water-	rich phase at equilibrium at 20°C was
reported to be $0.0036 g(1)/100g sln.$,
The corresponding mole fraction solubility, c	alculated by the compilers, is $x_1 = 4.0 \times 10^{-6}$.
AUXILIARY	INFORMATION
METHOD / APPARATUS / PROCEDURE :	SOURCE AND PURITY OF MATERIALS:
The surface tension of the saturated	(1) Lights Ltd;
water-rich phase was determined by vertical	b.p. 231°C/749 mm Hg, m.p. 6.0°C;
plate and expanding drop measurements, and extrapolation of a surface-tension-	no variation in properties of five
composition curve provided the solubility value.	fractions of vacuum distillation.
value.	(2) distilled.
	ESTIMATED ERROR:
}	
	REFERENCES :

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COMPONENTS :	ORIGINAL MEASUREMENTS:
(1) 1-Decanol; C ₁₀ H ₂₂ 0; [112-30-1]	Harkins, W.D.; Oppenheimer. H.
(2) Water; H ₂ 0; [7732-18-5]	J. Am. Chem. Soc. <u>1949</u> , 71, 808–11.
VARIABLES:	PREPARED BY:
One temperature: assumed to be ambient	S.C. Yalkowsky; S.C.Valvani; A.F.M. Barton
EXPERIMENTAL VALUES:	
The solubility of 1-decanol (1) in water was	reported to be $0.0003 \text{ mol}(1)/\text{kg}$ (2).
Corresponding values calculated by the compil and mole fraction $x_1 = 5 \times 10^{-6}$.	ers are mass percentage 0.005 g(l)/l00g sln
The temperature was not stated, but is assume	d to be ambient.
AUXILIARY	INFORMATION
METHOD / AP PARATUS / PROCEDURE :	SOURCE AND PURITY OF MATERIALS:
A turbidimetric method was used, with the aid of a photometer (turbidity increased	 Eastman Kodak Co. or Connecticut Hard Rubber Co.;
rapidly in the presence of the emulsified second phase). The study was concerned	purified by fractional distillation.
with the effect of long-chain electrolytes (soaps) on solubility. The components	(2) not stated
were weighed into a glass ampoule and shaken vigorously for at least 48 h. Equilibrium	
was approached from both undersaturation and supersation.	
	ESTIMATED ERROR:
	Not stated
	REFERENCES :

COMPONENTS :	ORIGINAL MEASUREMENTS:
(1) 1-Decanol; C ₁₀ H ₂₂ ; [112-30-1]	Erichsen, L. von
10 22	Brennst. Chem. 1952, 33, 166-72.
(2) Water; H ₂ O; [7732-18-5]	Dremov. Chem. 1552, 55, 100-72.
VARIABLES:	PREPARED BY:
Temperature: 0-260 ⁰ C	S. H. Yalkowsky and Z. Maczynska
EXPERIMENTAL VALUES: Proportion of 1-decanol (1) in alcohol-rich phase
t/ ⁰ C g(1)/100g	sln x ₁
0 97.	35 0.8065
10 96.	
20 96. 30 96.	
40 95.	
50 95.	
60 94.	85 0.6765
70 94.	
80 93.	
90 93.	
100	
120 91.	
130 90.	
140 89.	
150 89.	
160 88.	
170 87. 180 86	
180 86. 190 85.	
200 83.	
210 82.	
220 80.	
230 79.	20 0.3025
240 77.	
250 74. 260 72.	
	INFORMATION
METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
The synthetic method was used.	(1) Merck, or Ciba, or industrial product;
	distilled and chemically free from isomers;
The measurements were carried out in 2 mL glass ampules. These were placed in an	b.p. 236.0-236.1°C (764 mm Hg)
aluminium block equpped with two glass	$n_{\rm p}^{20}$ 1.4375.
windows. Cloud points were measured with	D 1.4373.
a thermocouple wound up around the ampule.	(2) not specified.
Each measurement was repeated twice.	
	NAMINAMED EDDOD
	ESTIMATED ERROR:
	Not specified
	Not specified.
	REFERENCES :

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) 1-Decanol; C ₁₀ H ₂₂ 0; 112-30-1 (2) Water; H ₂ 0; 7732-18-5	Kinoshita, K.; Ishikawa, H.; Shinoda, K. Bull. Chem. Soc. Jpn. <u>1958</u> , 31, 1081-4.
VARIABLES:	PREPARED BY:
One temperature: 25 [°] C	S.H. Yalkowsky; S.C. Valvani; A.F.M. Barton

The equilibrium concentration of 1-decanol (1) in the water-rich phase at 25° C was reported to be 0.000234 mol(1)/L sln. and the mass percentage solubility was reported as 0.0037 g(1)/100g sln.

The corresponding mole fraction solubility, calculated by the compilers, is $x_1 = 4.0 \times 10^{-6}$.

AUXILIARY INFORMATION

METHOD / APPARATUS / PROCEDURE : SOURCE AND PURITY OF MATERIALS: (1)purified by vacuum distillation The surface tension in aqueous solutions of through 50-100 cm column; alcohols monotonically decreases up to their saturation concentration and remains b.p. 101^oC/5 mm Hg constant in the heterogeneous region (ref 1-4). Surface tension was measured (2) not stated by the drop weight method, using a tip 6 mm in diameter, the measurements being carried out in a water thermostat. From the (surface tension)-(logarithm of concentration) curves the saturation points were determined as the intersections of the curves with the horizontal straight lines ESTIMATED ERROR: passing through the lowest experimental points. Temperature: $\pm 0.05^{\circ}C$ Solubility : within 4% **REFERENCES**: Z.Anorg. Chem. 1904,38, 410 Motylewski,S. 2. Taubamann, A. Z. physic. Chem. 1932, A161, 141. 3. Zimmerman, H.K., Jr. Chem. Rev. 1952, 51, 25. 4. Shinoda, K.; Yamanaka, I., Kinoshita, K. J. Phys. Chem. 1959, 63, 648.

COMPONENTS :	ORIGINAL MEASUREMENTS:
<pre>(1) 1-Decanol; C₁₀H₂₂0; [112-30-1]</pre>	Vochten, R.; Petre, G.
(2) Water; H ₂ 0; [7732-18-5]	J. Colloid Interface Sci. <u>1973</u> , 42, 320-7.
VARIABLES:	PREPARED BY:
One temperature: 15 ⁰ C	S.H. Yalkowsky; S.C. Valvani; A.F.M.Barton.

AWW-0

The equilibrium concentration of 1-decanol (1) in the water-rich phase at 15° C was reported to be 2.0 x 10^{-4} mol(1)/L sln.

The corresponding mass percentage solubility, calculated by the compilers with the assumption of a solution density equal to that of water, is 0.0032 g(1)/100 g sln, and the mole fraction solubility is $x_1 = 3.0 \times 10^{-6}$.

AUXILIARY	INFORMATION
METHOD/APPARATUS/PROCEDURE: The solubility was obtained from the surface tension of saturated solutions, measured by the static method of Wilhelmy (platinum plate). The apparatus consisted of an electrobalance (R.G. Cahn) connected with a high impedance mill detector (FLUKE type 845 AR). An all-pyrex vessel was used.	 SOURCE AND PURITY OF MATERIALS: (1) purified by distillation and preparative gas chromatography; b.p. 231.0°C/760 mm Hg (2) triply distilled from permanganate solution.
	ESTIMATED ERROR: Temperature: ± 0.1°C Solubility (probably standard deviation): 0.1 x 10 ⁻⁴ mol(1)/L sln. REFERENCES:

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) 1-Decanol; C ₁₀ H ₂₂ 0; [112-30-1]	Zhuravleva, I.K.; Zhuravlev, E.F.; Lomakina, N.G.
(2) Water; H ₂ 0; [7732-18-5]	Zh. Fiz. Khim. <u>1977</u> , 51, 1700-7;
2	Russ. J. Phys. Chem. <u>1977</u> , 51, 994-8.
VARIABLES :	PREPARED BY:
Temperature: $10.5 - 120.5^{\circ}C$	
lemperature: 10.5 - 120.5 C	A. Maczynski
EXPERIMENTAL VALUES:	
Solubility of water (2) in 1-decanol (1)
$t/^{\circ}$ C g(2)/100g sln	
10.5 3.5	0.24
62.5 5.0	0.32
82.5 6.0	0.36
02.5 0.0	0.50
Solubility of 1-decand	ol (1) in water (2)
$t/^{\circ}$ C g(1)/100g sln	$x_1^{(\text{compiler})}$
102.5 1.0	0.001
120.5 0.8	0.001
	INFORMATION
ME THOD/AP PARATUS / PROCEDURE :	SOURCE AND PURITY OF MATERIALS:
The 'polythermic' method (ref 1) was used.	(1) source not specified; 20 1 (270 2^{20} 0 6200
No details were reported in the paper.	$n_{\rm D}^{20}$ 1.4370; d_4^{20} 0.8300; purity not specified.
The results formed part of a report on the ternary system including nitromethane.	
	(2) $n_{\rm D}^{20}$ 1.333.
	ESTIMATED ERROR:
	Not specified.
	REFERENCES :
	1. Alekseev, W.F. Zh. russk. khim. o-va, <u>1876</u> , 8, 249.

(1) 1-Decanol, $C_{10}H_{22}^{0}$; [112-30-1] Tokunaga, S.; Manabe, M.; Koda, M. (2) Water; H_{2}^{0} ; [7732-18-5] Niihama Kogyo Koto Semmon Gakko Kiyo, Rikogakn Hen Memoire Niihama Technical College Sci. and Eng.) 1980, 16, 96-101. VARIABLES: PREPARED BY: A.F.M. Barton Temperature: 15-40°C Proportion of water (2) in the alcohol-rich phase $t/^{\circ}C$ g(2)/100g sln x_2 mol (1)/mol (2) 3.86 0.257 20 3.86 0.261 2.87 20 3.83 0.259 2.88 30 3.79 0.257 2.90
(2) Water; H_2^{0} ; [7732-18-5] Niihama Kogyo Koto Semmon Gakko Kiyo, Rikogakn Hen Memoirs Niihama Technical Colleg Sci. and Eng.) 1980, 16, 96-101. VARIABLES: PREPARED BY: A.F.M. Barton Temperature: 15-40°C A.F.M. Barton EXPERIMENTAL VALUES: Proportion of water (2) in the alcohol-rich phase $t/°C$ $t/°C$ $g(2)/100g sln$ x_2 $nol (1)/mol (2)$ 15 3.79 0.257 2.84 20 3.86 0.261 2.87 25 3.83 0.259 2.88
Rikogakn Hen Memoirs Wilhama Technical College Sci. and Eng.) 1980, 16, 96-101.VARIABLES: Temperature: $15-40^{\circ}C$ PREPARED BY: A.F.M. BartonEXPERIMENTAL VALUES:Proportion of water (2) in the alcohol-rich phase $t/^{\circ}C$ g(2)/100g sln x_2 t/^{\circ}Cg(2)/100g sln x_2 mol (1)/mol (2)153.790.2572.84203.860.2612.87253.830.2592.88
Sci. and Eng.) 1980, 16, 96-101. VARIABLES: PREPARED BY: Temperature: 15-40°C A.F.M. Barton EXPERIMENTAL VALUES: Proportion of water (2) in the alcohol-rich phase $t/^{\circ}$ C g(2)/100g sln x_2 mol (1)/mol (2) 15 3.79 0.257 2.84 20 3.86 0.261 2.87 25 3.83 0.259 2.88
Temperature: $15-40^{\circ}$ C A.F.M. Barton EXPERIMENTAL VALUES: Proportion of water (2) in the alcohol-rich phase $t/^{\circ}$ C g(2)/100g sln x_2 mol (1)/mol (2) 15 3.79 0.257 2.84 20 3.86 0.261 2.87 25 3.83 0.259 2.88
EXPERIMENTAL VALUES: Proportion of water (2) in the alcohol-rich phase $t/^{\circ}$ C g(2)/100g sln x_2 mol (1)/mol (2) 15 3.79 0.257 2.84 20 3.86 0.261 2.87 25 3.83 0.259 2.88
Proportion of water (2) in the alcohol-rich phase $t/^{0}$ Cg(2)/100g sln x_{2} mol (1)/mol (2)153.790.2572.84203.860.2612.87253.830.2592.88
$t/^{0}$ Cg(2)/100g sln x_{2} mol (1)/mol (2)153.790.2572.84203.860.2612.87253.830.2592.88
15 3.79 0.257 2.84 20 3.86 0.261 2.87 25 3.83 0.259 2.88
20 3.86 0.261 2.87 25 3.83 0.259 2.88
25 3.83 0.259 2.88
30 3.79 0.257 2.90
35 3.76 0.255 2.92
40 3.70 0.252 2.94
AUXILIARY INFORMATION
METHOD/APPARATUS/PROCEDURE: SOURCE AND PURITY OF MATERIALS:
The mixtures of 1-decanol (~5 mL) and water (1) Tokyo Kasei, GR > 98%; (~10 mL) were stirred magnetically in a used without further purification
stoppered vessel and allowed to stand for
10-12 h in a water thermostat. The (2) deionized; alcohol-rich phase was analyzed for water by Karl Fischer titration.
ESTIMATED ERROR:
Temperature: ± 0.1°C
Solubility: each result is the mean of three determinations
REFERENCES:
}

112	Ten-carbon and	Higher Alcoh	ols
COMPONENTS:		ORIGINAL MEA	ASUREMENTS:
	1; C ₁₁ H ₂₄ 0; [112-42-5] 0; [7732-18-5]	Tokınaga, S.; Manabe,M.; Koda, M. Niihama Kogyo Koto Semmon Gakko Kiyo, Rikogaku Hen (Memoirs Niihama Technical College, Sci. and Eng.) <u>1980</u> , 16, 96-101.	
VARIABLES:		PREPARED BY:	
Temperature: 15-40 ⁰ C		A.F.M. Bart	ton
EXPERIMENTAL VAL	UES:	<u> </u>	·····
	Proportion of wa	ter (2) in th	he alcohol-rich phase
t/ ^o c	g(2)/100g sln	<i>x</i> 2	mol (1)/mol (2)
15	3.45	0.255	2.92
20	3.40	0.252	2.94
25	3.43	0.254	2.97
30	3.39	0.251	3.00
35	3.37	0.250	3.02
40	3.29	0.245	3.04
	AUXILIARY	INFORMATION	
water (~10 mL) w in a stoppered w for 10-12 h in a	I-undecanol (~5 mL) and were stirred magnetically ressel and allowed to stand a water thermostat. The ase was analyzed for water	(1) disti (2) deion	
		ESTIMATED F Temperatu Solubilit REFERENCES	re: 0.1 ⁰ C y: each result is the mean of three determinations

COMPONENTS :	EVALUATOR:
(1) 1-Dodecanol (n-dodecyl alcohol);	A. Maczynski, Institute of Physical Chemistry
$C_{12}^{H}_{26}^{0}; [112-53-8]$	of the Polish Academy of Sciences, Warsaw,
(2) Water; H ₂ 0; [7732-18-5]	Poland; and A.F.M. Barton, Murdoch
(2)	University, Perth, Western Australia.
	November 1982

CRITICAL EVALUATION:

The proportion of 1-dodecanol (1) in the water-rich phase has been reported in two publications: Krause and Lange (ref 1) carried out measurements at 289K, 307K and 322K by the analytical method; and Robb (ref 2) determined one point only at 298K by a film balance technique. These values are in poor agreement, and equation 5 of the Editor's Preface has been used to provide an estimated figure of $2 \times 10^{-5} mol(1)/L sln$.

 $\log (c/mol(1)/L sln) = 2.722 - 0.6988n + 0.006418n^2,$

where n is the number of carbon atoms in the alcohol. The figure lies between that of refs 1 and 2, and is suggested as a tentative value.

The tentative value for the solubility of 1-dodecanol in water at 298K is 2×10^{-5} mol(1)/L sln or 4×10^{-4} g(1)/100g sln.

The proportion of water (2) in the alcohol-rich phase in equilibrium with the water rich-phase has also been reported in two publications: Zhuravleva *et al*. (ref 3) between 295K and 315K; and Tokunaga *et al*. (ref 4) between 303K and 313K by an analytical method. These reports disagree, not only with regard to the values but also in the sign of the temperature dependence, so only an estimate of the 298K value can be provided.

The tentative value for the solubility of water in 1-dodecanol at 298K is 3 g(2)/100g sln, $x_2 = 0.25$, with only a small dependence on temperature.

References:

- 1. Krause, F.P.; Lange, W. J. Phys. Chem. 1965, 69, 3171.
- 2. Robb, I.D. Aust. J. Chem. 1966, 19, 2281.
- 3. Zhuravleva, I.K.; Zhuravlev, E.F.; Salamatin, L.N. Zh. Obshch. Khim. 1976, 46, 1210.
- 4. Tokunaga, S.; Manabe, M.; Koda, M. Niihama Kogyo Koto Semmon Gakko Kiyo, Rikogaku Hen (Memoirs Niihama Technical College, Sci. and Eng.) <u>1980</u>, 16, 96.

Ten-carbon and Higher Alcohols			
COMPONENTS:		ORIGINAL MEASUREMENTS	3:
(1) 1-Dod	ecanol; C ₁₂ H ₂₆ 0 [112-53-8]	Krause, F.P.; Lange,	
(2) Water	; H ₂ 0; [7732-18-5]	J. Phys. Chem. 1965,	69, 3171-3.
VARIABLES:	2	PREPARED BY:	
Temperature	e: 16-49 [°] C	S.H. Yalkowsky; S.C.	Valvani; A.F.M. Barton
EXPERIMENTA			
	Solubility of]	l-dodecanol (1) in water	. (2)
t/°c	$10^{6}c_{1}^{2}/mol(1) (L sln)^{-1}$	$10^4 \text{ g(1)}/100 \text{ sln}^a$	$10^7 x_1^{a}$
16	9.1	1.7	1.6
34	15.6	2.9	2.8
49	19.3	3.6	3.5
	lated by the compilers with the a at of water.	assumption of a solution	n density equal

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
The isotopically labelled 1-dodecanol ((1-5 mg) was deposited on the surface film of the water in a closed vessel by evaporating the hexane solvent, and held there virtually stationary for 1-2 weeks in a thermostat box while equilibrium with the stirred water was achieved. Periodically samples were withdrawn, diluted with ethanol, extracted with hexane and counted. (The solubility of 1-hexadecanol, determined after equilibrating from both undersaturated and supersaturated solutions, was found to be the same within accuracy limits. Two solubility determinations with 1-dodecanol at 16°C, one with 1 mg and the other with 5 mg, gave the same results).	passed through 0.6 x 200 cm column of diglycolic acid polyethylen glycol on 60/80-mesh chromosorb W at 180°C with helium at 50 cm 3 min ⁻¹ ; diluted with 99.5% pure (1); m.p. 25°C free of comparatively water-soluble impurities; stored in hexane solution.

COMPONENTS :	ORIGINAL MEASUREMENTS:
(1) 1-Dodecanol; C ₁₂ H ₂₆ 0; [112-53-8]	Robb, I.D.
(2) Water; H ₂ 0; [7732-18-5]	Aust. J. Chem. <u>1966</u> , 19, 2281-4.
VARIABLES:	PREPARED BY:
One temperature: 25 [°] C	S.H. Yalkowsky; S.C. Valvani; A.F.M. Barton

The equilibrium concentration of 1-dodecanol (1) in the water-rich phase at 25° C was reported to be 2.3 x 10^{-5} mol(1)/L sln.

The corresponding mass percentage solubility, calculated by the compilers with the assumption of a solution density equal to that of water, is $4.3 \times 10^{-4} \text{ g(1)}/100 \text{ g sln}$, and the mole fraction solubility is $10^7 x_1 = 4.2$.

AUXILIARY	INFORMATION
METHOD/APPARATUS/PROCEDURE: In this method (described in detail in ref 1) crystals of (1) were stirred with (2) for 24 h at 25°C, and a solution filtered (Gooch sintered glass and 350-1000 Å nitro- cellulose under N ₂ pressure). The alcohol was extracted into hexane, and estimated by its surface properties on a film balance.	 SOURCE AND PURITY OF MATERIALS: (1) Fluka puriss. m.p. 23-24°C. (2) in equilibrium with air; pH 5.7 ± 0.1 specific conductivity 0.9-1.0 μS cm⁻¹.
	ESTIMATED ERROR: Solubility: 0.1 x 10 ⁻⁵ mol(1)/L sln on the basis of 16 determinations. REFERENCES: 1. Robb, I., Kolloidz. Z. Polymere <u>1966</u> , 209, 162.

COMPONENTS:	ORIGINAL MEASUREMENTS:	
(1) 1-Dodecanol; C ₁₂ H ₂₆ 0; [112-53-8]	Zhuravleva, I.K.; Zhuravlev, E.F.; Salamatin, L.N.	
(2) Water; H ₂ O; [7732-18-5]	Zh. Obshch. Khim. <u>1976</u> , 46, 1210-4.	
VARIABLES:	PREPARED BY:	
Temperature: 21.5 - 41.5 [°] C	A. Maczynski	
EXPERIMENTAL VALUES: Solubility of	water in 1-dodecanol	
t/ ^o c g(2)		
	/100g sln x_2 (compiler)	
21.5	0.7 0.07	
23.7	1.3 0.12	
24.2	1.4 0.13	
31.0 41.5	1.7 0.15 2.1 0.18	
AUXILIAF METHOD / APPARATUS / PROCEDURE :	Y INFORMATION SOURCE AND PURITY OF MATERIALS;	
Not specified.	1	
	(1) source not specified; b.p. 101.0°C, m.p. 22.6°C, $n_{\rm D}^{24}$ 1.4420, d_4^{20} 0.8310	
	(2) not specified.	
	ESTIMATED ERROR:	
	Not specified.	
	REFERENCES:	

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) 1-Dodecanol; C ₁₂ H ₂₆ 0; 112-53-8	Tokunaga, S.; Manabe, M.; Koda, M.
	Niihama Kogyo Koto Semmon Gakko Kiyo,
(2) Water; H ₂ 0; 7732-18-5	Rikogaku Hen (Memoirs Niihama Technical
	College, Sci. and Eng.) 1980, 16, 96-101.
	······································
VARIABLES:	PREPARED BY:
Temperature: 30-40 [°] C	A.F.M. Barton
EXPERIMENTAL VALUES:	1
Proportion of w	water (2) in the alcohol-rich phase
t/ ^o C g(2)/100g	$\sin x_2 \mod(1)/\mod(2)$
30 3.09	0.248 3.03
35 3.06	0.246 3.06
40 3.03	0.244 3.09
	JARY INFORMATION
METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
The mixtures of 1-dodecanol (~5 mL) and water (~10 mL) were stirred magnetically	(1) distilled
a stoppered vessel and allowed to stand	for (2) deionized;
10-12 h in a water thermostat. The alcohol-rich phase was analyzed for wate	distilled prior to use
by Karl Fischer titration.	
	ESTIMATED ERROR:
	Temperature: ±0.1°C
	Solubility: each result is the mean of
	three determinations.
	REFERENCES:

COMPONENTS :	EVALUATOR:
 (1) 1-Tetradecanol (<i>n</i>-tetradecyl alcohol); C₁₄H₃₀0; [112-72-1] (2) Water; H₂0: [7732-18-5] 	A. Maczynski, Institute of Physical Chemistry of Polish Academy of Sciences, Warsaw, Poland; and A.F.M. Barton, Murdoch Univer- sity, Perth, Western Australia November 1982

CRITICAL EVALUATION:

The proportion of 1-tetradecanol (1) in the water-rich phase has been reported in two publications: Robb (ref 1) determined the solubility of (1) in (2) at 298K by a film balance technique; and Hoffman and Anacker (ref 2) used the analytical method at four temperatures between 277K and 334K. The two reports are in marked disagreement, but the result of Robb is supported by comparison with the solubilities of other normal aliphatic alcohols in water, as discussed in the Editor's Preface. If the equation

 $\log (c/mol L^{-1}) = -0.57n + 2.14$

is used to relate the solubility of 1-alkanols in water at 298K to the carbon number n (ref 1), the solubility of 1-tetradecanol is found to be 1.5 x 10^{-6} mol(1)/L sln or 3×10^{-5} g(1)/100g sln. Equation 5 of the Editor's Preface yields a marginally higher value.

The tentative value for the solubility of 1-tetradecanol in water at 298K is 3×10^{-5} g(1)/100g sln or 2 x 10^{-6} mol(1)/L sln.

The proportion of water in the alcohol-rich phase in equilibrium with the water-rich phase has not been reported in the literature.

References:

1. Robb, I.D. Aust. J. Chem. 1966, 19, 2281.

2. Hoffman, C.S.; Anacker, E.W. J. Chromatogr. 1967, 30, 390.

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) 1-Tetradecanol; C ₁₄ H ₃₀ 0; [112-72-1] (2) Water; H ₂ 0; [7732-18-5]	Robb, I.D. Aust. J. Chem. <u>1966</u> , 19, 2281-4,
VARIABLES:	PREPARED BY:
One temperature: 25 [°] C	S.H. Yalkowsky; S.C. Valvani; A.F.M. Barton

EXPERIMENTAL VALUES:

The equilibrium concentration of 1-tetradecanol (1) in the water-rich phase at $25^{\circ}C$ was reported to be 1.46 x 10^{-6} mol(1)/L sln.

The corresponding mass percentage solubility, calculated by the compilers with the assumption of a solution density equal to that of water, is $3.1 \times 10^{-5} \text{ g(1)/l00g sln}$, and the mole fraction solubility is $x_1 \approx 2.6 \times 10^{-8}$.

AUXILIARY	INFORMATION
METHOD/APPARATUS/PROCEDURE: In this method (described in detail in ref 1) crystals of (1) were stirred with (2) for 24h at 25° C, and the solution was then filtered (Gooch sintered glass and 350-1000 Å nitro- cellulose under N ₂ pressures). The alcohol was extracted into hexane, and estimated by its surface properties on a film balance.	 SOURCE AND PURITY OF MATERIALS: (1) Fluka puriss. m.p. 38-39°C (2) in equilibrium with air; pH 5.7 ± 0.1 specific conductivity 0.9-1.0 μS cm⁻¹. ESTIMATED ERROR: Solubility: 0.1 x 10⁻⁶ mol(1)/L sln on the basis of 9 determinations.
	REFERENCES: 1. Robb, I. Kolloidz. Z. Polymere <u>1966</u> 209, 162.

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) 1-Tetradecanol; C ₁₄ H ₃₀ 0; [112-72-1] (2) Water; H ₂ 0; [7732-18-5]	Hoffman, C.S.; Anacker, E.W. J. Chromatogr. <u>1967</u> , 30, 390-6.
VARIABLES: Temperature: 4-61 [°] C	PREPARED BY: A. Maczynski; A. Szafranski; A.F.M. Barton
EXPERIMENTAL VALUES:	······································
Solubility of l-tetrad	ecanol (1) in water (2)
$t/^{\circ}$ C 10 ⁶ g(1) (L sln) ⁻¹	$10^{5}g(1)/100g \sin^{a}$ $10^{8}x_{1}^{a}$
4 0.194 32 1.23 45 2.37 61 4.49 <i>a</i> Calculated by the compilers with the equal to that of water.	0.42 0.35 2.6 2.2 5.1 4.3 9.6 7.5 assumption of a solution density
AUXILIARY	INFORMATION
METHOD/APPARATUS/PROCEDURE: The analytical method was used. Saturated solutions of (1) in (2) free from colloidal particles were prepared by using the Krause and Lange (ref 1) procedure. To 1000 mL (2) containing 50 ppb AgNO ₃ (to prevent bacteria) in a 2000-mL flask 1-29 mg (1) was added with minimum agitation, the flask stoppered, the solution stirred gently at a constant temperature and sampled. The 2nd sample was retained, weighed and 10-12 mL aliquots collected, each aliquot shaken 18 h with 5 mL hexane. The hexane was evaporated the (1) residue redissolved in 25-200 mL hexane and analyzed by gas-liquid chromatography.	 SOURCE AND PURITY OF MATERIALS: (1) Matheson, Coleman and Bell; 99.5+%; purified by preparative gas chromatography. (2) double distilled.

COMPONENTS:	ORIGINAL MEASUREMENTS:
<pre>(1) 1-Pentadecanol; C₁₅H₃₂0; [629-76-5] (2) Water; H₂0; [7732-18-5]</pre>	Robb, I.D. Aust. J. Chem. <u>1966</u> , 19, 2281-4.
VARIABLES:	PREPARED BY:
One temperature: 25 ⁰ C	S.H. Yalkowsky; S.C. Valvani; A.F.M. Barton
EXPERIMENTAL VALUES:	
The equilibrium concentration of 1-pentadecal was reported to be 4.5 x 10^{-7} mol(1)/L sln.	nol (1) in the water-rich phase at 25° C

The corresponding mass percentage solubility, calculated by the compilers with the assumption of a solution density equal to that of water, is 1.0×10^{-5} g(1)/100g sln, and the mole fraction solubility is $x_1 = 7.9 \times 10^{-9}$.

(The water-solubilities of the higher normal alcohols may also be estimated from the number of carbon atoms, as discussed in the Editor's Preface). This predicts $3.9 \times 10^{-7} \text{ mol}(1)/\text{L sln}$.

AUXILIARY	INFORMATION
METHOD/APPARATUS/PROCEDURE: In this method (described in detail in ref 1) crystals of (1) were stirred with (2) for 24 h at 25°C and the solution filtered (Gooch sintered glass and 350-1000 Å nitro- cellulose under N ₂ pressure). The alcohol was extracted into hexane, and estimated by its surface properties on a film balance.	<pre>SOURCE AND PURITY OF MATERIALS: (1) Fluka purum; m.p. 42-44°C (2) in equilibrium with air; pH 5.7±0.1 specific conductivity 0.9-1.0 µS cm⁻¹.</pre> ESTIMATED ERROR: Solubility: 0.3 x 10 ⁻⁷ mol(1)/L sln. on the basis of 8 determinations. REFERENCES: 1. Robb, I. Kolloidz. Z. Polymere 1966, 209, 162.

COMPONENTS:	EVALUATOR:
 (1) 1-Hexadecanol (n-hexadecyl alcohol); C₁₆H₃₄0; [36653-82-4] (2) Water; H₂0; [7732-18-5] 	A. Maczynski, Institute of Physical Chemistry of the Polish Academy of Sciences, Warsaw, Poland; and A.F.M. Barton, Murdoch University, Perth, Western Australia November 1982

CRITICAL EVALUATION:

The proportion of 1-hexadecanol (1) in the water-rich phase has been reported in three publications: Krause and Lange (ref 1) carried out measurements of the solubility of (1) in (2) at 307K and 328K by the analytical method; Robb (ref 2) determined one point only at 298K by a film balance technique; and Hoffman and Anacker (ref 3) determined the solubility of (1) in (2) at 316K and 334K by the analytical method.

These data from refs 1-3 are in poor agreement. However, the solubilities of normal aliphatic alcohols in water may be correlated as discussed in the Editor's Preface. The solubility of 1-alkanols in water at 298K is related to the carbon number n, by (ref 2)

 $\log (c/mol L^{-1}) = -0.57n + 2.14$

For 1-hexadecanol this gives $1 \times 10^{-7} \text{ mol}(1)/\text{L} \sin$, or $3 \times 10^{-6} \text{ g}(1)/100\text{g} \sin$, which is slightly lower than Robb's experimental value.

The tentative range of values for the solubility of 1-hexadecanol in water at 298K is thus (3 to 4) x 10^{-6} g(1)/100g sln or (1-2) x 10^{-7} mol(1)/L sln.

The proportion of water in the alcohol-rich phase in equilibrium with the water-rich phase has not been reported.

References:

1. Krause, F.P.; Lange, W. J. Phys. Chem. 1965, 69, 3171.

2. Robb, I.D. Aust. J. Chem. 1966, 19, 2281.

3. Hoffman, C.S.; Anacker, E.W. J. Chromatogr. 1967, 30, 390.

	1-Hexad	ecanol	423
COMPONENTS:		ORIGINAL MEASUREMENTS:	
 1-Hexadecanol; Water; H₂0; [7 	C ₁₆ H ₃₄ 0; [36653-82-4] 732-18-5]	Krause, F.P.; Lange, W. J. Phys. Chem. <u>1965</u> , 69, 31	71-3.
VARIABLES:		PREPARED BY:	
Temperature: 33 ⁰ C a	nd 127 ⁰ C	S.H. Yalkowsky; S.C. Valvan	i; A.F.M. Barton
EXPERIMENTAL VALUES:		· · · · · · · · · · · · · · · · · · ·	
	Solubility of 1-h	exadecanol (1) in water (2)	
t/ ^o c	10 ⁸ c ₁ /mol(1) (L sln)	$10^7 \text{ g(1)/100g sln}^a$	10 ¹⁰ x ₁ ^a
34	3.3	8.0	6.0
55	12.7	31	23
		INFORMATION	
(0.2 mg) was deposit of the water in a c ting the hexane solvirtually stationar thermostat box while stirred bulk water ically, samples were with ethanol, extra counted. (The solu equilibrating from b supersaturated solu the same within accu solubility determina	belled l-hexadecanol ted on the surface film losed vessel by evapora- vent, and held there y for 1-2 weeks in a e equilibrium with the was achieved. Period- e withdrawn, diluted cted with hexane and ubility determined after both undersaturated and tions, was found to be uracy limits. Two ations with 1-dodecanol mg and the other with	<pre>SOURCE AND PURITY OF MATERI (1) Isotopes Specialities passed through 0.5 x 10% Dow-Corning silic stopcock grease on 60 Chromosorb W at 162°C 62 cm min⁻¹; free of comparatively impurities, stored in m.p. 40°C (2) distilled; sterilized ESTIMATED ERROR: Temperature: uncertain by Solubility: within ± 10% REFERENCES:</pre>	Co, Burbank, Cal. 75 cm column of a-free silicone /80 mesh with helium at water-soluble hexane solution; by boiling.

COMPONENTS:	ORIGINAL MEASUREMENTS:
<pre>(1) 1-Hexadecano1; C₁₆H₃₄0; [36653-82-4] (2) Water; H₂0; [7732-18-5]</pre>	Robb, I.D. Aust. J. Chem. <u>1966</u> , 19, 2281-4
VARIABLES:	PREPARED BY:
One temperature: 25 [°] C	S.H. Yalkowsky; S.C. Valvani; A.F.M. Barton

EXPERIMENTAL VALUES:

This equilibrium concentration of 1-hexadecanol (1) in the water-rich phase at 25° C was reported to be 1.7 x 10^{-7} mol(1)/L sln.

The corresponding mass percentage solubility, calculated by the compilers with the assumption of a solution density equal to that of water, is $4.1 \times 10^{-6} \text{ g(1)}/100 \text{ g sln}$, and the mole fraction solubility is $x_1 = 3.1 \times 10^{-9}$.

AUXILIARY	INFORMATION
METHOD/APPARATUS/PROCEDURE: In this method (described in detail in ref 1) crystals of (1) were stirred with (2) for 24 h at 25°C and the solution was then filtered (Gooch sintered glass and 350-100 Å nitrocellulose under N ₂ pressure). The alcohol was extracted into hexane, and estimated by its surface properties on a film balance.	<pre>SOURCE AND PURITY OF MATERIALS: (1) Fluka puriss., > 99%; m.p. 49-50°C (2) in equilibrium with air; pH 5.7 ± 0.1 specific conductivity 0.9-1.0 µS cm⁻¹.</pre>
	ESTIMATED ERROR: Solubility: 0.2 x 10 ⁻⁷ mol(1)/L sln on the basis of 14 determinations. REFERENCES: 1. Robb, I. Kolloidz. Z. Polymere, <u>1966</u> , 209, 162.

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) 1-Hexadecanol; C ₁₆ ^H ₃₄ 0; [36653-82-4]	Hoffman, C.S.; Anacker, E.W.
(2) Water; H ₂ 0; [7732-18-5]	J. Chromatogr. <u>1967</u> , 30, 390-6.
(2) water, ¹² 2, ¹⁷⁷² ¹⁰ ⁵	
VARIABLES:	PREPARED BY:
Temperature: 43 and 61 ⁰ C	A. Maczynski; A. Szafranski; A.F.M. Barton
EXPERIMENTAL VALUES:	
Solubility of 1-hex	adecanol (1) in water (2)
$t/^{\circ}$ C $10^{7}g(1)(L sln)^{-1}$	$10^{6}g(1)/100g sln^{a}$ $10^{9}x_{1}^{a}$
43 1.55	3.8 2.8
61 4.06	9.8 7.3
AUXILIARY	INFORMATION
METHOD/APPARATUS/PROCEDURE:	SOURCE AND DURITY OF MATERIALS.
	SOURCE AND PURITY OF MATERIALS:
The analytical method was used.	
,	(1) Applied Science Laboratory; 99.8+ %
Saturated solutions of (1) in (2) free from	
Saturated solutions of (1) in (2) free from colloidal particles were prepared by using	 (1) Applied Science Laboratory; 99.8+ % pure by thin layer and gas-liquid chromatography; used as received.
Saturated solutions of (1) in (2) free from	 (1) Applied Science Laboratory; 99.8+ % pure by thin layer and gas-liquid chromatography; used as received.
Saturated solutions of (1) in (2) free from colloidal particles were prepared by using the Krause and Lange (ref 1) procedure. To 1000 mL (2) containing 50 ppb AgNO ₃ (to prevent bacteria) in a 2000mL flask 1-25 mg	 (1) Applied Science Laboratory; 99.8+ % pure by thin layer and gas-liquid chromatography; used as received.
Saturated solutions of (1) in (2) free from colloidal particles were prepared by using the Krause and Lange (ref 1) procedure. To 1000 mL (2) containing 50 ppb AgNO ₃ (to prevent bacteria) in a 2000mL flask 1-25 mg (1) was added with minimum agitation, the	 (1) Applied Science Laboratory; 99.8+ % pure by thin layer and gas-liquid chromatography; used as received. (2) doubly distilled.
Saturated solutions of (1) in (2) free from colloidal particles were prepared by using the Krause and Lange (ref 1) procedure. To 1000 mL (2) containing 50 ppb AgNO, (to prevent bacteria) in a 2000mL flask 1-25 mg (1) was added with minimum agitation, the flask stoppered, the solution stirred gently at a constant temperature, sampled, the	 (1) Applied Science Laboratory; 99.8+ % pure by thin layer and gas-liquid chromatography; used as received. (2) doubly distilled.
Saturated solutions of (1) in (2) free from colloidal particles were prepared by using the Krause and Lange (ref 1) procedure. To 1000 mL (2) containing 50 ppb AgNO ₃ (to prevent bacteria) in a 2000mL flask 1-25 mg (1) was added with minimum agitation, the flask stoppered, the solution stirred gently	 (1) Applied Science Laboratory; 99.8+ % pure by thin layer and gas-liquid chromatography; used as received. (2) doubly distilled.
Saturated solutions of (1) in (2) free from colloidal particles were prepared by using the Krause and Lange (ref 1) procedure. To 1000 mL (2) containing 50 ppb AgNO ₃ (to prevent bacteria) in a 2000mL flask 1-25 mg (1) was added with minimum agitation, the flask stoppered, the solution stirred gently at a constant temperature, sampled, the 2nd sample retained, weighed and 80 mL aliquots collected, each aliquot shaken 18 h with 20 mL hexane, the hexane evaporated,	 (1) Applied Science Laboratory; 99.8+ % pure by thin layer and gas-liquid chromatography; used as received. (2) doubly distilled.
Saturated solutions of (1) in (2) free from colloidal particles were prepared by using the Krause and Lange (ref 1) procedure. To 1000 mL (2) containing 50 ppb AgNO ₃ (to prevent bacteria) in a 2000mL flask 1-25 mg (1) was added with minimum agitation, the flask stoppered, the solution stirred gently at a constant temperature, sampled, the 2nd sample retained, weighed and 80 mL aliquots collected, each aliquot shaken 18 h	 (1) Applied Science Laboratory; 99.8+ % pure by thin layer and gas-liquid chromatography; used as received. (2) doubly distilled.
Saturated solutions of (1) in (2) free from colloidal particles were prepared by using the Krause and Lange (ref 1) procedure. To 1000 mL (2) containing 50 ppb AgNO ₃ (to prevent bacteria) in a 2000mL flask 1-25 mg (1) was added with minimum agitation, the flask stoppered, the solution stirred gently at a constant temperature, sampled, the 2nd sample retained, weighed and 80 mL aliquots collected, each aliquot shaken 18 h with 20 mL hexane, the hexane evaporated, the (1) residue redissolved in 25-200 mL	 Applied Science Laboratory; 99.8+ % pure by thin layer and gas-liquid chromatography; used as received. doubly distilled. ESTIMATED ERROR:
Saturated solutions of (1) in (2) free from colloidal particles were prepared by using the Krause and Lange (ref 1) procedure. To 1000 mL (2) containing 50 ppb AgNO ₃ (to prevent bacteria) in a 2000mL flask 1-25 mg (1) was added with minimum agitation, the flask stoppered, the solution stirred gently at a constant temperature, sampled, the 2nd sample retained, weighed and 80 mL aliquots collected, each aliquot shaken 18 h with 20 mL hexane, the hexane evaporated, the (1) residue redissolved in 25-200 mL hexane and analyzed by gas-liquid	 (1) Applied Science Laboratory; 99.8+ % pure by thin layer and gas-liquid chromatography; used as received. (2) doubly distilled. ESTIMATED ERROR: Not specified
Saturated solutions of (1) in (2) free from colloidal particles were prepared by using the Krause and Lange (ref 1) procedure. To 1000 mL (2) containing 50 ppb AgNO ₃ (to prevent bacteria) in a 2000mL flask 1-25 mg (1) was added with minimum agitation, the flask stoppered, the solution stirred gently at a constant temperature, sampled, the 2nd sample retained, weighed and 80 mL aliquots collected, each aliquot shaken 18 h with 20 mL hexane, the hexane evaporated, the (1) residue redissolved in 25-200 mL hexane and analyzed by gas-liquid	 (1) Applied Science Laboratory; 99.8+ % pure by thin layer and gas-liquid chromatography; used as received. (2) doubly distilled. ESTIMATED ERROR: Not specified REFERENCES:
Saturated solutions of (1) in (2) free from colloidal particles were prepared by using the Krause and Lange (ref 1) procedure. To 1000 mL (2) containing 50 ppb AgNO ₃ (to prevent bacteria) in a 2000mL flask 1-25 mg (1) was added with minimum agitation, the flask stoppered, the solution stirred gently at a constant temperature, sampled, the 2nd sample retained, weighed and 80 mL aliquots collected, each aliquot shaken 18 h with 20 mL hexane, the hexane evaporated, the (1) residue redissolved in 25-200 mL hexane and analyzed by gas-liquid	 (1) Applied Science Laboratory; 99.8+ % pure by thin layer and gas-liquid chromatography; used as received. (2) doubly distilled. ESTIMATED ERROR: Not specified
Saturated solutions of (1) in (2) free from colloidal particles were prepared by using the Krause and Lange (ref 1) procedure. To 1000 mL (2) containing 50 ppb AgNO ₃ (to prevent bacteria) in a 2000mL flask 1-25 mg (1) was added with minimum agitation, the flask stoppered, the solution stirred gently at a constant temperature, sampled, the 2nd sample retained, weighed and 80 mL aliquots collected, each aliquot shaken 18 h with 20 mL hexane, the hexane evaporated, the (1) residue redissolved in 25-200 mL hexane and analyzed by gas-liquid	 (1) Applied Science Laboratory; 99.8+ % pure by thin layer and gas-liquid chromatography; used as received. (2) doubly distilled. ESTIMATED ERROR: Not specified REFERENCES: 1. Krause, F.P.; Lange, W.
Saturated solutions of (1) in (2) free from colloidal particles were prepared by using the Krause and Lange (ref 1) procedure. To 1000 mL (2) containing 50 ppb AgNO ₃ (to prevent bacteria) in a 2000mL flask 1-25 mg (1) was added with minimum agitation, the flask stoppered, the solution stirred gently at a constant temperature, sampled, the 2nd sample retained, weighed and 80 mL aliquots collected, each aliquot shaken 18 h with 20 mL hexane, the hexane evaporated, the (1) residue redissolved in 25-200 mL hexane and analyzed by gas-liquid	 (1) Applied Science Laboratory; 99.8+ % pure by thin layer and gas-liquid chromatography; used as received. (2) doubly distilled. ESTIMATED ERROR: Not specified REFERENCES: 1. Krause, F.P.; Lange, W.

426 Ten-carbon and	Higher Alcohols
COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) 1-Heptadecanol; C ₁₇ H ₃₆ 0; [1454-85-9]	Robb, I.D.
(2) Water; H ₂ 0; [7732-18-5]	Aust. J. Chem. <u>1966</u> , 19, 2281-4.
VARIABLES:	PREPARED BY:
One temperature: 25 [°] C	A.F.M. Barton
EXPERIMENTAL VALUES: The equilibrium concentration of 1-heptadecar was reported to be no more than 10^{-7} mol(1)/j The corresponding limiting mass percentage so is 3 x 10^{-6} g(1)/100g sln, and the mole frac (The water-solubility of the higher normal a number of carbon atoms, as discussed in the 3 x 10^{-8} mol(1)/L sln).	L sln. olubility, calculated by the compilers, tion solubility is $x_1 \le 7 \ge 10^{-10}$. lcohols may also be estimated from the

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
In this method (described in detail in ref 1) crystals of (1) were stirred with (2) for 24 h at 25° C and the solution was then filtered (Gooch sintered glass and $350-1000$ Å nitrocellulose under N ₂ pressure). The alcohol was extracted ² into hexane, and estimated by its surface properties on a film balance. The solubility of (1) was found to be too low to be measured by this method.	 (1) Fluka purum., > 97%: m.p. 50-53°C. (2) in equilibrium with air pH 5.7 ± 0.1 specific conductivity 0.9-1.0 μS cm⁻¹.
	ESTIMATED ERROR:
	Not specified
	REFERENCES: 1. Robb, I., Kolloidz. Z. Polymere <u>1966</u> , 209, 162.

COMPONENTS:	ORIGINAL MEASUREMENTS:
<pre>(1) 1-Octadecanol; C₁₈H₃₈0 [112-92-5] (2) Water; H₂0; [7732-18-5]</pre>	Krause, F.P.; Lange, W. J. Phys. Chem. <u>1965</u> , 69, 3171-3.
VARIABLES: Temperature: 34 [°] C and 65 [°] C	PREPARED BY: S.H. Yalkowsky; S.C. Valvani; A.F.M. Barton
EXPERIMENTAL VALUES:	•
Solubility of 1-octa	adecanol (1) in water (2)
	-1 10 ⁵ (1) (100 - 1) ^a 10 ⁹ a

t/ ⁰ C	$10^{2}c_{1}^{mol(1)}(L \ sln)^{-1}$	10 g(1)/100g sln"	$10^{7}x_{1}^{4}$
34	4	1.1	7.3
63	22	6.0	40

 $\overset{a}{\text{Calculated}}$ by the compilers with the assumption of a solution density equal to that of water.

(The water solubilities of the higher normal alcohols may also be estimated from the number of carbon atoms, as discussed in the Editor's Preface).

AUXILIARY	INFORMATION
METHOD/APPARATUS/PROCEDURE: The isotopically-labelled 1-octadecanol (0.1 mg) was deposited on the surface film of the water in a closed vessel by evapor- ating the hexane solvent, and held there virtually stationary for 1-2 weeks in a thermostat box while equilibrium with the stored bulk water was achieved. Period- ically samples were withdrawn, diluted with ethanol, extracted with hexane and counted. (The solubility of 1-hexadecanol, deter- mined after equilibrating from both undersaturated and supersaturated solutions, was found to be the same within accuracy limits. Two solubility determinations with 1-dodecanol at 16°C, one with 1 mg and the other with 5 mg, gave the same results. No comparable checks were reported for 1-octadecanol).	 SOURCE AND PURITY OF MATERIALS: (1) Isotope Specialities Co., Burbank, Cal., passed through 0.6 x 75 cm column of 20% Tween 80 on 60/80-mesh HMDS-Chromosorb W at 180°C with a helium flow rate of 67 cm³ min ⁻¹; free of comparatively water-soluble impurities; stored in hexane solution m.p. 59°C. (2) distilled; sterilized by boiling.

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Underlined page numbers refer to evaluation text and those not underlined to compiled tables. All compounds are listed as in Chemical Abstracts.

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